

Real-time gauge theory simulations from stochastic quantisation

Dénes Sexty

Darmstadt University of Technology

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Collaborators: J. Berges, Sz. Borsányi, I.-O. Stamatescu

1. Complex Langevin method and real time evolution
2. Results for a scalar oscillator
3. Results for SU(2) gauge theory
4. Connection with Schwinger Dyson equations
5. Methods to improve convergence:
 Reweighting and using gauge fixing

J. Berges, Sz. Borsányi, D. Sexty, I.-O. Stamatescu PRD75 045007

J. Berges, D. Sexty. NPB

Motivations

Understanding heavy ion collisions

Not weakly coupled system

High occupation numbers prevent perturbative treatment even for weak couplings

At $n = O(1/\alpha)$ all diagrams become large

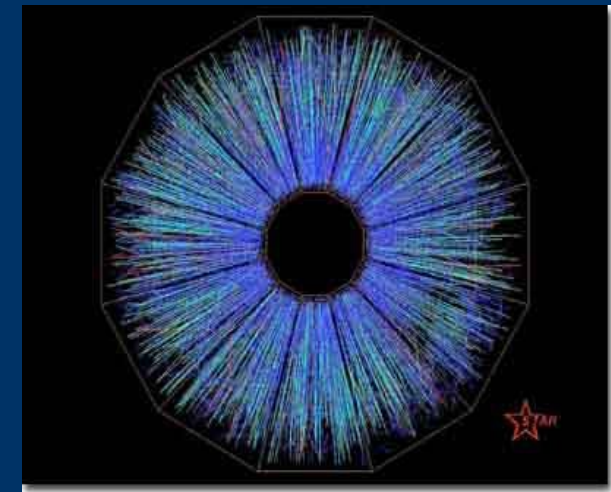
On the lattice: mainly equilibrium methods so far, static quantities with few exceptions

High occupation numbers

Classical-statistical description at earliest times

Cannot describe approach to thermal equilibrium

First principle calculations of QFT needed



Non equilibrium + Quantum fields=?

Late times approaching thermal equilibrium:

quantum effects become important

Classical approximation breaks down

Direct Method: Schrödinger equation for the wave function: $\Psi[A_\mu^a(x)]$

Impossible!

Formulation with non-equilibrium generator function $Z[J] = \int D\Phi e^{i \int_C L(\Phi, J) dt}$

averages with complex weight is needed! e^{iS_M}

Importance sampling doesn't work

Stochastic Quantization Parisi, Wu (1981)

Weighted, normalized average:
$$\frac{\int O(x) \exp(-S(x)) dx}{\int \exp(-S(x)) dx} = \langle O \rangle$$

Stochastic process for x
$$\frac{dx}{d\tau} = -\frac{\partial S}{\partial x} + \eta(\tau)$$

Gaussian noise $\langle \eta(\tau) \rangle = 0$ $\langle \eta(\tau) \eta(\tau') \rangle = 2 \delta(\tau - \tau')$

Averages are calculated along the trajectories:

$$\langle O \rangle = \frac{1}{T} \int_0^T O(x(\tau)) d\tau$$

Fokker-Planck equation for the probability distribution of $P(x)$:

$$\frac{\partial P}{\partial \tau} = \frac{\partial}{\partial x} \left(\frac{\partial P}{\partial x} + P \frac{\partial S}{\partial x} \right) = -H_{FP} P$$

Real action \rightarrow positive eigenvalues

for real action the Langevin method is convergent

Real-time evolution

$$\langle O(t) \rangle = \langle i | U(0, t) O U(t, 0) | i \rangle$$

Schwinger-Keldysh contour

Nonequilibrium generating functional $Z[J] = \int D\Phi e^{i \int_c L(\Phi, J) dt}$

Real time = Langevin method with complex action!

$$\frac{d\phi}{d\tau} = i \frac{\partial S}{\partial \phi} + \eta(\tau)$$

Klauder '83, Parisi '83, Hueffel, Rumpf '83,
Okano, Schuelke, Zeng '91, ...

applied to nonequilibrium: Berges, Stamatescu '05, ...

5D classical langevin system



4D quantum averages

The field is complexified

real scalar \rightarrow complex scalar

link variables: SU(2) \rightarrow SL(2,C)
compact non-compact

Is it still the same theory?

Yes: real (SU(2)) averages
Schwinger-Dyson equations fulfilled

No general proof of convergence

Runaway trajectories present (supressed by small Langevin time-step)

Scalar Theory

Complex contour given by: C_t , $\Delta_t = C_{t+1} - C_t$, $C_0 = 0$, $C_{N_t} = -i\beta$

action discretised
on the contour $S = \sum_t \left(\frac{(\phi_{t+1} - \phi_t)^2}{2\Delta_t} - \Delta_t \frac{V(\phi_t) + V(\phi_{t+1})}{2} \right)$

Langevin updating
in "5th" coordinate $\frac{d\phi_t}{d\tau} = \frac{\partial S}{\partial \phi_t} + \eta_t(\tau)$ $\langle \eta_t(\tau) \rangle = 0$
 $\langle \eta_t(\tau) \eta_{t'}(\tau') \rangle = 2\delta(\tau - \tau')\delta_{tt'}$

discretised: $\phi_t(\tau + \epsilon) = \phi_t(\tau) + i\epsilon \frac{\partial S}{\partial \phi_t} + \sqrt{\epsilon} \eta_t(\tau)$

Interacting scalar
oscillator

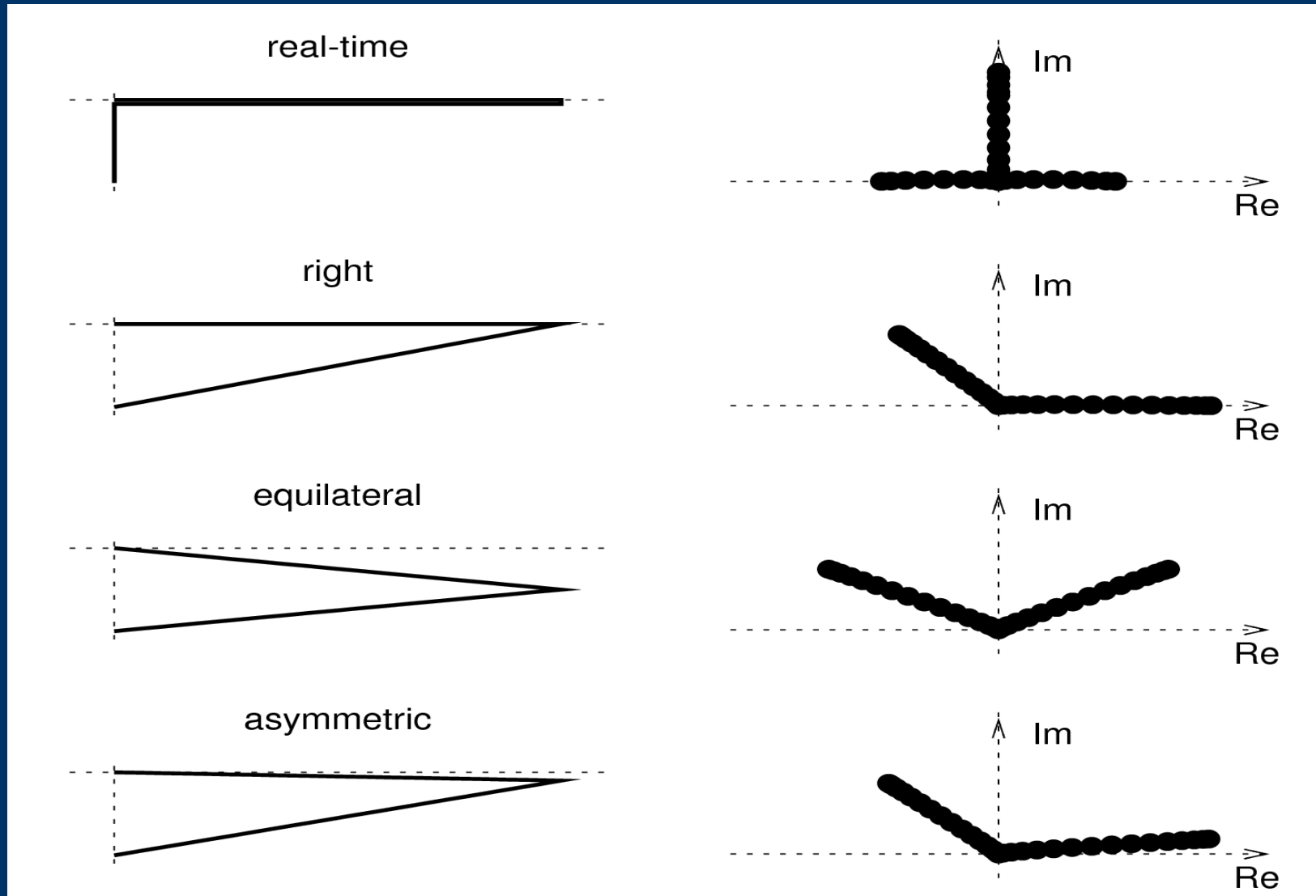
$$V(\phi) = \frac{1}{2} m^2 \phi^2 + \frac{\lambda}{24} \phi^4$$

Thermal equilibrium \longrightarrow periodic boundary conditions

$$\phi_0 = \phi_{N_t}$$

Type of contours

Eigenvalues of the free action
(positive Imaginary part = convergence)



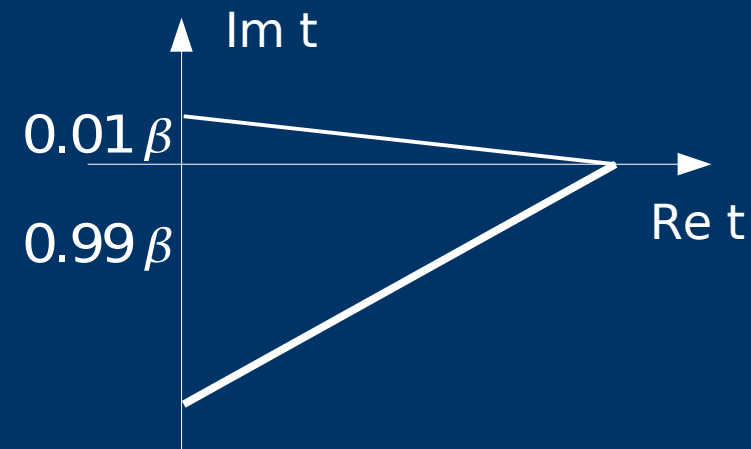
downwards sloped contour: regulator

Real-time two point function

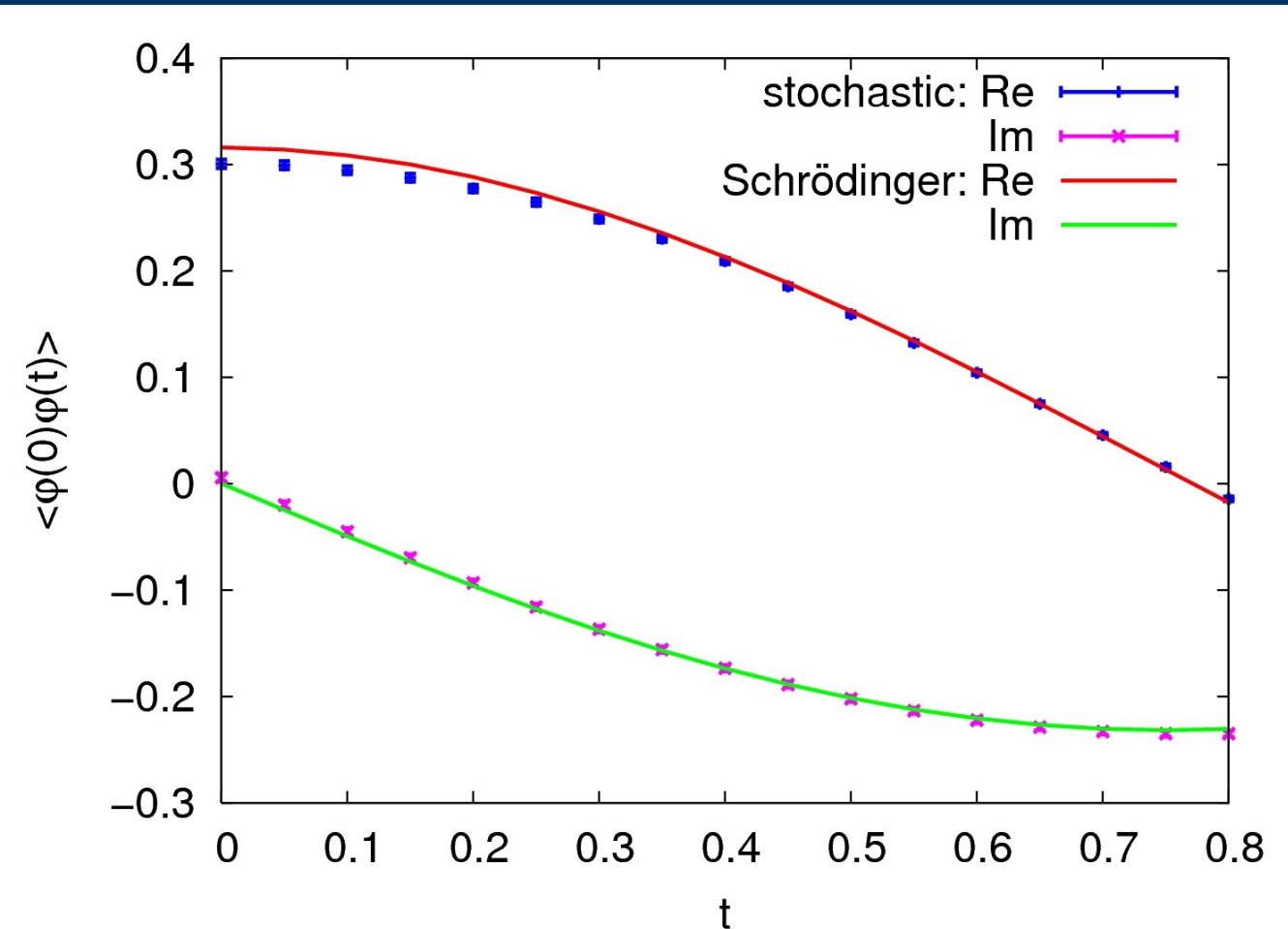
Thermal equilibrium:
periodic boundary cond.

Imaginary extent
gives $\beta = \frac{1}{T}$

Asymmetric
contour:



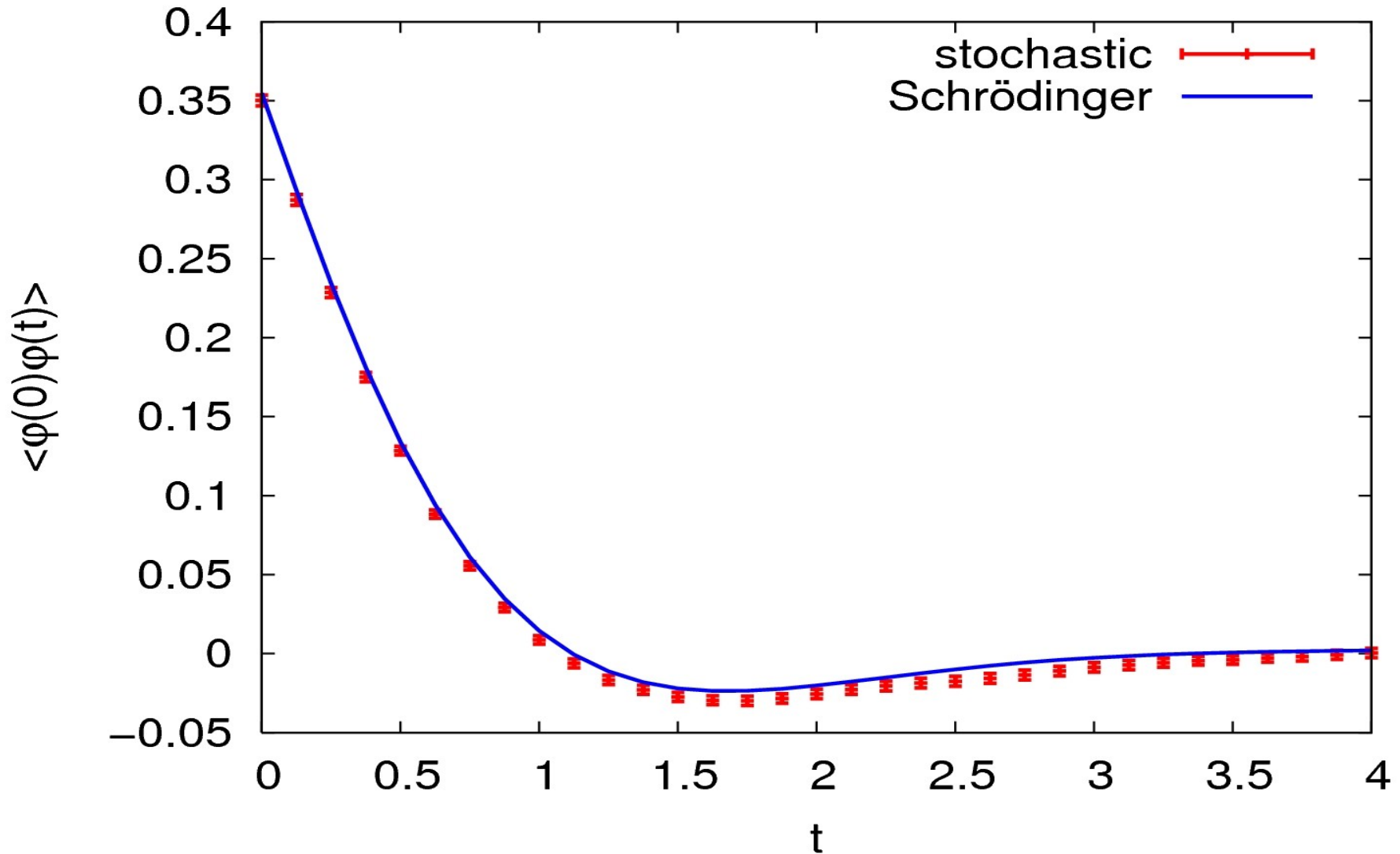
$$\lambda = 24, \beta = 1$$



Reproduces the Schrodinger equation result.

Two point function in thermal equilibrium with longer contour

$$\lambda=6, \beta=8$$



Non-equilibrium time evolution

Generating functional with initial density matrix:

$$Z(J, \rho) = \text{Tr} \left(\rho T_c e^{i \int_c J(x) \Phi(x)} \right) = \int d\varphi_1 d\varphi_2 \rho(\varphi_1, \varphi_2) \int_{\varphi_1}^{\varphi_2} D' \varphi e^{i \int_c L(x) + J(x) \varphi(x)}$$

Exponentializing the density matrix

Including φ_1, φ_2 in the path integral

$$\langle A(\varphi) \rangle = \int D\varphi_u D\varphi_l \exp(iS_\rho(\varphi_u, \varphi_l)) A(\varphi_u)$$

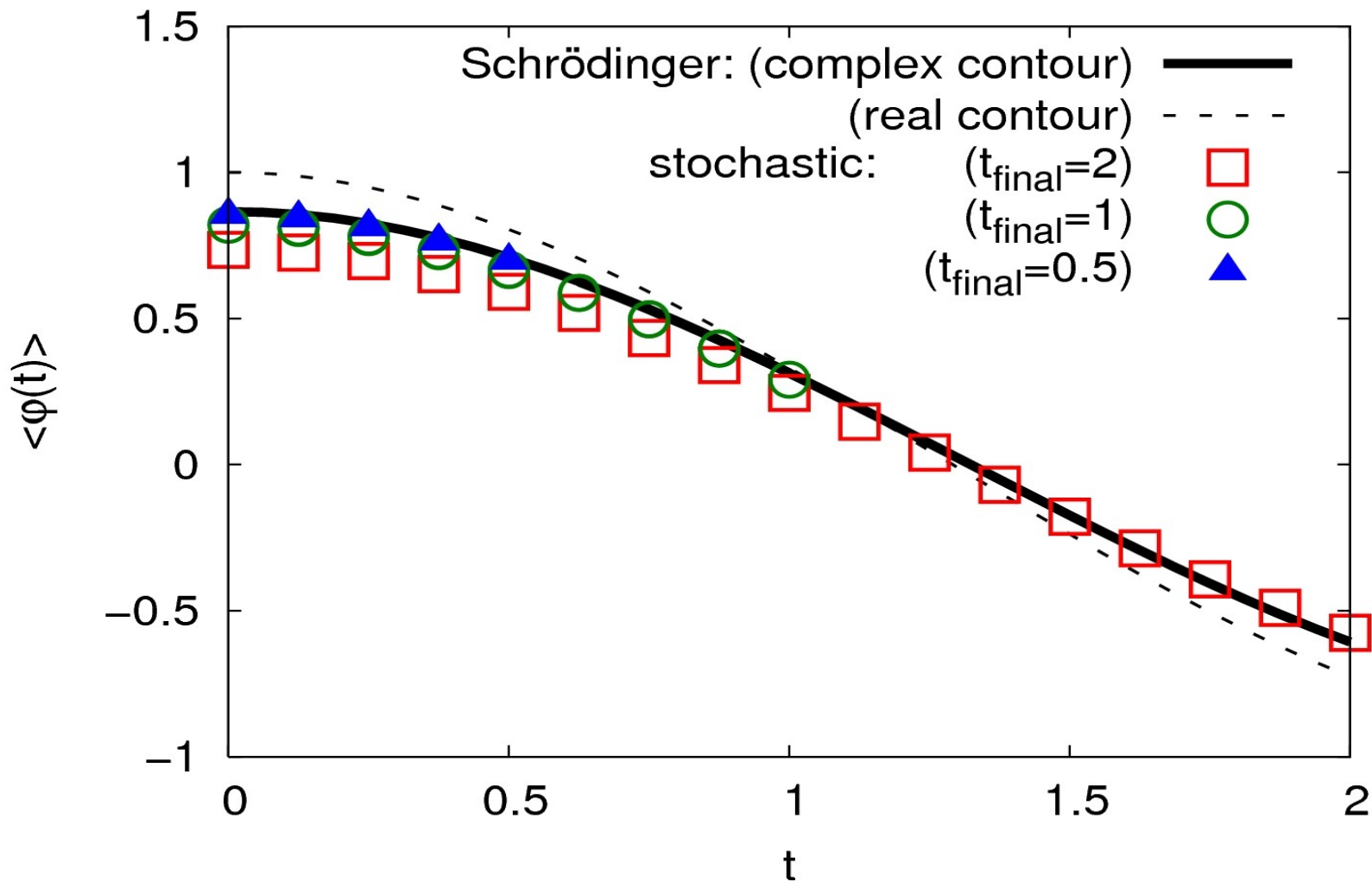
Langevin simulation with new "action":

$$S_\rho[\varphi_u, \varphi_l] = S[\varphi_u] - S[\varphi_l] - \frac{i}{a_t} S_0(\varphi_u, \varphi_l)$$

Most general gaussian density matrix with 5 parameters:

$$S_0(\varphi_u, \varphi_l) = i \dot{\phi}(\varphi_u - \varphi_l) - \frac{\sigma^2 + 1}{8 \xi^2} \left((\varphi_u - \phi)^2 + (\varphi_l - \phi)^2 \right) + \frac{i \eta}{2 \xi} \left((\varphi_u - \phi)^2 - (\varphi_l - \phi)^2 \right) + \frac{\sigma^2 - 1}{4 \xi^2} (\varphi_u - \phi)(\varphi_l - \phi)$$

Non-equilibrium time evolution



Contour with 5% slope

Bigger real time extent \longrightarrow worse agreement

SU(2) pure gauge theory

$$S = -\beta_0 \sum_{x,i} \frac{1}{2 \text{Tr} \mathbf{1}} (\text{Tr} U_{x,0i} + \text{Tr} U_{x,0i}^{-1}) - 1$$

$$+ \beta_s \sum_{x,i < j} \frac{1}{2 \text{Tr} \mathbf{1}} (\text{Tr} U_{x,ij} + \text{Tr} U_{x,ij}^{-1}) - 1$$

$$\beta_0 = \frac{2 \text{Tr} \mathbf{1} a_s}{g_0^2 a_t}$$

$$\beta_s = \frac{2 \text{Tr} \mathbf{1} a_t}{g_0^2 a_s}$$

Updating the link variables:

$$U'_{x,\mu} = \exp(i \lambda_a (\epsilon i D_{x\mu a} S[U] + \sqrt{\epsilon} \eta_{x\mu a})) U_{x\mu}$$

$$\langle \eta_{x\mu a} \rangle = 0$$

$$\langle \eta_{x\mu a} \eta_{y\nu b} \rangle = 2 \delta_{xy} \delta_{\mu\nu} \delta_{ab}$$

Left derivative: $D_a f(U) = \left. \frac{\partial}{\partial \alpha} f(e^{i \lambda_a \alpha} U) \right|_{\alpha=0}$

complexified link variables

SU(2) \longrightarrow SL(2,C)

compact \longrightarrow non-compact

$$U = \exp\left(i \frac{\varphi \hat{n} \hat{\sigma}}{2}\right) = \left(\cos \frac{\varphi}{2}\right) \mathbf{1} + i \left(\sin \frac{\varphi}{2}\right) \hat{n} \hat{\sigma}$$

$$U = a \mathbf{1} + i b_i \sigma_i \quad a^2 + b_i b_i = 1$$

a, b_i become complex variables

Schwinger Dyson equations for lattice gauge theory

Langevin-time equilibrium reached:

$$\langle U_{x\mu a}(\tau + d\tau) \rangle = \langle U_{x\mu a}(\tau) \rangle \Rightarrow \langle D_{x\mu a} S \rangle = 0 \quad \text{First Schwinger Dyson equation}$$

Plaquette average is Langevin time independent

$$\langle U_{x,\mu\nu}(\tau + d\tau) \rangle = \langle U_{x,\mu\nu}(\tau) \rangle \quad \text{Schwinger Dyson equation for plaquette average}$$

can also be derived using the properties of Haar integration in the original integration over group space

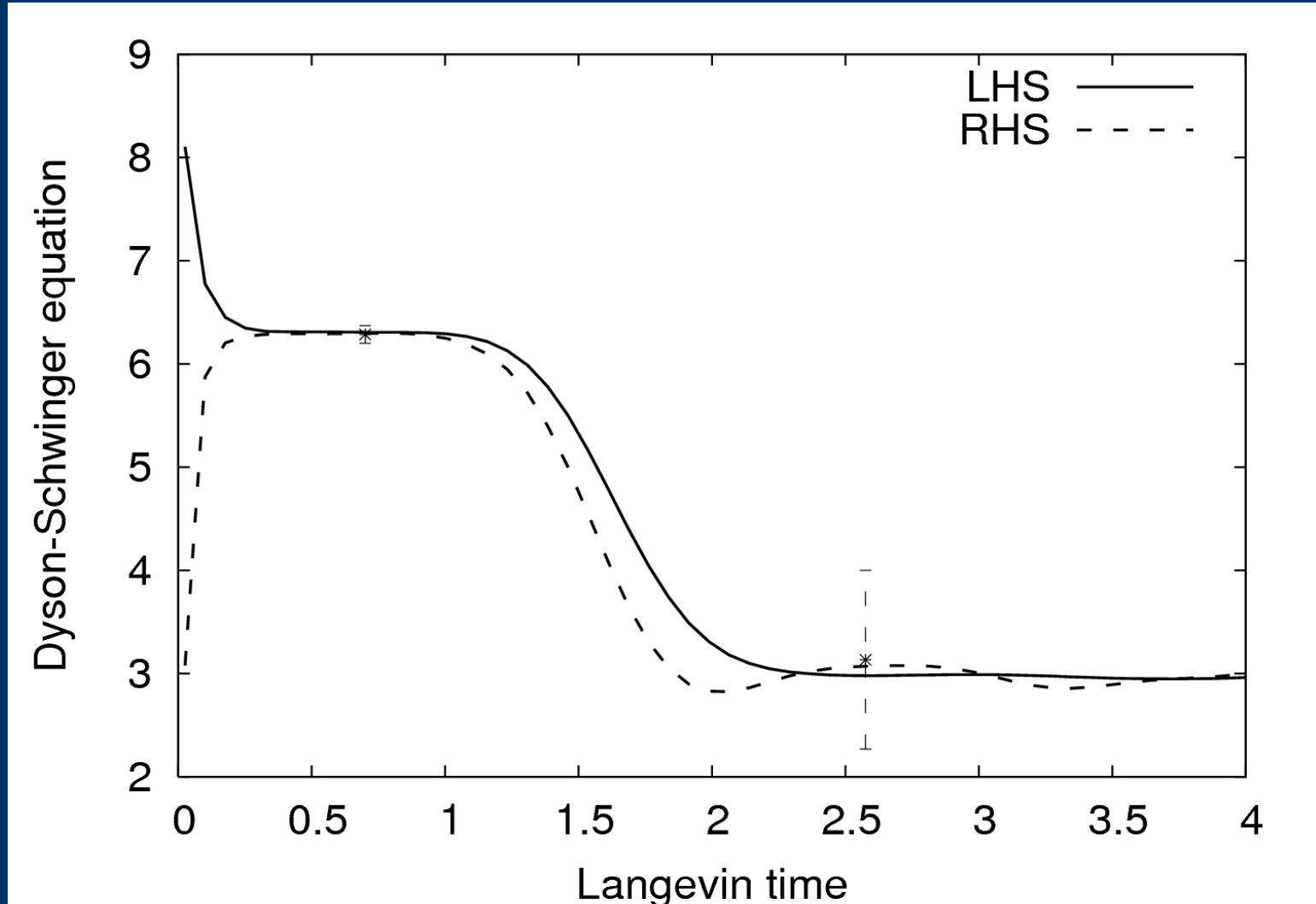
$$\frac{2(N^2 - 1)}{N} \left\langle \left[\begin{array}{|c|} \hline \mu \\ \hline \end{array} \right] \right\rangle = \frac{i}{N} \sum_{\pm\gamma} \beta_{\mu\gamma} \left\{ \left\langle \left[\begin{array}{|c|} \hline \mu \\ \hline \end{array} \right] \right\rangle - \left\langle \left[\begin{array}{|c|} \hline \mu \\ \hline \end{array} \right] \right\rangle \right. \\ \left. - \frac{1}{N} \left\langle \left[\begin{array}{|c|} \hline \mu \\ \hline \end{array} \right] \right\rangle - \left\langle \left[\begin{array}{|c|} \hline \mu \\ \hline \end{array} \right] \right\rangle \right\}$$

This method gives solutions of SD equations (all of them!)

(loophole: one might get unphysical solution)

SU(2) field theory

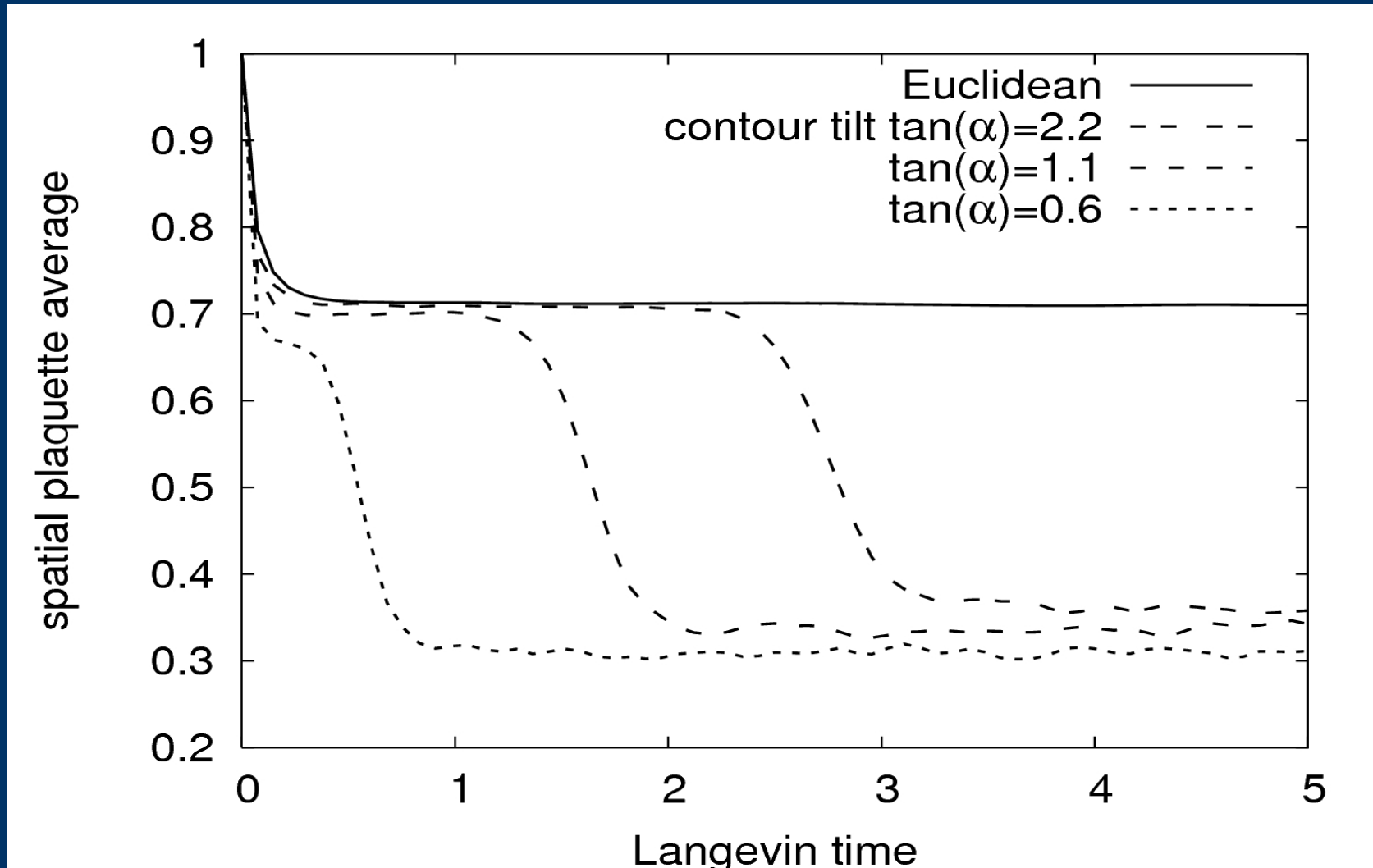
Numerical check of the Schwinger-Dyson equation



SD equations are fulfilled in both regions

SU(2) gauge theory without gaugefixing

without gauge fixing, non-physical fixpoint is always present



How to stabilize the first (physical) result?

U(1) One plaquette model

$$S_0 = i\beta \cos(\varphi)$$

We are interested
in averages:

$$\langle f(\varphi) \rangle = \frac{1}{Z} \int_0^{2\pi} d\varphi e^{i\beta \cos \varphi} f(\varphi)$$

Langevin equation: $\frac{d\varphi}{d\tau} = -i\beta \sin \varphi + \eta(\tau)$

Distribution of φ on the complex plane

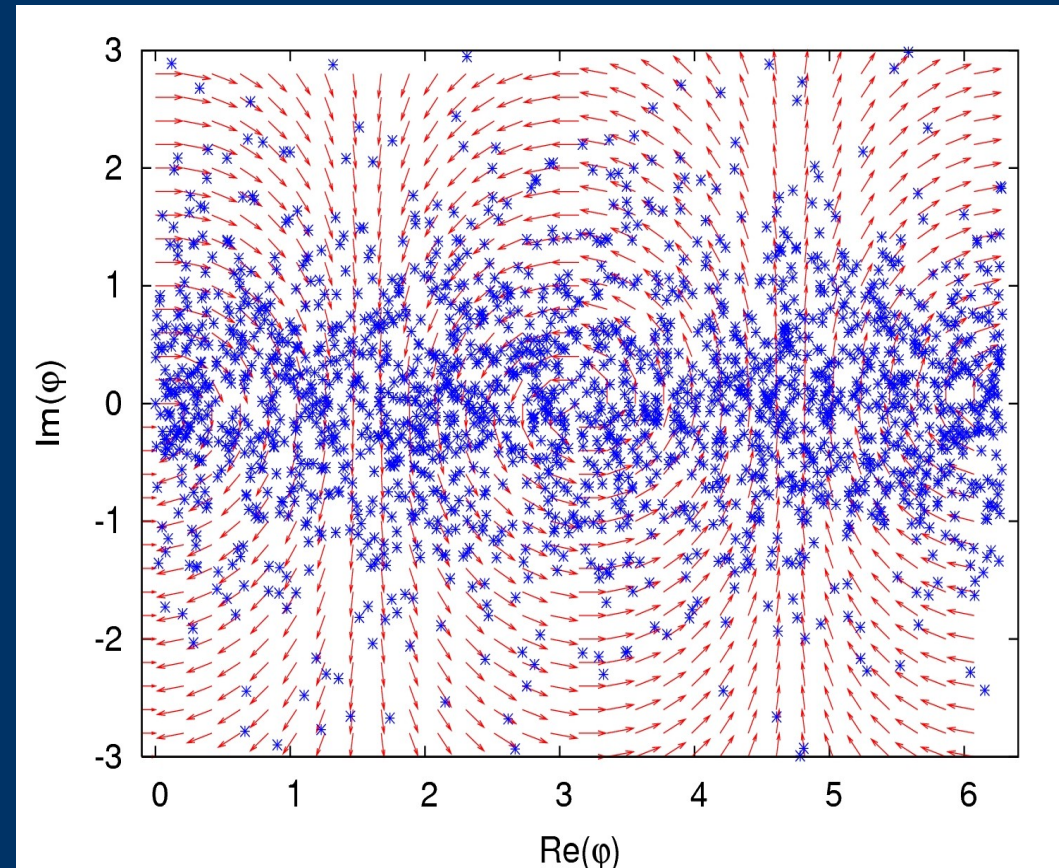
Failure of the naïve method

exact result: $\langle e^{i\varphi} \rangle = i0.575$

stochastic result:

$$-0.009 \pm 0.006 + i(0.00006 \pm 0.00007)$$

symmetric distribution
result compatible with zero



Stochastic reweighting

generalization: $S_p = i\beta \cos(\varphi) + i p \varphi$

$$\langle O \rangle_p = \frac{1}{Z_p} \int_0^{2\pi} d\varphi e^{S_p} O(\varphi)$$

Langevin equation: $\frac{d\varphi}{d\tau} = -i\beta \sin \varphi + i p + \eta(\tau)$

reweighting factor: $\omega_p = \exp(S_0 - S_p)$

Reweighting formula

averages with S_0 calculated
from averages with S_p

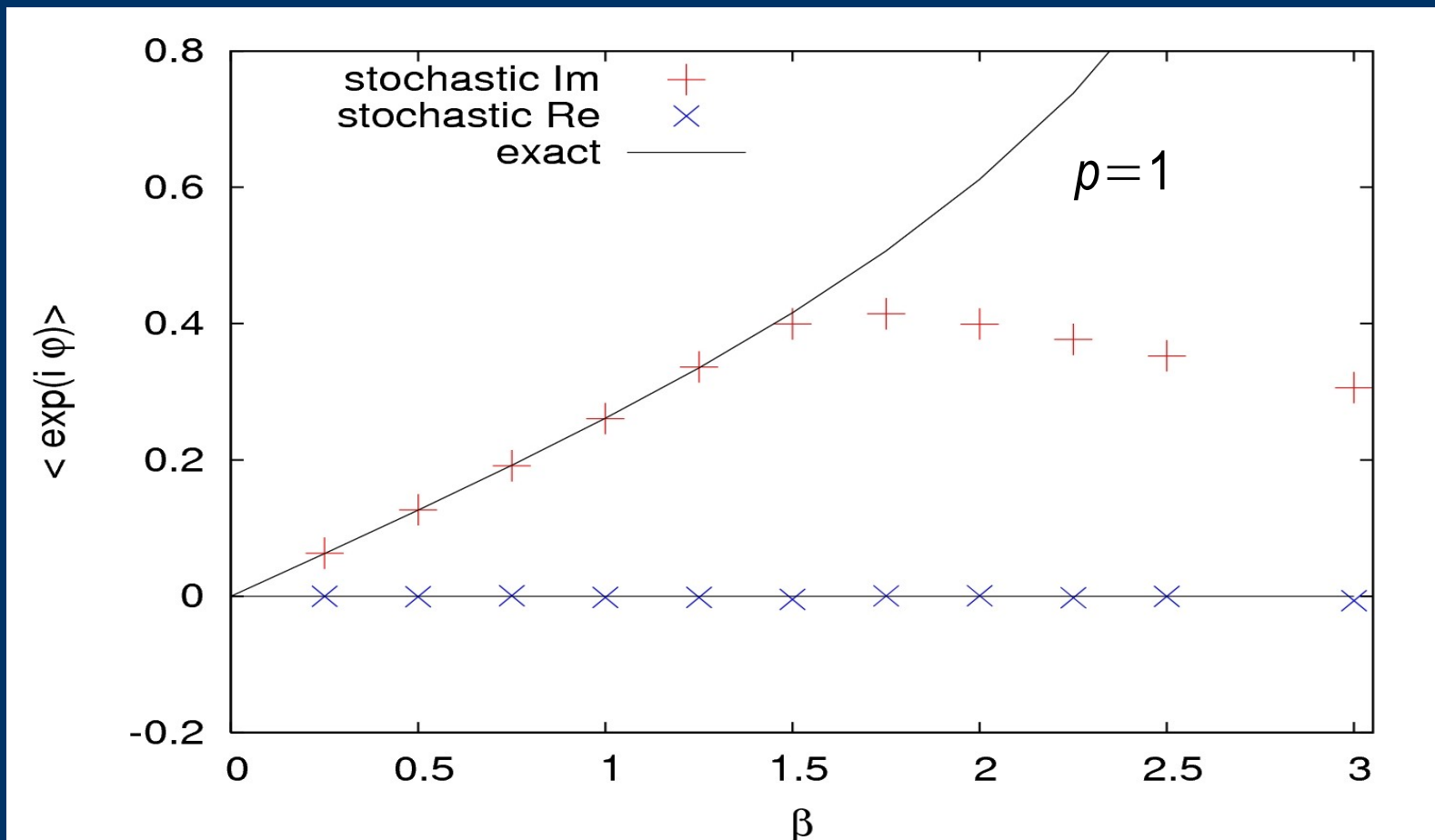
$$\langle O \rangle_0 = \frac{\int_0^{2\pi} d\varphi e^{iS_p} \omega_p O(\varphi)}{\int_0^{2\pi} d\varphi e^{iS_p} \omega_p} = \frac{\langle \omega_p O \rangle_p}{\langle \omega_p \rangle_p}$$

$$\langle e^{i\varphi} \rangle_0 = \frac{\langle 1 \rangle_{p=1}}{\langle e^{-i\varphi} \rangle_{p=1}} = (-0.02 \pm 0.02) + i(0.574 \pm 0.001)$$

Exact result: $\langle e^{i\varphi} \rangle_{p=0} = i 0.575$ with reweighting it works!

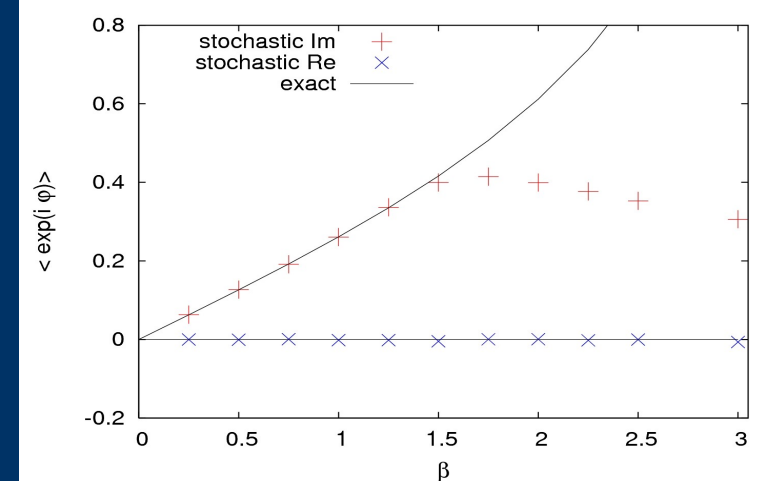
Using the generalized action $S_p = i\beta \cos(\varphi) + i\rho\varphi$

Correct results obtained for $\langle \exp(i\varphi) \rangle$ in the region: $\beta \leq \rho$



Flowchart: normalized drift vectors on the complex plane

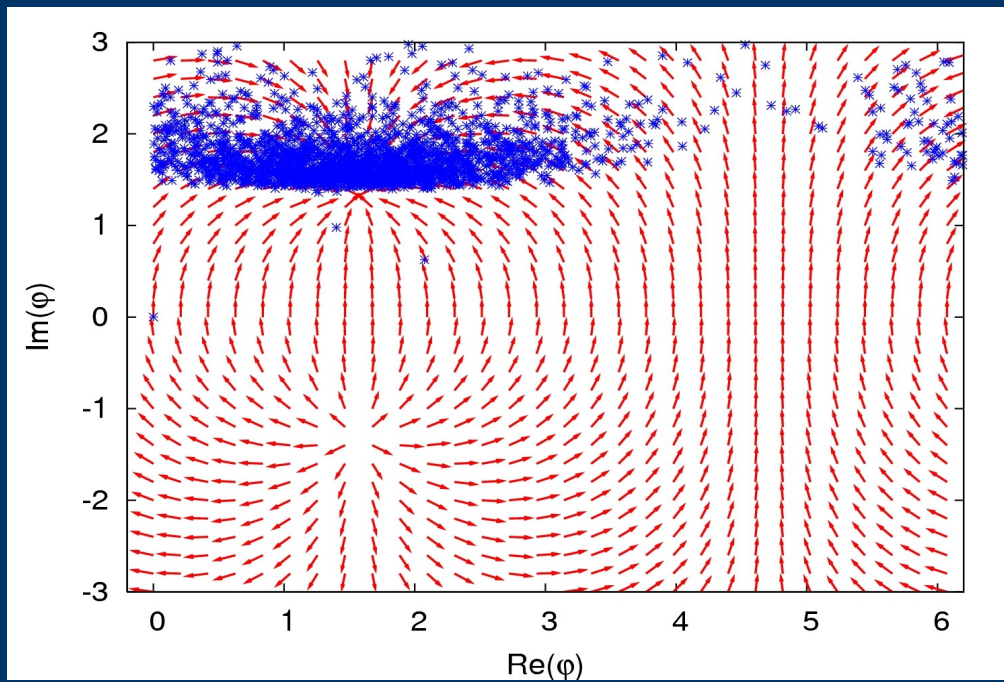
shows fixedpoint (zero drift term) structure on the complex φ plane



Attractive fixedpoint present

smaller distribution
correct results

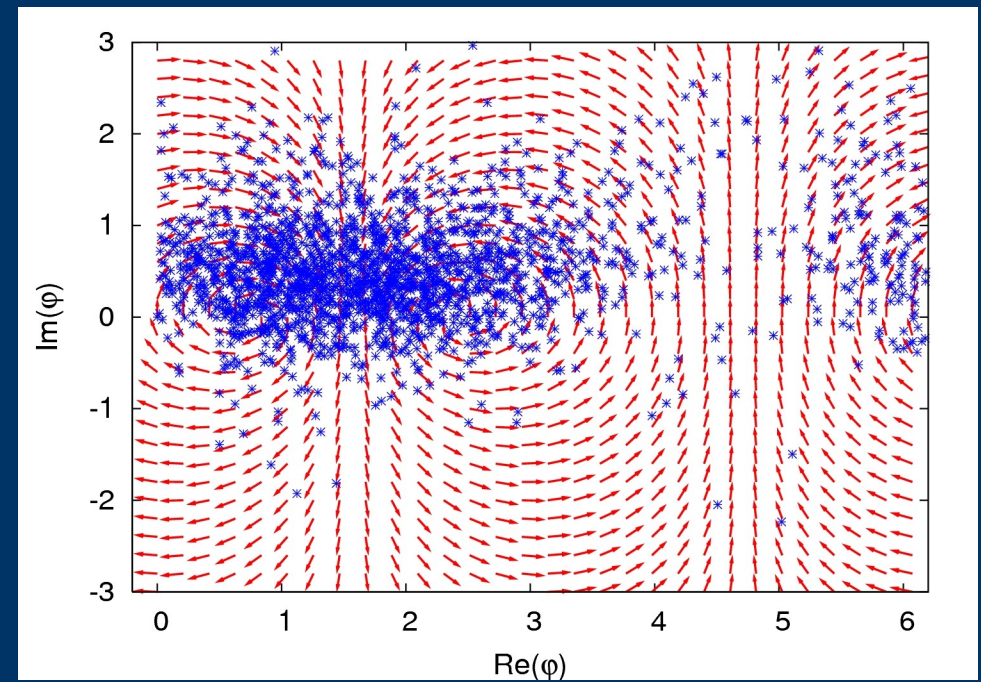
$$\beta=0.5, \rho=1$$



No attractive fixedpoint present
(only indifferent)

larger distribution
incorrect results

$$\beta=1.5, \rho=1$$



One-plaquette model in classical limit

$$S = i\beta \cos(\varphi) + i\rho\varphi$$

$$\text{Langevin equation: } \frac{d\varphi}{d\tau} = -i\beta \sin\varphi + i\rho + \eta(\tau)$$

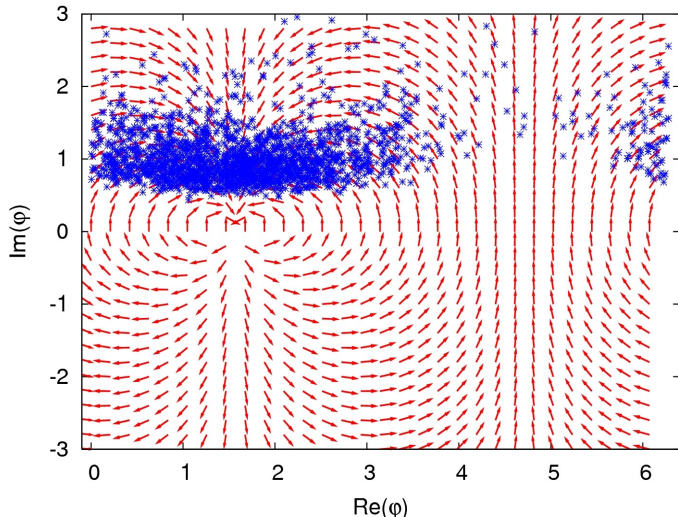
Classical limit: $(\beta = \rho) \rightarrow \infty$

fluctuations suppressed

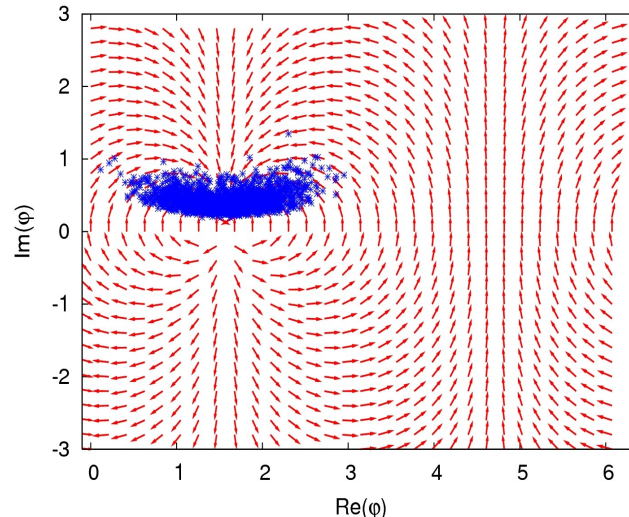
classical averages in the limit $\beta = \rho \rightarrow \infty$

Distributions of φ on the complex plane

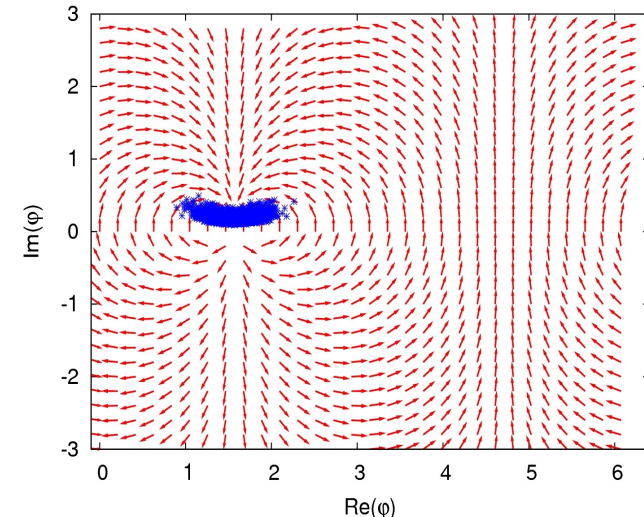
$\beta = \rho = 1$



$\beta = \rho = 10$



$\beta = \rho = 100$



Gaugefixing in SU(2) one plaquette model

SU(2) one plaquette model: $S = i\beta \text{Tr} U \quad U \in \text{SU}(2)$

“gauge” symmetry: $U \rightarrow W U W^{-1}$ complexified theory: $U, W \in \text{SL}(2, \mathbb{C})$

exact averages by numerical integration: $\langle f(U) \rangle = \frac{1}{Z} \int_0^{2\pi} d\varphi \int d\Omega \sin^2 \frac{\varphi}{2} e^{i\beta \cos \frac{\varphi}{2}} f(U(\varphi, \hat{n}))$

Langevin updating $U' = \exp(i\lambda_a (\epsilon i D_a S[U] + \sqrt{\epsilon} \eta_a)) U$

parametrized with Pauli matrices

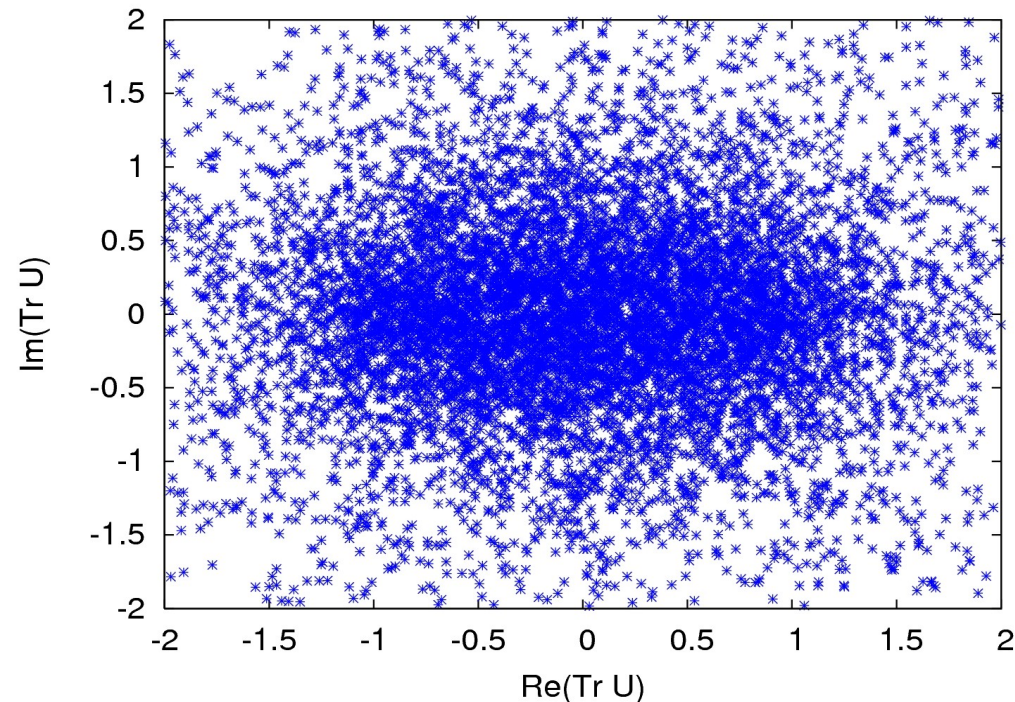
$$U = \exp\left(i \frac{\varphi \hat{n} \hat{\sigma}}{2}\right) = \left(\cos \frac{\varphi}{2}\right) \mathbf{1} + i \left(\sin \frac{\varphi}{2}\right) \hat{n} \hat{\sigma}$$
$$U = a \mathbf{1} + i b_i \sigma_i \quad a^2 + b_i b_i = 1$$

After each Langevin timestep: fix gauge condition

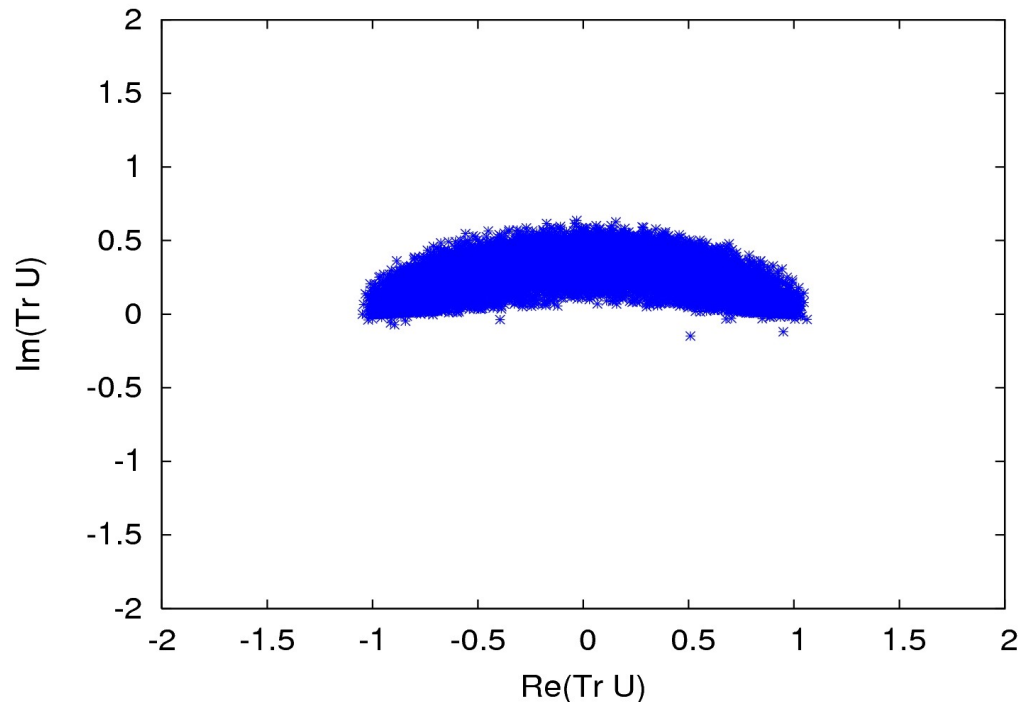
$$U = a \mathbf{1} + i \sqrt{1 - a^2} \sigma_3 \quad b_i = (0, 0, \sqrt{1 - a^2})$$

SU(2) one-plaquette model

Distributions of $\text{Tr}(U)$ on the complex plane



Without gaugefixing



With gaugefixing

Exact result from integration: $\langle \text{Tr } U \rangle = i0.2611$

From simulation:

$$(-0.02 \pm 0.02) + i(-0.01 \pm 0.02)$$

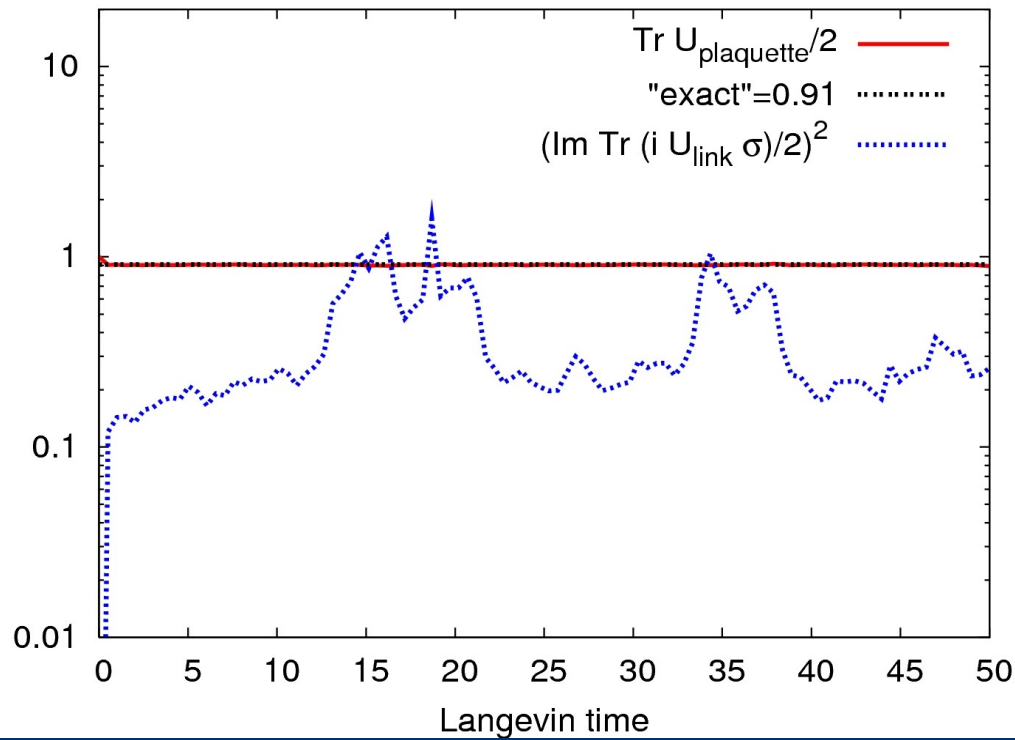
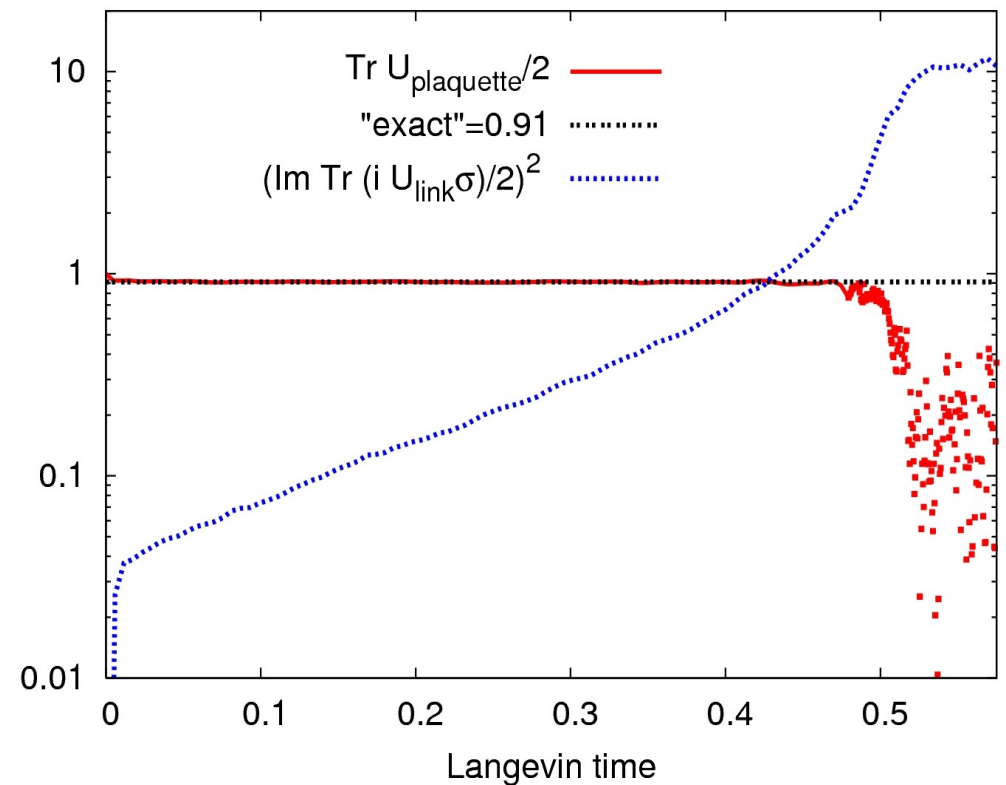
$$(-0.004 \pm 0.006) + i(0.260 \pm 0.001)$$

With gauge fixing, all averages are correctly reproduced

SU(2) field theory

$(\text{Im Tr} U)^2$ measures size of distribution

Without gauge fixing
non physical fixed point



Gauge fixing
small lattice coupling \rightarrow large β

Correct result stabilizes

However: $a \sim \exp(-b_0/g^2)$

With the coupling $g = 0.5$

$$1/m_{\text{pion}} \sim 10^{15} a_{\text{lat}}$$

Conclusions

Without optimization: short real time simulation of scalar oscillator in equilibrium and non-equilibrium gives correct results (Schrodinger)

Langevin method: Schwinger Dyson equation solver

Optimization methods to reduce fluctuations:
reweighting
gaugefixing
using small lattice-coupling

with optimization:

Method gives physical solution for SU(2) lattice gauge theory

Scalar Theory

Complex contour given by: C_t , $\Delta_t = C_{t+1} - C_t$, $C_0 = 0$, $C_{N_t} = -i\beta$

action discretised
on the contour $S = \sum_t \left(\frac{(\phi_{t+1} - \phi_t)^2}{2 \Delta_t} - \Delta_t \frac{V(\phi_t) + V(\phi_{t+1})}{2} \right)$

Langevin updating
in "5th" coordinate $\frac{d\phi_t}{d\tau} = \frac{\partial S}{\partial \phi_t} + \eta_t(\tau)$

Free theory: $v(\phi) = \frac{m^2 \phi^2}{2}$

The action can be diagonalized: $S = \frac{1}{2} \sum_a c^a \chi^a \chi^a$, $\chi^a = \sum_t \psi_t^a \phi_t$

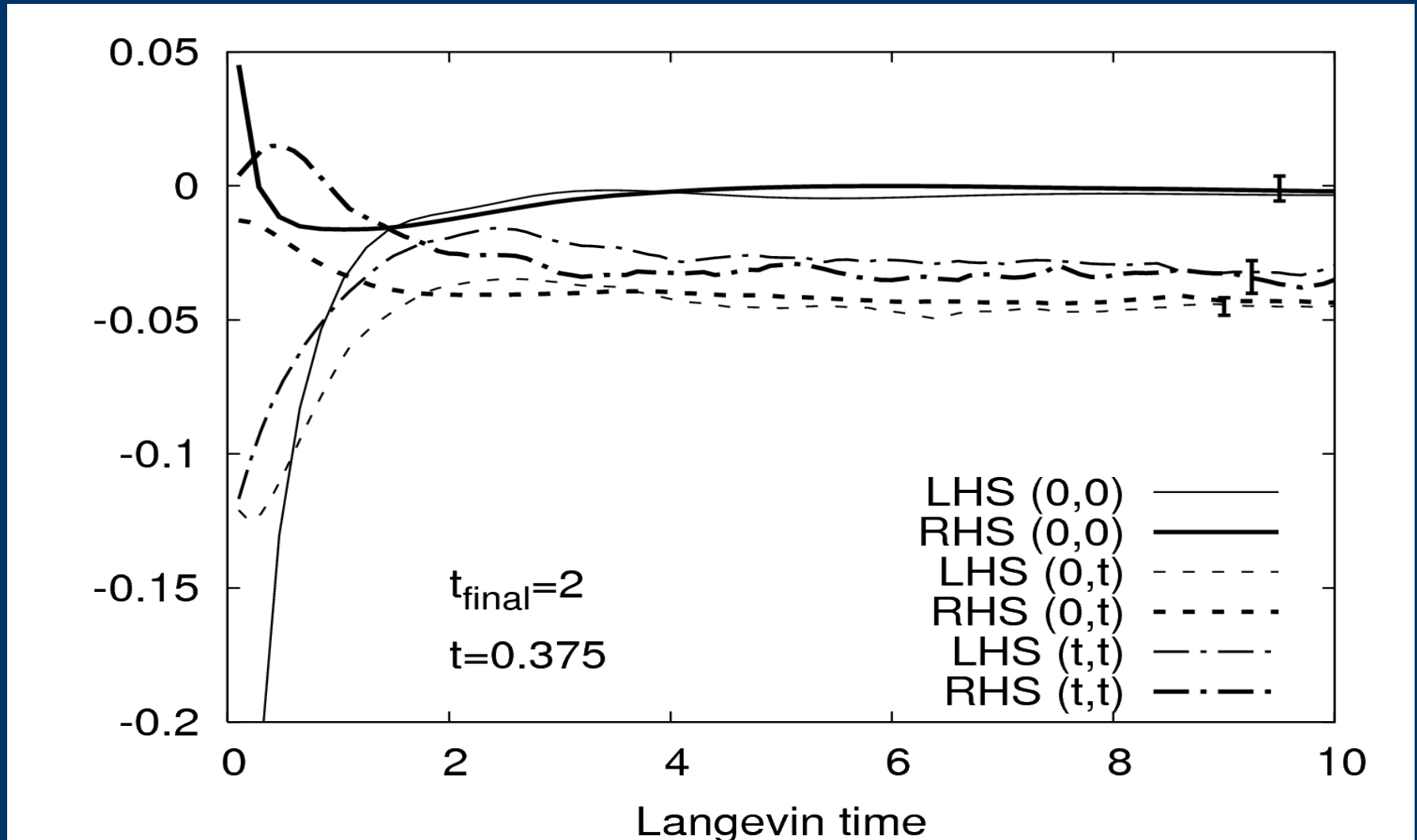
Langevin equation diagonalized coords.:

$$\frac{d\chi^a}{d\tau} = i c^a \chi^a + \eta^a$$

convergent if $\text{Im}(c^a) > 0$

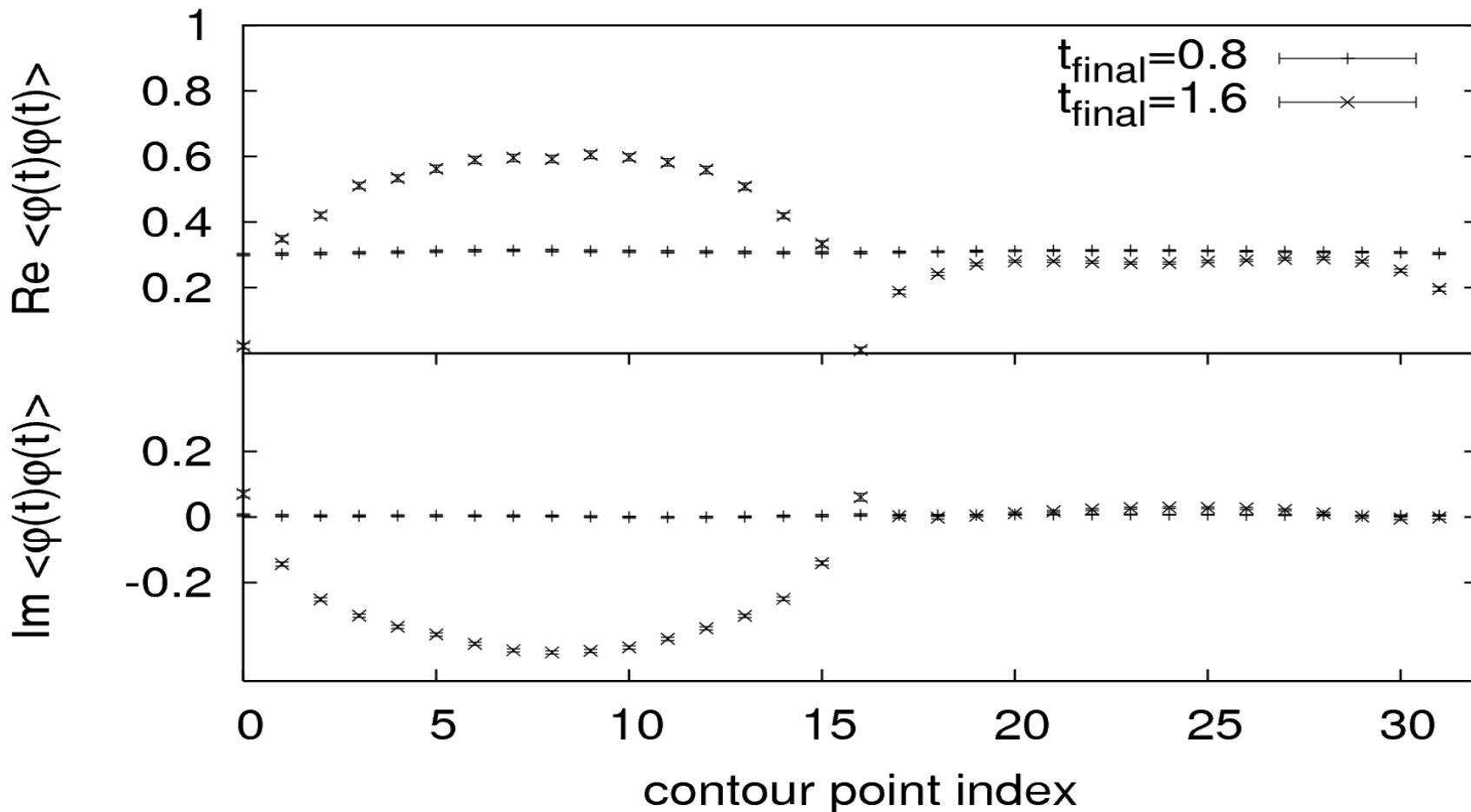
Numerical check of the Schwinger-Dyson equation

$$\sum_{\tau} G_{0,t\tau}^{-1} \langle \varphi_{\tau} \varphi_{t'} \rangle - \delta_{tt'} = -i\lambda \langle \varphi_t \varphi_t \varphi_t \varphi_{t'} \rangle$$



Non-Physical fixpoints

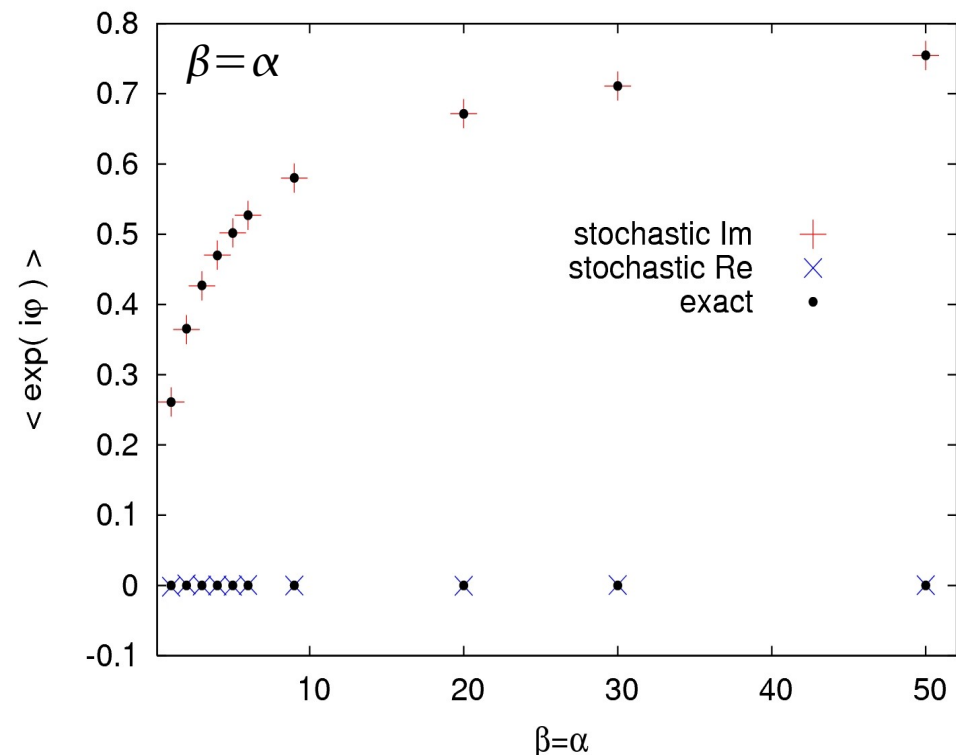
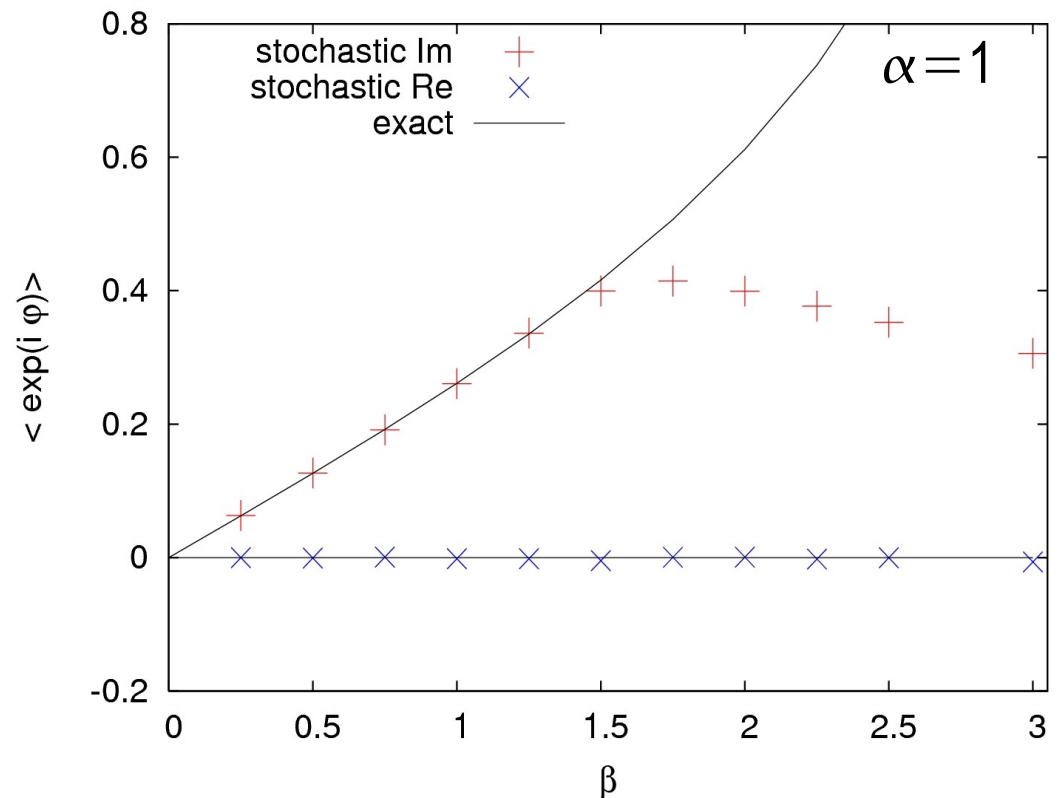
long contour \rightarrow non-time translation invariant solution



Using the generalized action S_α

Correct results obtained for $\beta \leq \alpha$

With reweighting correct results for S_0



S_α for $\beta=\alpha$

classical fixed point (zero drift term)
on the real axis

$\alpha = \text{integer}$

action can be uniquely written as

$$S(U) \quad U \in U(1)$$

Correct results for $\langle f(U) \rangle_\alpha \quad U \in U(1)$