Towards Sampling Complex Actions

Kades, Gärttner, Gasenzer, Pawlowski, arXiv:2106.09367

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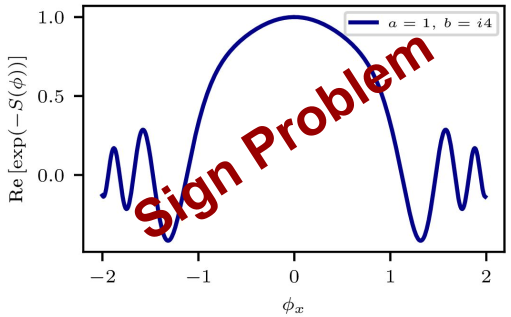
LATTICE 21

Motivation

Sign problem



➢ Goal: Numerically access observables

$$\langle \mathcal{O}(\phi) \rangle = \frac{1}{Z} \int \mathcal{D}\phi \, \mathcal{O}(\phi) e^{-S(\phi)}$$

with $S(\phi) \in \mathbb{C}$

➢ Problem: No probability distribution!

➢ Standard Monte Carlo algorithms fail, with one exception: Langevin dynamics

$$\langle \mathcal{O}(\phi) \rangle_\rho = \int_a^b \mathrm{d}\phi\, \mathcal{O}(\phi)\rho(\phi)$$

Complex Langevin dynamics

G. Parisi, Phys. Lett. B 131, 393–395 (1983)

Klauder, Recent Developments in High-Energy Physics (1983) pp. 251–281.

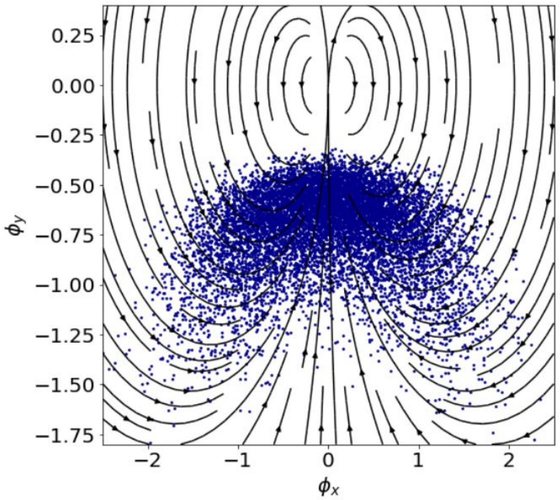
What is complex Langevin dynamics:

➢ A sampling process that allows the numerical computation of complex action problems.

Update rules (CLE)

$$\frac{\mathrm{d}\phi_x}{\mathrm{d}\tau} = -\frac{\delta S_{\mathrm{Re}}(\phi)}{\delta \phi}\bigg|_{\phi_x + i\phi_y} + \eta$$

$$\frac{\mathrm{d}\phi_y}{\mathrm{d}\tau} = -\frac{\delta S_{\mathrm{Im}}(\phi)}{\delta \phi}\bigg|_{\phi_x + i\phi_y}$$

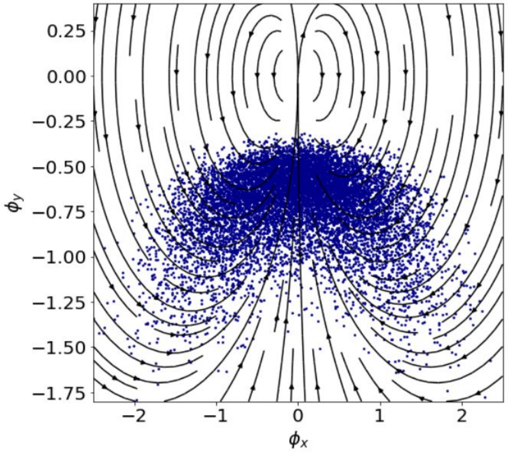


$$P(\phi_x, \phi_y; \theta)$$

Observables

$$\langle \mathcal{O}(\phi) \rangle_\rho = \langle \mathcal{O}(\phi_x + i\phi_y) \rangle_P \simeq \frac{1}{N}\sum_i^N \mathcal{O}(\phi_{x,i} + i\phi_{y,i})$$

Complex Langevin dynamics



Big advantage:

➢ Appeal of general applicability (model-independent)

Problems (model-specific):

➢ Potential convergence to unphysical fixed points / solutions

➢ Numerical instabilities

Ambjørn and S.-K. Yang, Phys. Lett. B 165, 140–146 (1985)

Nishimura and S. Shimasaki, Phys. Rev. D 92, 011501 (2015)

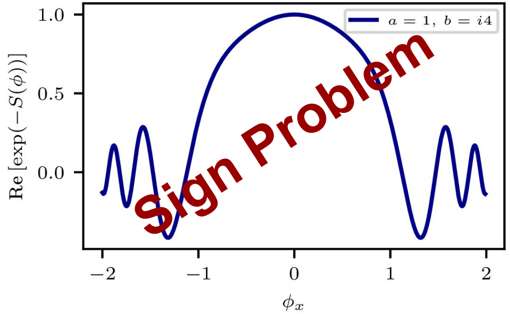
Hayata et al., Nucl. Phys. B 911, 94–105 (2016)

Salcedo, Phys. Rev. D 94, 114505 (2016)

E. Seiler, EPJ Web Conf. 175, 01019 (2018)

Nagata et al., J. High Energ. Phys. 2018, 4 (2018)

Complex Langevin dynamics



$S(\phi) \in \mathbb{C}$

Theoretical understanding:

- ➢ Rather heuristic derivation from Langevin dynamics
- ➢ Subsequent theoretical justification and derivation of criteria for correctness based on Fokker-Planck equation
  Aarts, J. High Energ. Phys. 2008, 018–018 (2008)
  Aarts et al., Phys. Rev. D 81, 054508 (2010).
- ➢ No thorough understanding in terms of a Markov chain Monte Carlo algorithm

Key question:

- ➢ How to define a sampling process based on the first principles of a Markov chain Monte Carlo algorithm (detailed-balance equation) for complex action problems?

Key insights

$$\langle \mathcal{O}(\phi) \rangle = \frac{1}{Z} \int \mathcal{D}\phi \, \mathcal{O}(\phi) e^{-S(\phi)}$$

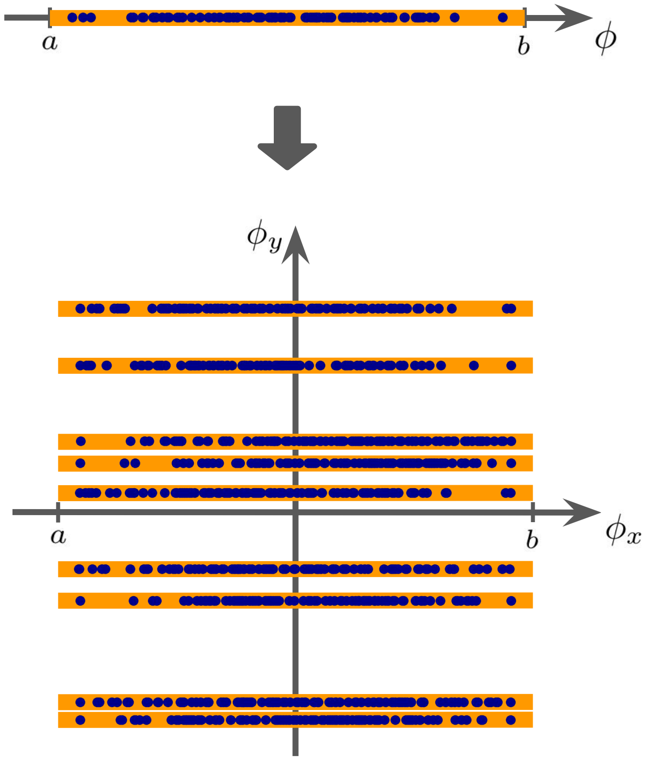
Key insights for a possible sampling process

➢ Reformulation as a **mean over several integrals in the complex plane**

$$\langle \mathcal{O}(\phi) \rangle_\rho = \int_a^b \mathrm{d}\phi \, \mathcal{O}(\phi)\rho(\phi)$$

$$\phi = \phi(\phi_x) = \phi_x + i\phi_{y,i} \, , \quad \mathrm{d}\phi = \mathrm{d}\phi_x$$

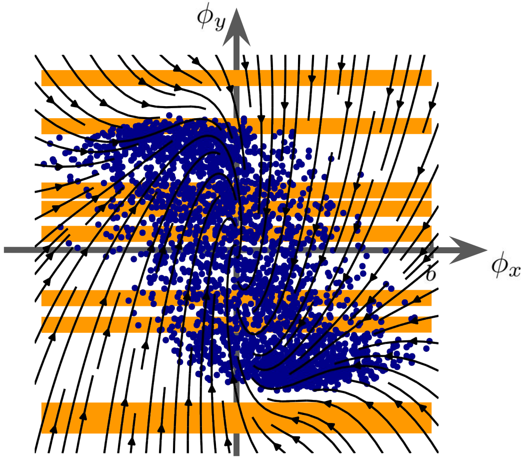
$$\langle \mathcal{O}(\phi) \rangle_\rho = \frac{1}{N} \sum_{i=1}^{N} \int_{a-i\phi_{y,i}}^{b-i\phi_{y,i}} \mathrm{d}\phi_x \, \mathcal{O}(\phi_x + i\phi_{y,i})\rho(\phi_x + i\phi_{y,i})$$



$$\langle \mathcal{O}(\phi) \rangle = \frac{1}{Z} \int \mathcal{D}\phi \, \mathcal{O}(\phi) e^{-S(\phi)}$$

Key insights for a possible sampling process

- Mixing the sampling process of each integral allows the definition of **real-valued transition probabilities**



- Key for an interpretation as a Markov chain Monte Carlo algorithm

- Basis for a numerical sampling scheme in the complex plane

$$\langle \mathcal{O}(\phi) \rangle_\rho = \frac{1}{MN} \sum_{i=1}^{MN} \mathcal{O}(\phi_{x;i} + i\phi_{y;i})$$

Implications

$$\langle \mathcal{O}(\phi) \rangle_\rho = \frac{1}{MN} \sum_{i=1}^{MN} \mathcal{O}(\phi_{x;i} + i\phi_{y;i})$$

Main Results

➢ Mathematical framework for a Markov chain Monte Carlo sampling algorithm for complex action problems based on **four constraints**:

1. Satisfaction of the following detailed-balance equation for a fixed hidden state w:

Adapted detailed-balance equation

$$= p(v', w) g(w'|v, v', w) T(v|v', w) \,. \qquad (37)$$

2. Th… updated with an infinites-im…

Infinitesimally small step sizes in imaginary direction

3. The … the b… den s… ple, i… the i…

$$\langle \mathcal{O}(\phi) \rangle_\rho = \int_{a-i\phi_y}^{b-i\phi_y} \mathrm{d}\phi_x \, \mathcal{O}(\phi_x + i\phi_y) \rho(\phi_x + i\phi_y)$$

$$\langle \mathcal{O}(\phi) \rangle_\rho = \int_{a}^{b} \mathrm{d}\phi_x \, \mathcal{O}(\phi_x + i\phi_y) \rho(\phi_x + i\phi_y)$$

4. The distribution $p(v, w)$ and the transition probabilities T and g need to satisf… constraint, cf. Eq. (26),

Equilibrium

$$p(v', w', \tau) \stackrel{!}{=} \ldots$$

$$\times \, p(v, w, \tau) \, g(w'|v', v, w) T(v'|v, w) \,. \qquad (38)$$

➢ Substitution sampling algorithm

Main Results

The substitution sampling algorithm

- ➢ allows a novel **mathematically well-founded** derivation of complex Langevin dynamics as a Markov chain Monte Carlo algorithm

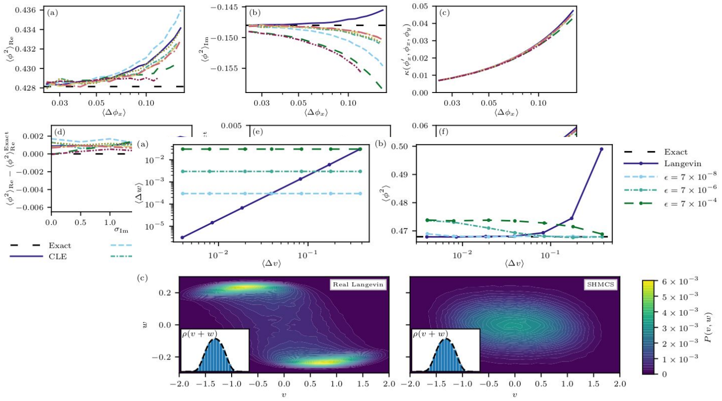
$$\frac{\mathrm{d}\phi_x}{\mathrm{d}\tau} = -\frac{\delta S_{\mathrm{Re}}(\phi)}{\delta\phi}\bigg|_{\phi_x+i\phi_y} + \eta$$
$$\frac{\mathrm{d}\phi_y}{\mathrm{d}\tau} = -\frac{\delta S_{\mathrm{Im}}(\phi)}{\delta\phi}\bigg|_{\phi_x+i\phi_y}$$

- ➢ is in strong contrast to the standard, rather heuristic derivation from Langevin dynamics

Main Results

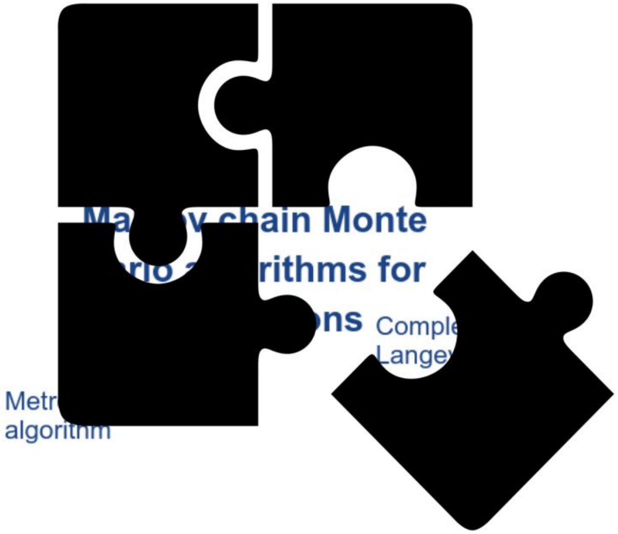
Proof of concept of the mathematical framework by the derivation of

- ➢ complex Langevin-like algorithms (similar to CLD)
- ➢ another algorithm called substitution Hamiltonian Monte Carlo algorithm (only for real actions)



➢ Why is it interesting to take a closer look at a Markov chain Monte Carlo framework for complex action problems?

Conclusion and Outlook



Appeal of a Markov chain Monte Carlo algorithm for complex action problems:

- ➢ Explicit access to the underlying sampling process
- ➢ Finite step sizes in configuration space
- ➢ Potential solution to the problem of wrong convergence

Possible future developments:

- ➢ Derivation of novel sampling algorithms for complex action problems
- ➢ Potential improvement of the presented sampling framework by more theoretical insights

Thank you!