Kernels and integration cycles in complex Langevin simulations
(handout version)

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talk on Wednesday talk on Tuesday

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UNI GRAZ

Handout version*

- This handout is a slightly modified version of the talk given at Lattice 2024. Some additional comments have been added in order to give context to the slides shown.
- Slides marked by an asterisk (*) were not part of the original talk.

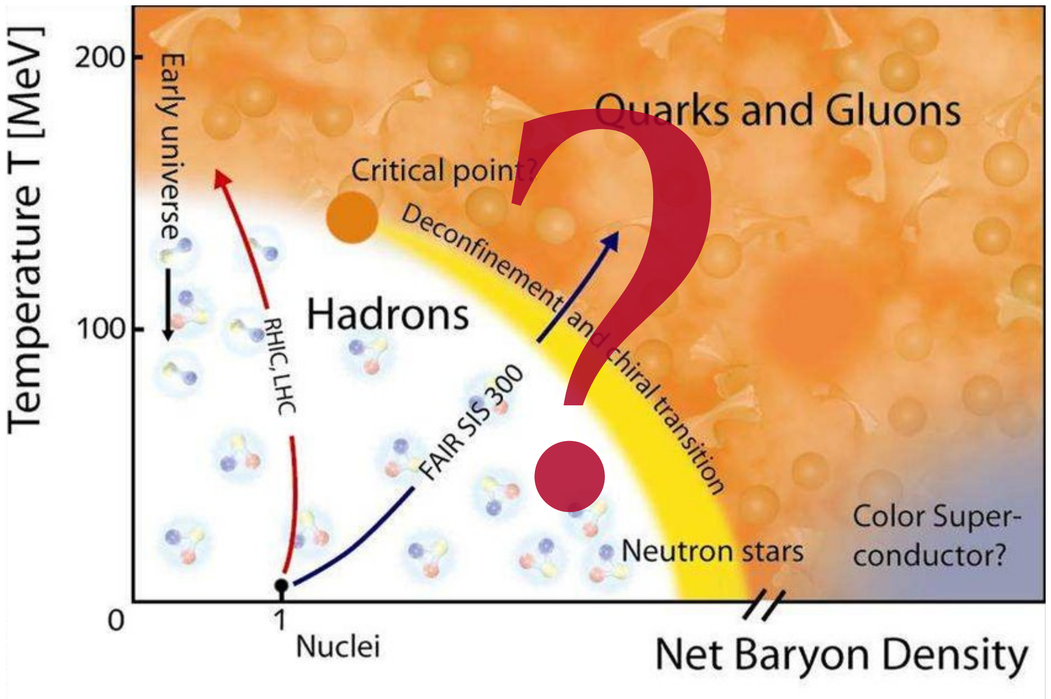
Motivation

- QCD at finite density poorly understood.
- Lattice methods based on importance sampling fail due to the sign problem:

$$\langle \mathcal{O} \rangle = \int dx \mathcal{O}(x) \rho(x)$$

$$\rho(x) \propto e^{-S(x)} \notin \mathbb{R}$$

$\Longrightarrow$ probabilistic interpretation lost.



Motivation

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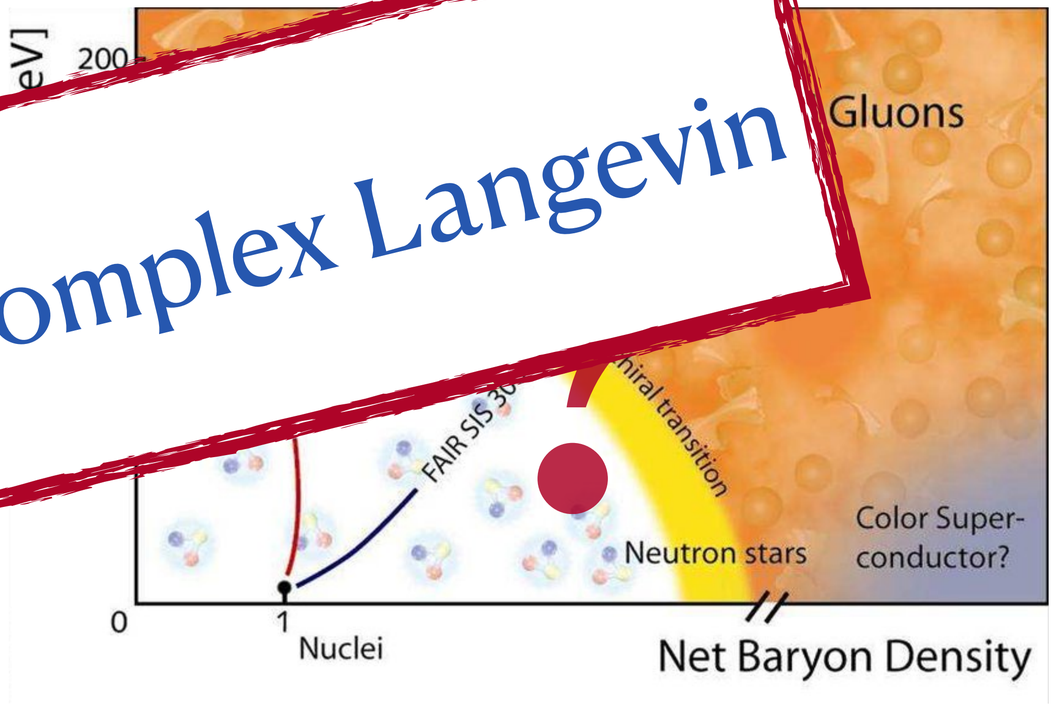
$\Longrightarrow$ probability interpretation lost.

Possible solution: Complex Langevin



Motivation*

- The main motivation for this work is to understand the phase diagram of QCD, one conjectured version of which is shown on the previous slide. The finite-temperature region close to the T-axis is under good theoretical control, mostly due to first principles lattice calculations.
- In the finite-densite region, however, lattice methods based on importance sampling cannot be applied in a straightforward way due to the infamous sign problem. There, the (Euclidean) action S of the theory becomes complex. The conventional lattice approach, which is based on drawing samples from a "probability distribution" e^{-S}, can thus no longer be applied.

The complex Langevin equation

Klauder '83; Parisi '83

- Complexify $x \to z = x + iy$, evolve statistical system in fictitious time direction τ.

Complex Langevin equation

$$\frac{dz}{d\tau} = -\frac{\partial S(z)}{\partial z} + \eta(\tau)$$

drift term

Gaussian noise:

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

- Obtain target theory $e^{-S(z)}$ in equilibrium limit $\tau \to \infty$.

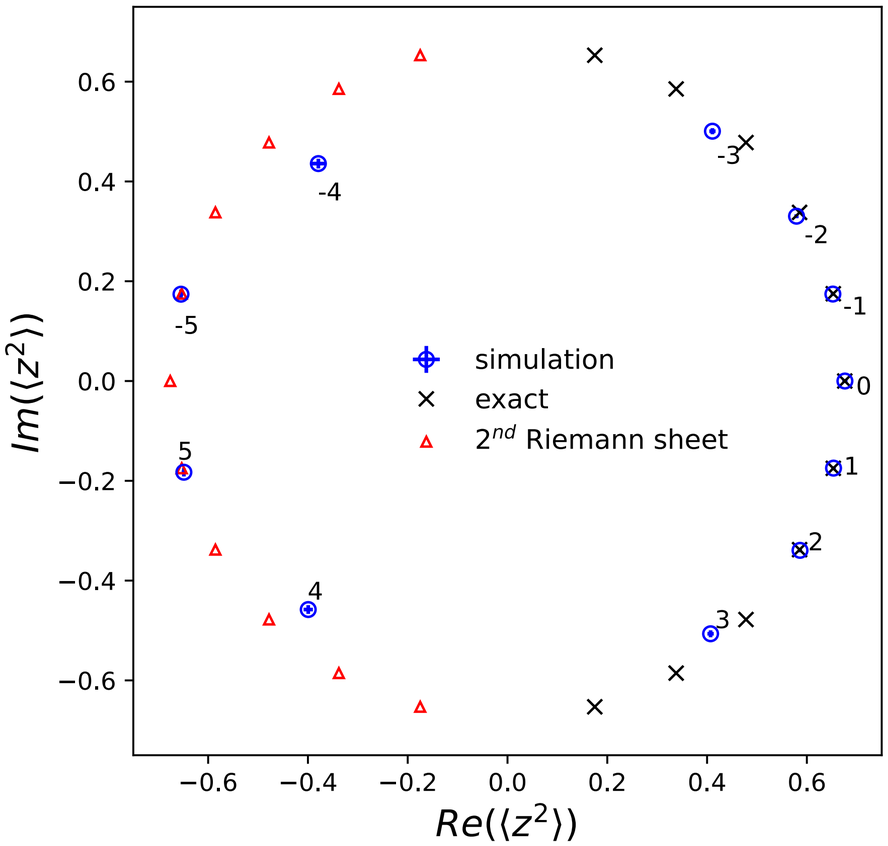
The complex Langevin equation*

- The complex Langevin approach — like a few other attempts of solving the sign problem — is based upon the complexification of the underlying field manifold.
- Moreover, one introduces an artificial time dimension (the "Langevin time") τ and interprets the system of interest as a statistical one coupled to a heat reservoir at fixed temperature and reaching equilibrium as $\tau \to \infty$. The evolution in τ is controlled by the Langevin (stochastic differential) equation. Since the Langevin equation is a stochastic one, there is a corresponding probability density for z, whose τ -evolution is governed by a so-called Fokker-Planck equation.
- For real S, this probability density can — under mild assumptions — be shown to converge to the desired weight e^{-S}. For complex S, on the other hand, the τ-evolution produces a probability density $P(x, y)$ in the complex plane, which — ideally — would reproduce the desired expectation values via $\int dx \mathcal{O}(x) e^{-S(x)} = \int dx dy \mathcal{O}(x + iy) P(x, y)$. As is discussed next, however, this is not always true.

Drawbacks and pitfalls

Wrong convergence

- Complex Langevin simulations can give wrong results despite converging properly.
- Example: $S(z) = \frac{\lambda}{4} z^4, \lambda = e^{\frac{i\pi l}{6}}$.
- Correct convergence only for $|l| \leq 2$.
  Okamoto et al. '89
- In general, we do not know if results are correct.
- Want: Correctness criterion.



Drawbacks and pitfalls*

Wrong convergence

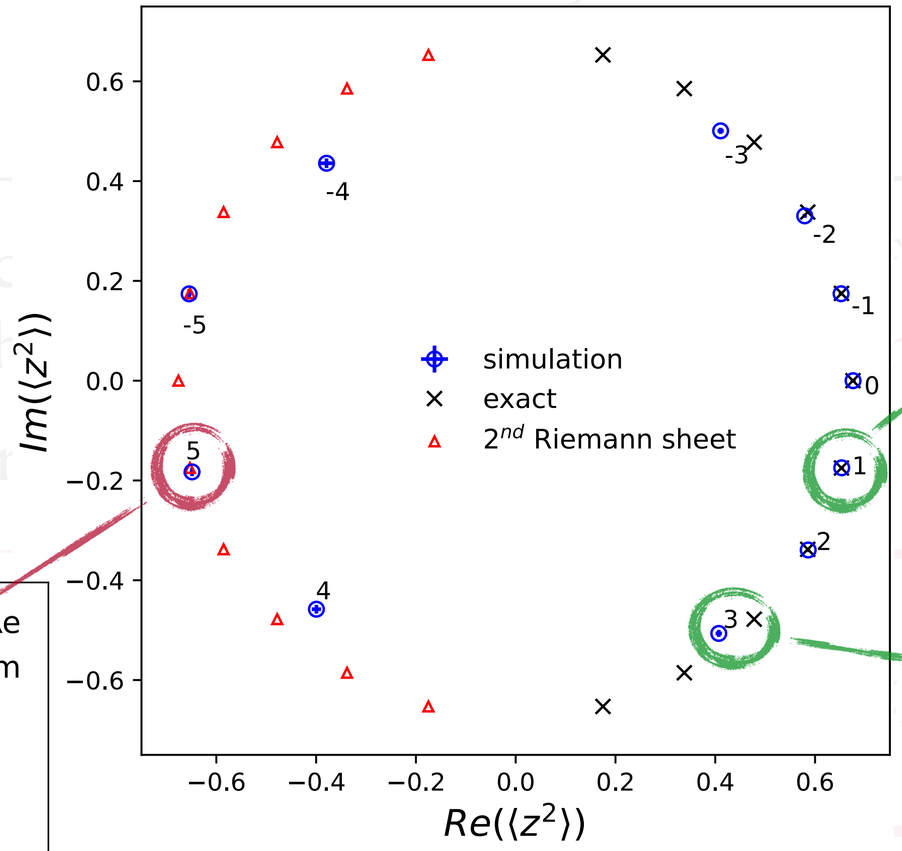
- As the simple example on the previous slide, where we discuss $\langle z^2 \rangle$, computed both analytically and in a complex Langevin simulation, shows, the complex Langevin equation can sometimes produce incorrect solutions despite converging to a proper equilibrium distribution.
- The main problem with this is that — in general — we cannot tell whether the results we obtain from a complex Langevin simulation are correct, since we cannot compare to exact results or to other methods. One thus would like to have some correctness criterion that can distinguish between correct and incorrect results.
- It is curious to note that if one continues λ in the analytical solution to the second Riemann sheet, one does find agreement with complex Langevin results for $l = 5$, where one otherwise would not. This will be discussed further later.

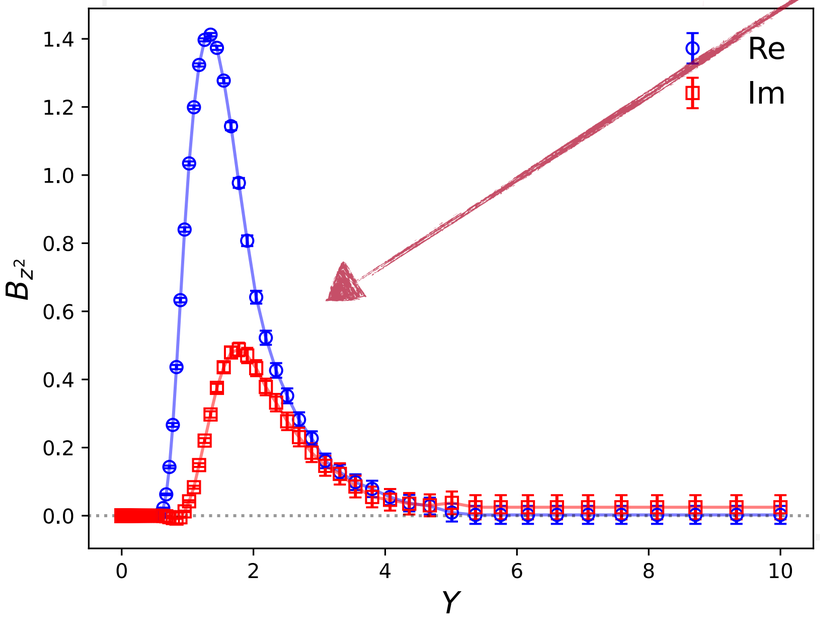
Boundary terms

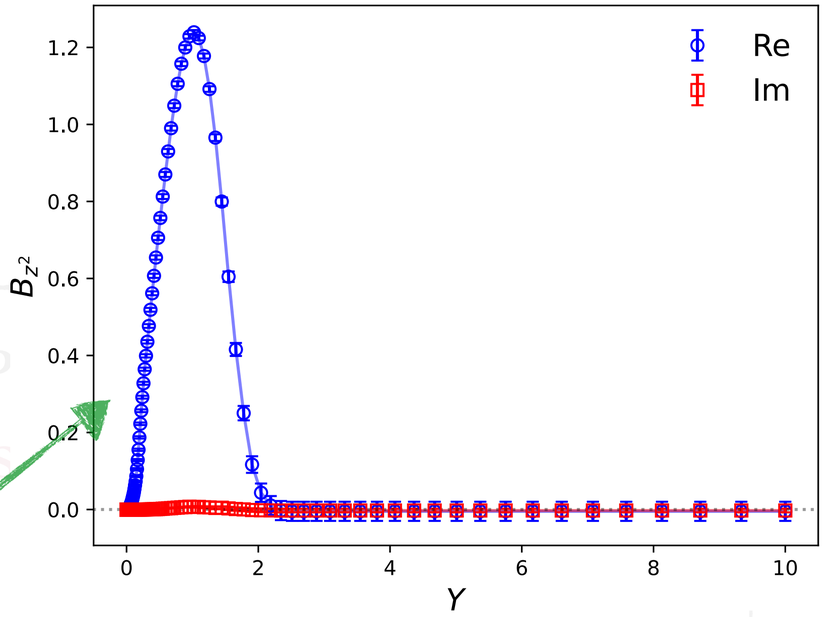
Aarts et al. ’11; Scherzer et al. ‘19

- Formal argument for correctness relies on fast decay of $P\mathcal{O}$, such that one can integrate by parts without appearance of boundary terms.
- Can measure boundary terms:

$$B_{\mathcal{O}(z)}(Y) = \left\langle \Theta\left(Y - |z|\right) L\mathcal{O}(z) \right\rangle$$


simulation
exact
2nd Riemann sheet
-5
-4
-3
-2
-1
0
1
2
3
4
5
$Im(\langle z^2 \rangle)$
$Re(\langle z^2 \rangle)$


Re
Im
B_{z^2}
Y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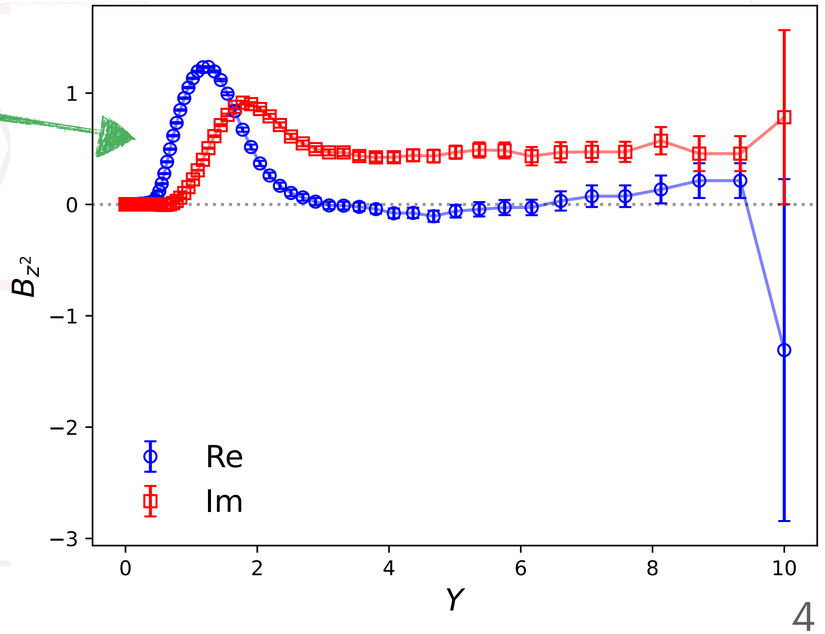
Re
Im
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Boundary terms

Aarts et al. ’11; Scherzer et al. ‘19

- Formal argument for correctness relies on fast decay of $P\mathcal{O}$, such that one can integrate by parts without appearance of boundary terms.
- Can measure boundary terms:

$$B_{\mathcal{O}(z)}(Y) = \left\langle \Theta\left(Y - |z|\right) L\mathcal{O}(z) \right\rangle$$

- Can infer incorrect solutions from non-vanishing boundary terms.
- Cannot infer correct solutions from vanishing boundary terms.

Boundary terms*

- On the previous slide, I introduced so-called boundary terms as possible correctness criteria. Namely, a formal proof of correctness of the complex Langevin approach relies on the absence of boundary terms such that one can integrate by parts in certain integrals. The presence of boundary terms spoils this requirement.
- Now, one can measure the (possibly) appearing boundary terms in a simulation and — ideally — use them to distinguish correct from incorrect results. For this, one typically introduces a cutoff Y in the complex plane and looks for a plateau of the boundary terms in Y, which one then extrapolates to $Y \to \infty$.
- Indeed, non-vanishing boundary terms (i.e., a plateau at non-vanishing values) imply incorrect solutions, a desirable property. Unfortunately, however, the absence of boundary terms does not imply that the obtained results are correct, as I show via a counter example.

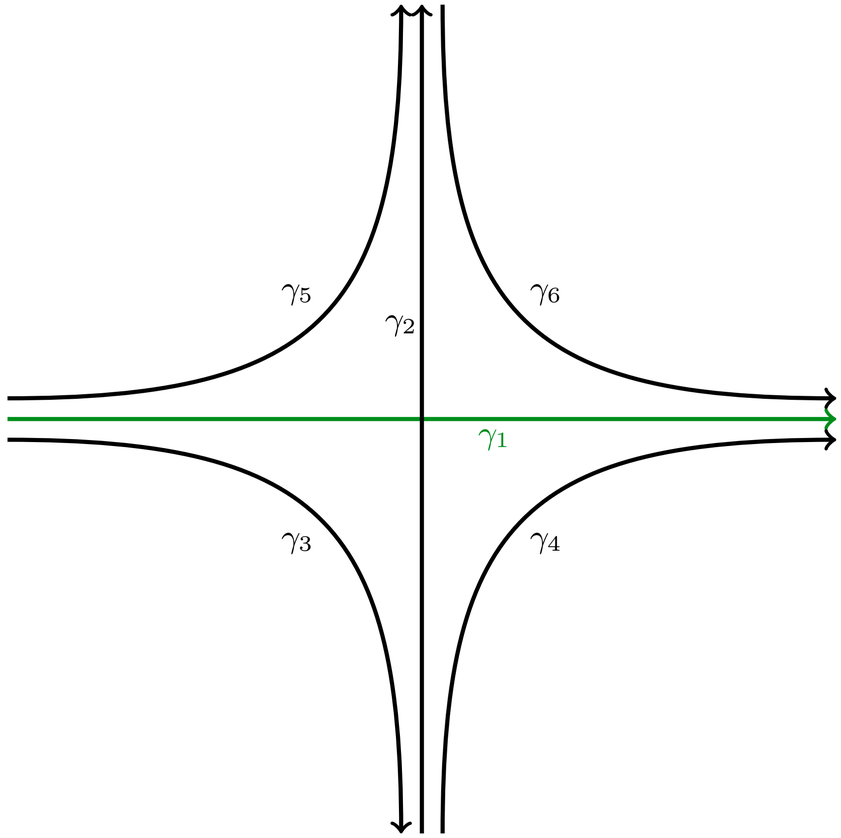
Integration cycles

see also Witten ‘11

- Integration paths connecting zeros of $\rho(z)$.
- Example: $\rho(z) = e^{-\frac{z^4}{4}}$.
- Three independent cycles, γ_1 is the relevant one.
- Vanishing boundary terms only imply that result is linear combination of integration cycles:

$$\langle \mathcal{O} \rangle_{\text{CL}} = \sum_{i=1}^{3} a_i \langle \mathcal{O} \rangle_{\gamma_i}$$

Salcedo, Seiler ’19



Integration cycles*

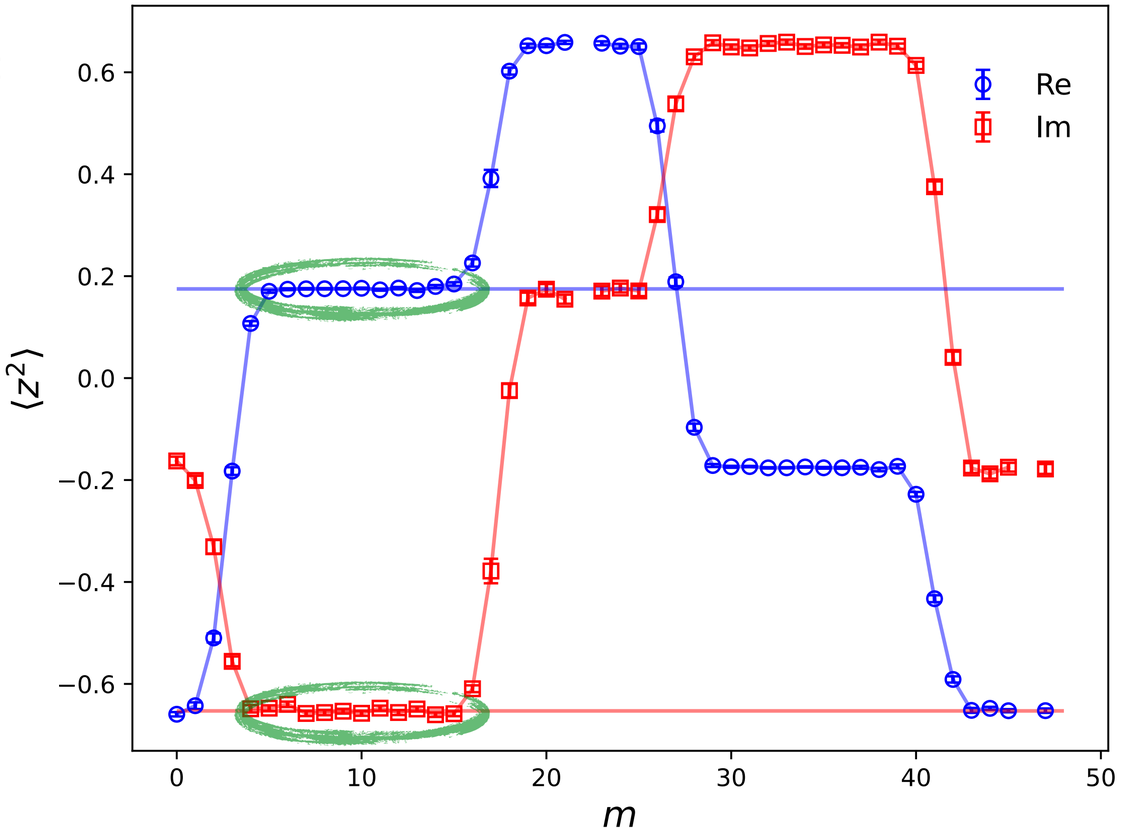
- In general, the absence of boundary terms does not indicate that the obtained results are correct, but only that they are a linear combination of observables computed along all (independent) integration cycles (defined on the previous slide) of the theory.
- In practical applications one neither knows what the observables computed along cycles are (if one did, one would have solved the theory because $\langle \mathcal{O} \rangle_{\gamma_1}$ is the result of interest), nor the values of the coefficients.
- In the example shown, there are six possible integration cycles. However, only three of them are independent, since, e.g., $\int_{\gamma_5} + \int_{\gamma_6} = \int_{\gamma_1}$.

Complex Langevin evolution with a kernel

- May introduce kernel into Langevin equation:
  Parisi, Wu ’81; Söderberg ‘88

$$\frac{\partial z}{\partial \tau} = -K\frac{\partial S(z)}{\partial z} + \sqrt{K}\,\eta(\tau)$$

- Example: $S = \frac{\lambda}{4}z^4$, $\lambda = e^{\frac{5i\pi}{6}}$, $K = e^{-\frac{i\pi m}{24}}$.
- Kernel can restore correct convergence.
  Okamoto et al. ’89

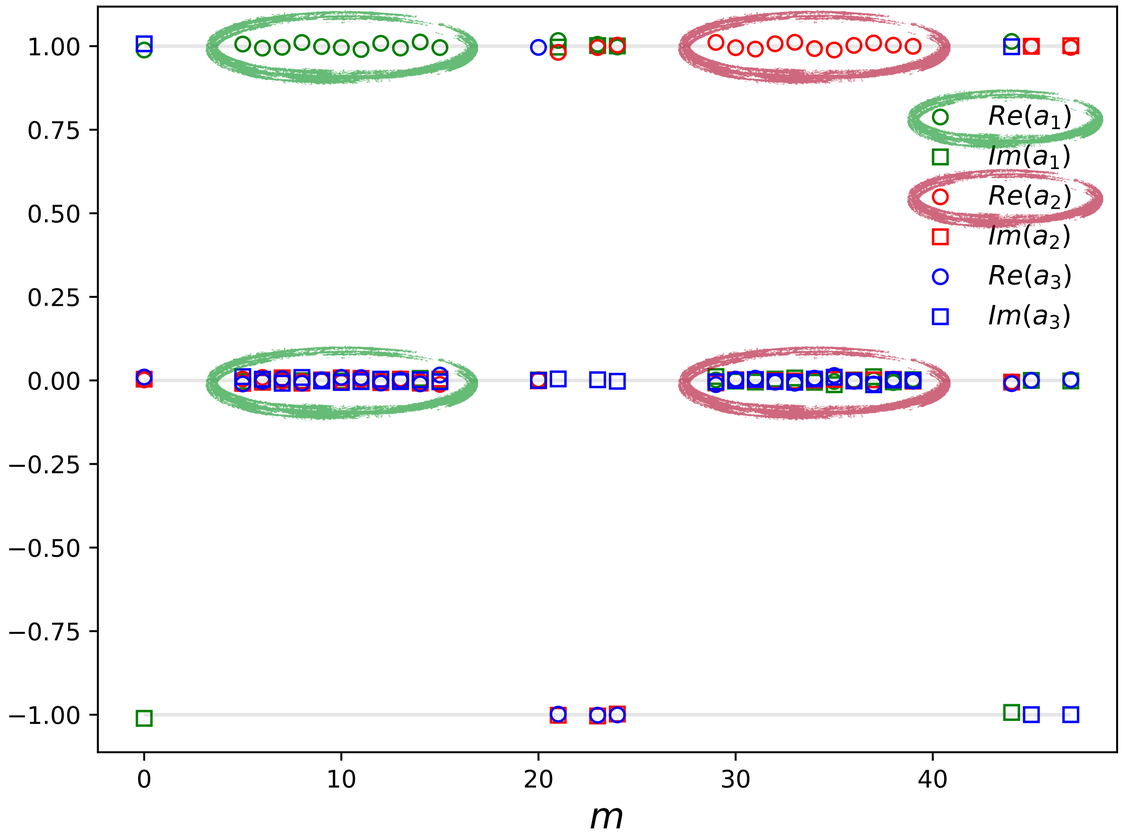


Complex Langevin evolution with a kernel*

- The introduction of kernels provides a generalization to the (real or complex) Langevin equation. For real S, one can show that its introduction leaves the stationary distribution e^{-S} unchanged, but convergence might be improved. For complex S, the situation is less clear since a kernel in general changes the equilibrium distribution in the complex plane, $P(x, y)$.
- Nonetheless, as shown on the previous slide, a correctly chosen kernel can indeed lead to correct convergence where the complex Langevin approach would otherwise fail.
- Note that we consider the simplest choice of kernel here. In general, it can depend on z, in which case there would be an additional term $\dfrac{\partial K}{\partial z}$ in the Langevin equation.

Kernels and integration cycles

- Recall: $$\langle \mathcal{O} \rangle_{\mathrm{CL}} = \sum_{i=1}^{3} a_i \langle \mathcal{O} \rangle_{\gamma_i}$$
- γ_1 is the real integration cycle.
- Kernel can favor certain cycles.
  see also Salcedo '93
- Only proven for a single degree of freedom.



Kernels and integration cycles*

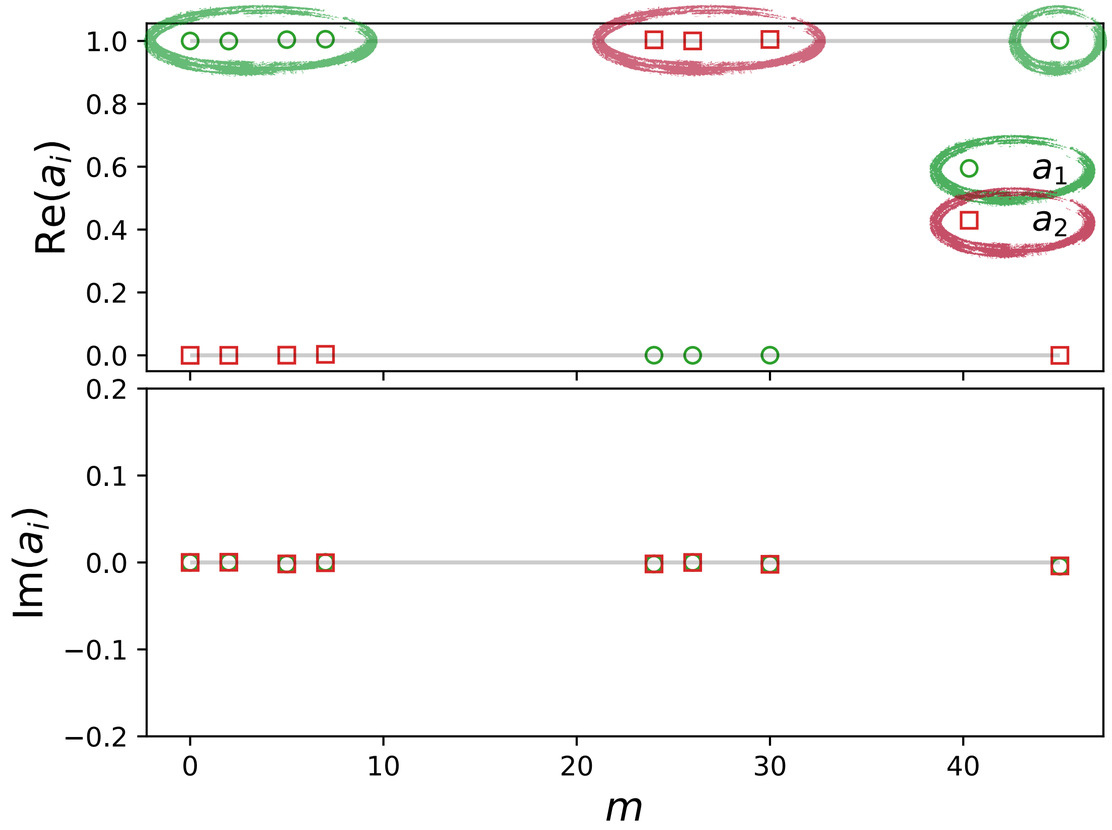
- Here we explore the relation between kernels, which can restore correct convergence, and integration cycles. Recall that incorrect convergence (in the absence of boundary terms, which we shall always assume from now on) can be traced back to contributions from integration cycles other than the real one.
- Indeed, we find that the kernel can be chosen in such a way that only the real cycle contributes, thus guaranteeing correct results. On the other hand, a bad choice of kernel can lead to other cycles becoming dominant, thus giving incorrect results, but nonetheless vanishing boundary terms. In the example shown, γ_2 corresponds to an integration over the imaginary axis.
- The fact that the complex Langevin simulation for $K = 0$ and $\lambda = e^{\pm 5i\pi/6}$ on slide 3 reproduces the "2nd Riemann sheet" result can be traced back to non-vanishing contributions from cycles other than the real one.

Integration cycles in higher dimensions

- Consider $S(z_1, z_2) = \frac{\lambda}{4}(z_1^2 + z_2^2)^2$.
- $e^{-S(z_1,z_2)}$ has 16 zeros but there are only 2 independent integration cycles.
- $$\langle \mathcal{O} \rangle_{\mathrm{CL}} \stackrel{?}{=} \sum_{i=1}^{2} a_i \langle \mathcal{O} \rangle_{\gamma_i}$$

$$\lambda = e^{\frac{i\pi}{6}}$$

$$K = e^{-\frac{i\pi m}{24}}$$



Integration cycles in higher dimensions*

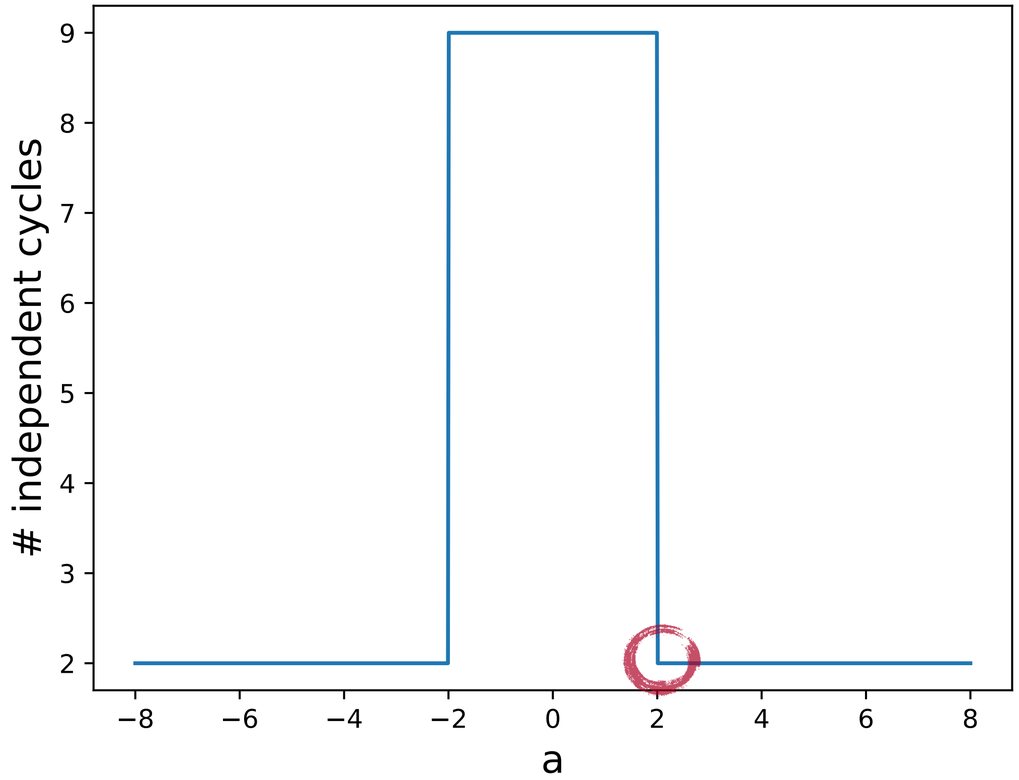
- Since the theorem relating the absence of boundary terms to a linear combination of integration cycles was only proven for a single degree of freedom, we tried to verify its validity in higher dimensions. Here we consider two degrees of freedom and a straightforward extension of the model studied previously.
- Curiously, for the O(2)-symmetric model discussed on the previous slide there are only two independent integration cycles despite e^{-S} having 16 zeros in the complex plane.
- We aimed at verifying the aforementioned theorem and indeed succeeded in doing so. We find that for our choice of kernel (which is the most simple one, being independent of z_i and acting the same on z_1 and z_2), either γ_1 or γ_2 contribute in an exclusive way, but there is no mixing. We emphasize, however, that this does not need to be the case in general and we have found counter-examples in different two-variable theories.
- We also mention that there are large regions (in the parameter m characterizing the kernel) in which we find boundary terms, i.e., expect the theorem to not be applicable, and thus refrain from showing results.

Number of independent cycles

- Consider the more general model

$$S(z_1, z_2) = \frac{\lambda}{4}(z_1^4 + z_2^4 + a z_1^2 z_2^2).$$

- Number of independent cycles depends on a.
- The O(2)-symmetric point $a = 2$ is "critical".



Number of independent cycles*

- We find that the number of independent integration cycles can depend on the "coupling" of a theory. The model on the previous slide, which reduces to the one discussed before for $a = 2$, either has 9 independent cycles (for small $|a|$) or 2 (for larger $|a|$). The "transition" happens precisely at the symmetric point $a = 2$, where the number of independent cycles happens to be 2.
- It would be interesting to study to which extent — if at all — non-real integration cycles play a role in more realistic theories, i.e., lattice models or even QCD. If they turn out to be relevant generically, one has to be careful in designing appropriate kernels since boundary terms are then not a reliable correctness criterion.

Summary & Outlook

- CL promising approach for systems with a complex-action problem.
- Major drawbacks: Runaways (adaptive step size) and wrong convergence.
- Wrong convergence can in principle be fixed by kernels.
  - How to construct them?
  - How to verify convergence?
- Outlook:
  - Understand relevance of integration cycles in realistic theories.
  - (Heavy-dense) QCD with kernels.

Contact*

- For any questions/discussion, please do not hesitate to contact the author via michael.mandl@uni-graz.at .