Kernels and Integration Cycles in Complex Langevin Simulations

(handout version)

Michael Mandl

with Michael Hansen, Dénes Sexty and Erhard Seiler

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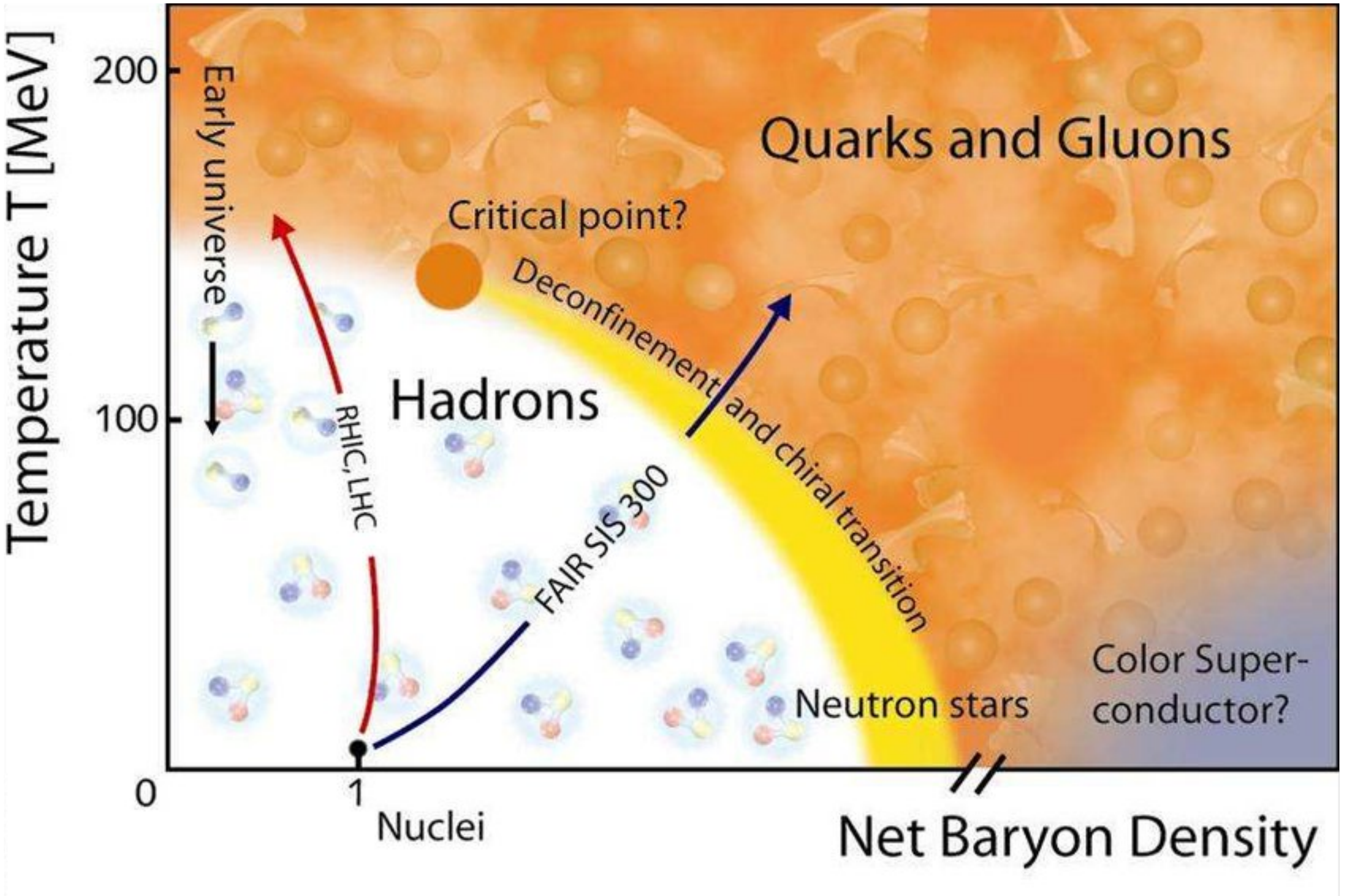
Handout version*

- This handout is a slightly modified version of the talk given at ACHT 25: some additional comments have been added to give context to the slides.
- Slides with a title marked with an asterisk (*) were not part of the original talk.

Motivation

- QCD at finite density:
  - Heavy-ion collisions
  - Neutron stars
- Real-time evolution of QFTs:
  - Transport coefficients
  - Non-equilibrium properties



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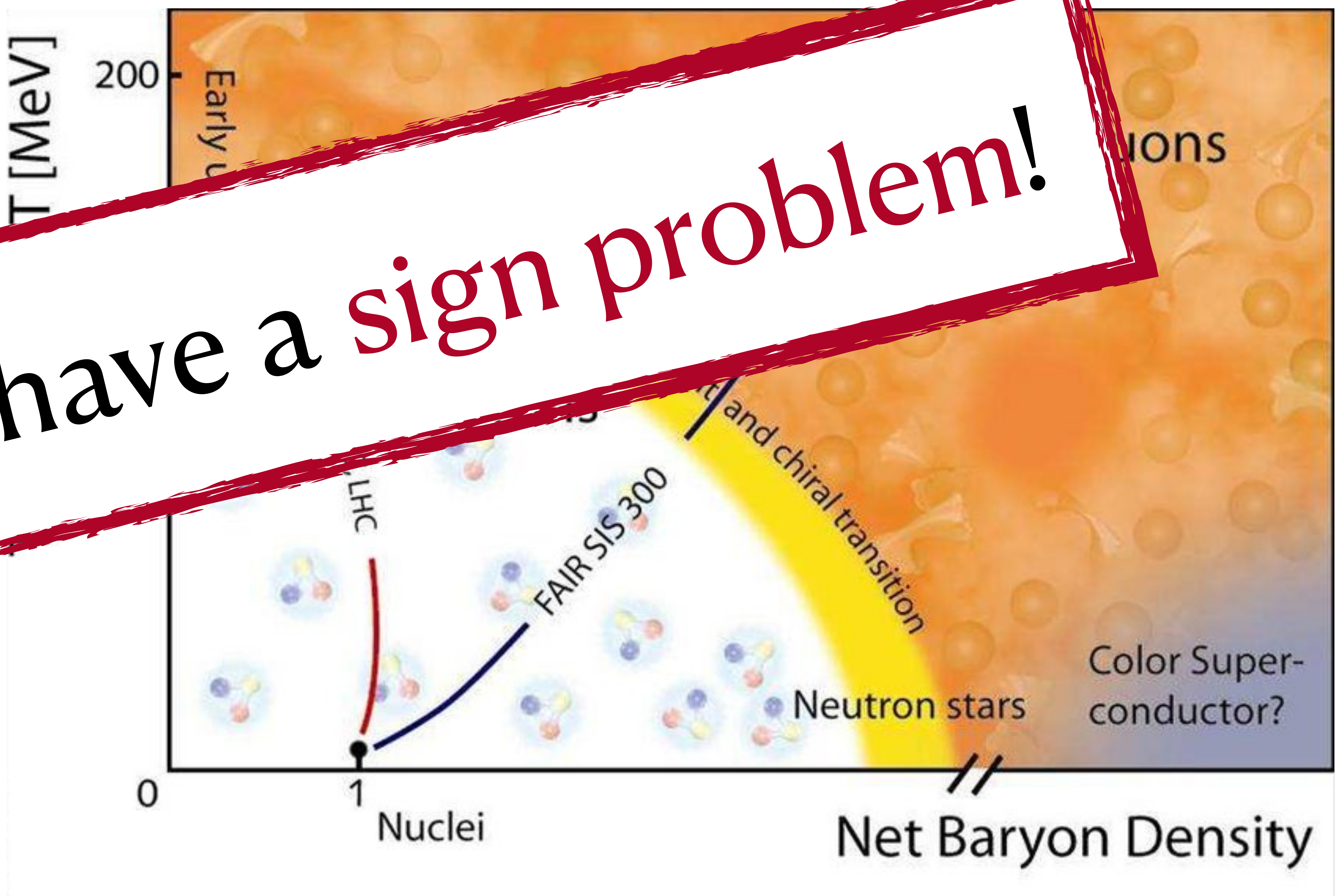


These systems have a sign problem!

Motivation*

- Lattice studies of (e.g.) quantum chromodynamics (QCD) at finite chemical potential or quantum field theories in real time are examples of theories that suffer from a sign (or complex-action) problem: the path integral measure is not real and positive definite, which prevents the straightforward application of conventional lattice methods based on importance sampling.

- Our method of choice to tackle the sign problem is the complex Langevin approach.

The complex Langevin equation

Klauder '83; Parisi '83

$z = x + iy$

Complex Langevin equation

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

Gaussian noise:

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

drift term

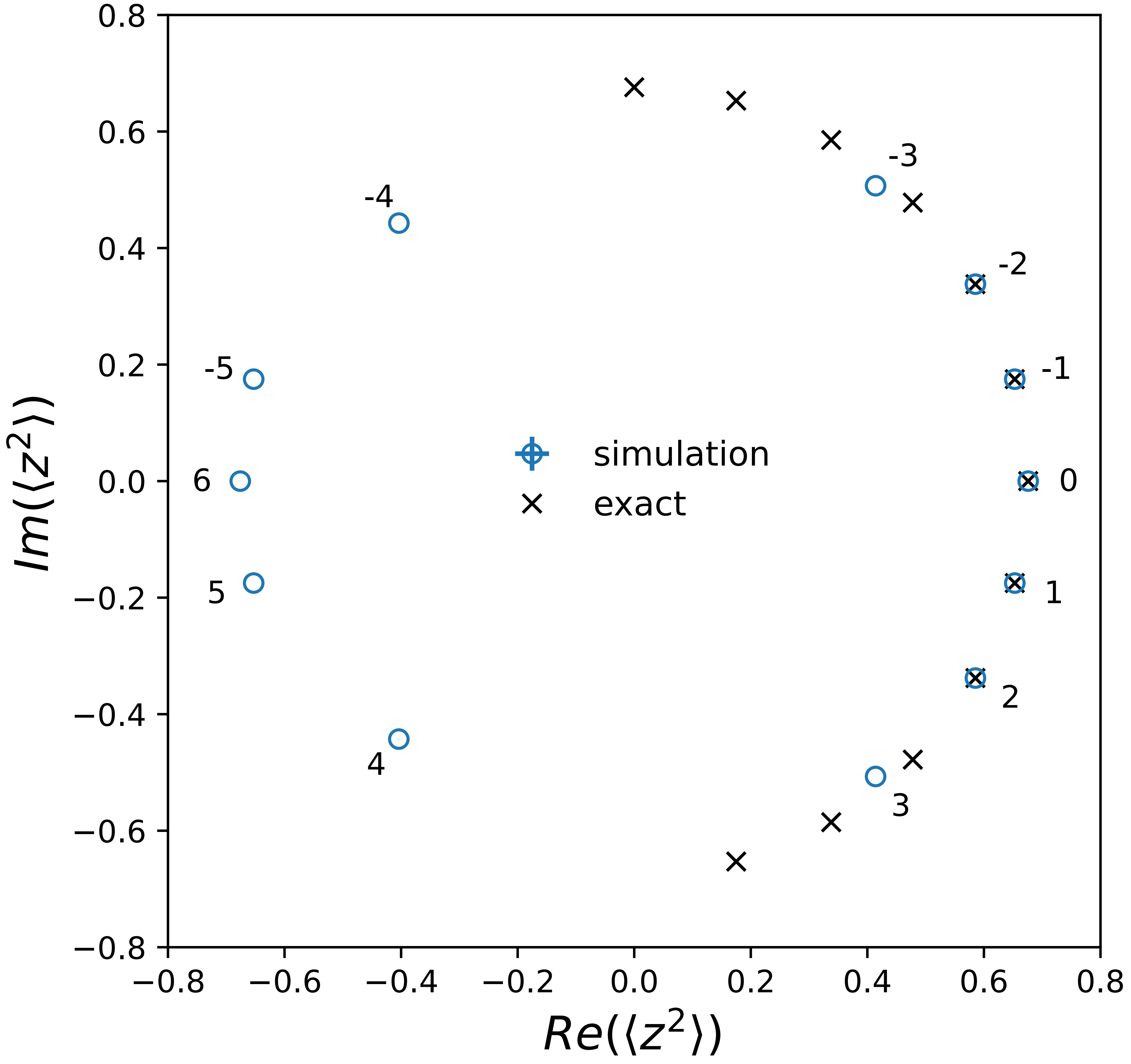
- $\Longrightarrow^*$ probability density $P(x, y, \tau)$.
- Does it obey $$\lim_{\tau\to\infty} \int dxdy\, \mathcal{O}(x + \mathrm{i}y) P(x, y, \tau) = \int dx \mathcal{O}(x) e^{-S(x)}$$?

The complex Langevin equation*

- The complex Langevin equation is a stochastic differential equation describing the evolution of complexified degrees of freedom in an auxiliary time dimension.
- For a theory with a single real degree of freedom x, the complex Langevin approach introduces the complexified variable $z = x + iy$ and studies its evolution in the Langevin time τ. This evolution gives rise to a probability density P in the complex plane.
- The question that is posed in the last bullet point of the previous slide is whether the observables that the complex Langevin approach provides (l.h.s.) can reproduce the desired results (r.h.s.).

The wrong convergence problem

- 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.



The wrong convergence problem*

- Complex Langevin simulations can give wrong results despite apparently converging to a reasonable equilibrium distribution. In the simple model considered here, one can compare with exact results to assess the convergence properties. In general, however, there is no simple *a-priori* way to tell whether results are correct or not.

- On the previous slide, the numbers in the plot represent different values of the integer l.

How to restore correct convergence?

Parisi, Wu '81; Söderberg '88

- May introduce kernel into Langevin equation:

Kernelled complex Langevin equation

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

- For real dynamics: leaves equilibrium distribution unchanged.
- Alters the probability distribution $P(x, y, \tau)$.

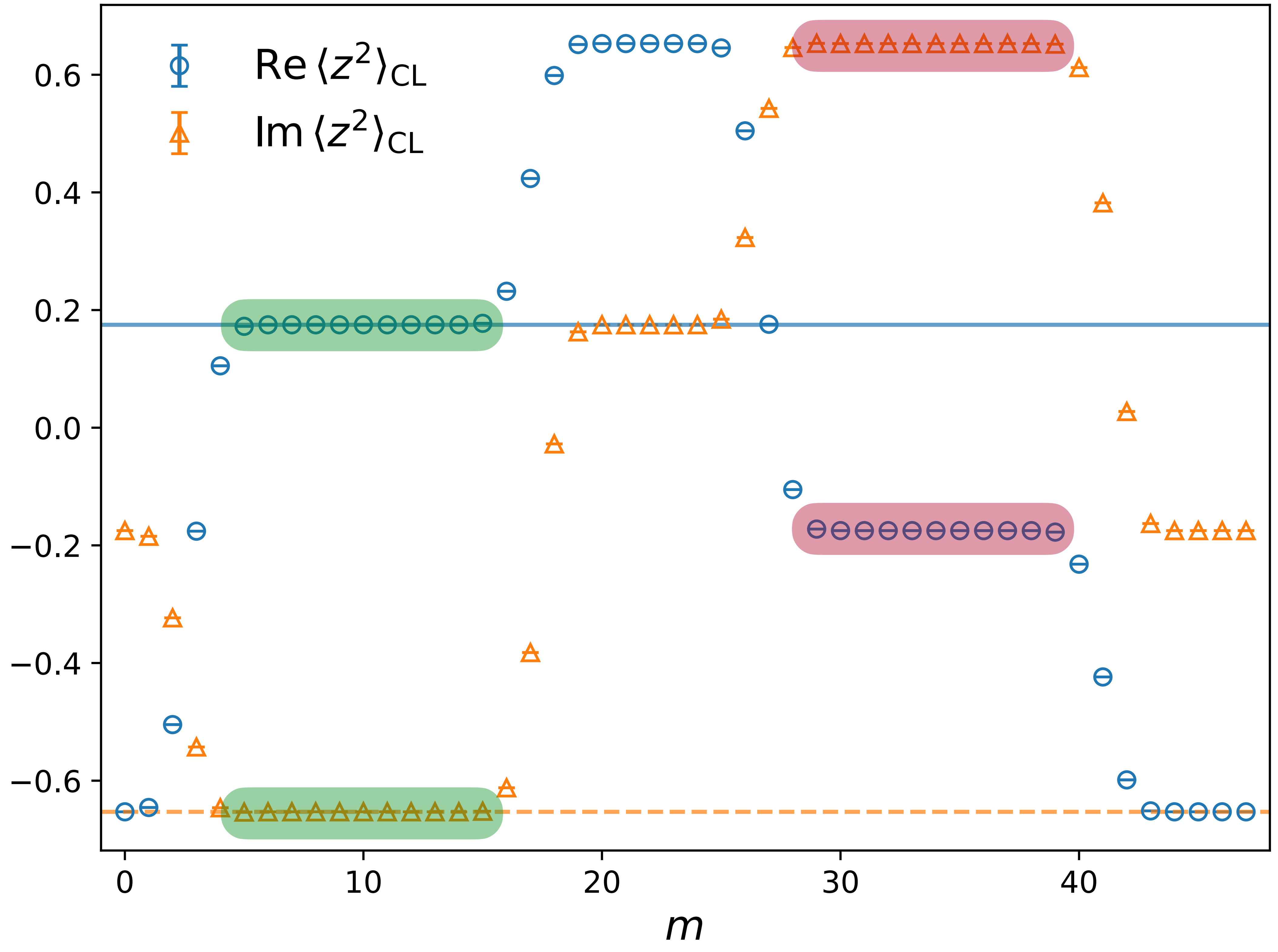
How to restore correct convergence?*

- In order to restore correct convergence, one may introduce a so-called kernel into the complex Langevin equation. It essentially represents a non-trivial diffusion term. Apart from having to be holomorphic, its form is in principle arbitrary.
- While for real actions the introduction of a kernel leaves the stationary (equilibrium) distribution invariant and, thus, the physics unchanged, for complex actions the distribution will — in general — change. In the case of wrong convergence, this is, of course, desirable.
- For this talk, we assume the kernel to not depend on z.

Complex Langevin evolution with a kernel

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

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

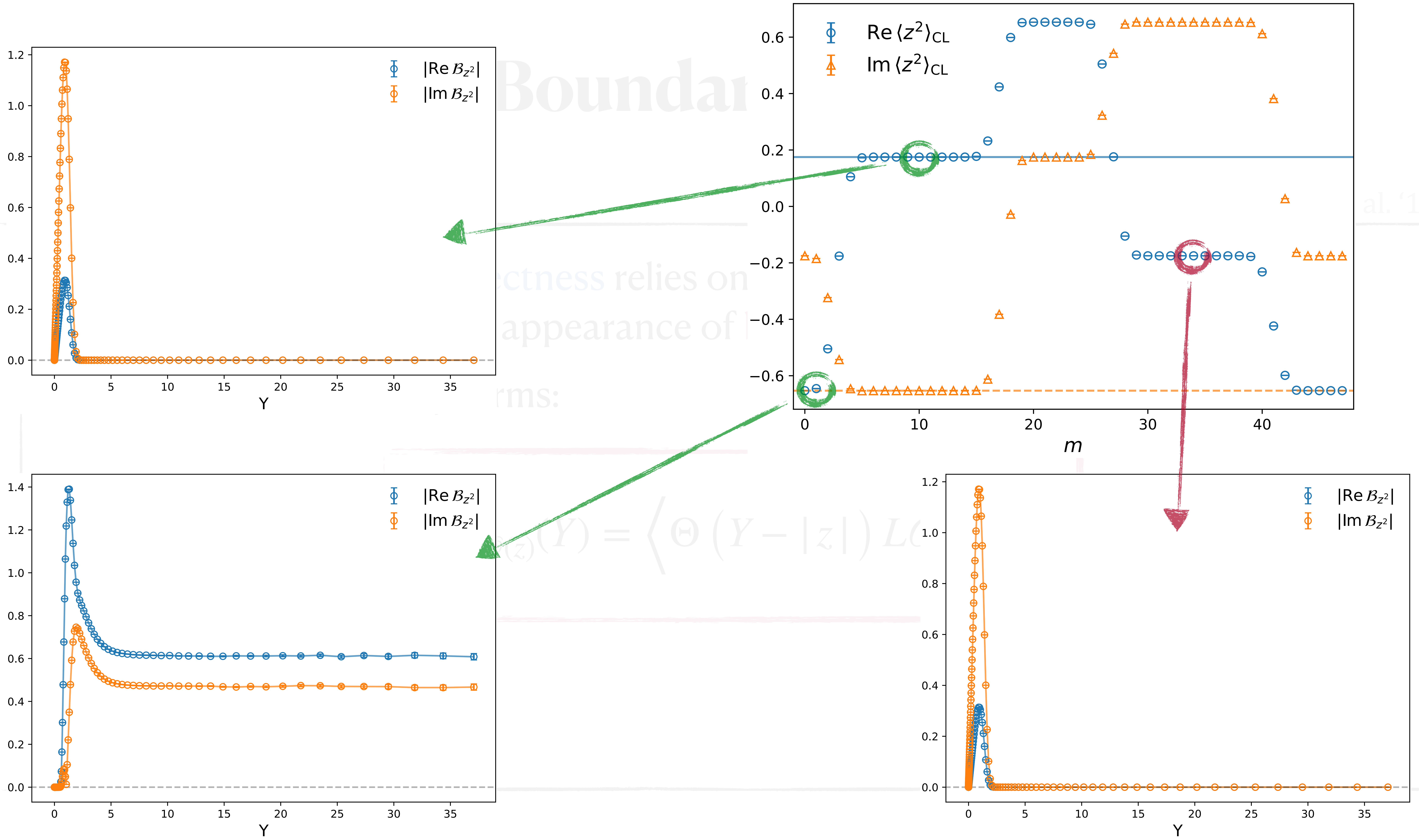


Boundary terms

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:

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



$|\mathrm{Re}\,\mathcal{B}_{z^2}|$
$|\mathrm{Im}\,\mathcal{B}_{z^2}|$
Y
$\mathrm{Re}\,\langle z^2\rangle_{\mathrm{CL}}$
$\mathrm{Im}\,\langle z^2\rangle_{\mathrm{CL}}$
m

Boundary terms

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

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

Boundary terms*

- Measuring boundary terms (as a function of the cutoff Y on the magnitude of z) is a common way to investigate the convergence properties of a complex Langevin simulation.

- In practice, one studies the Y-dependence of $\mathscr{B}_{\mathcal{O}(z)}$ and extrapolates to $Y \to \infty$. If there is a plateau at a non-zero value (or no plateau at all), one concludes that boundary terms are non-zero and the obtained complex Langevin results are incorrect. The converse, unfortunately, is not true, however. An example of this is seen on the previous two slides, where for certain values of the kernel boundary terms vanish but the results are still incorrect.

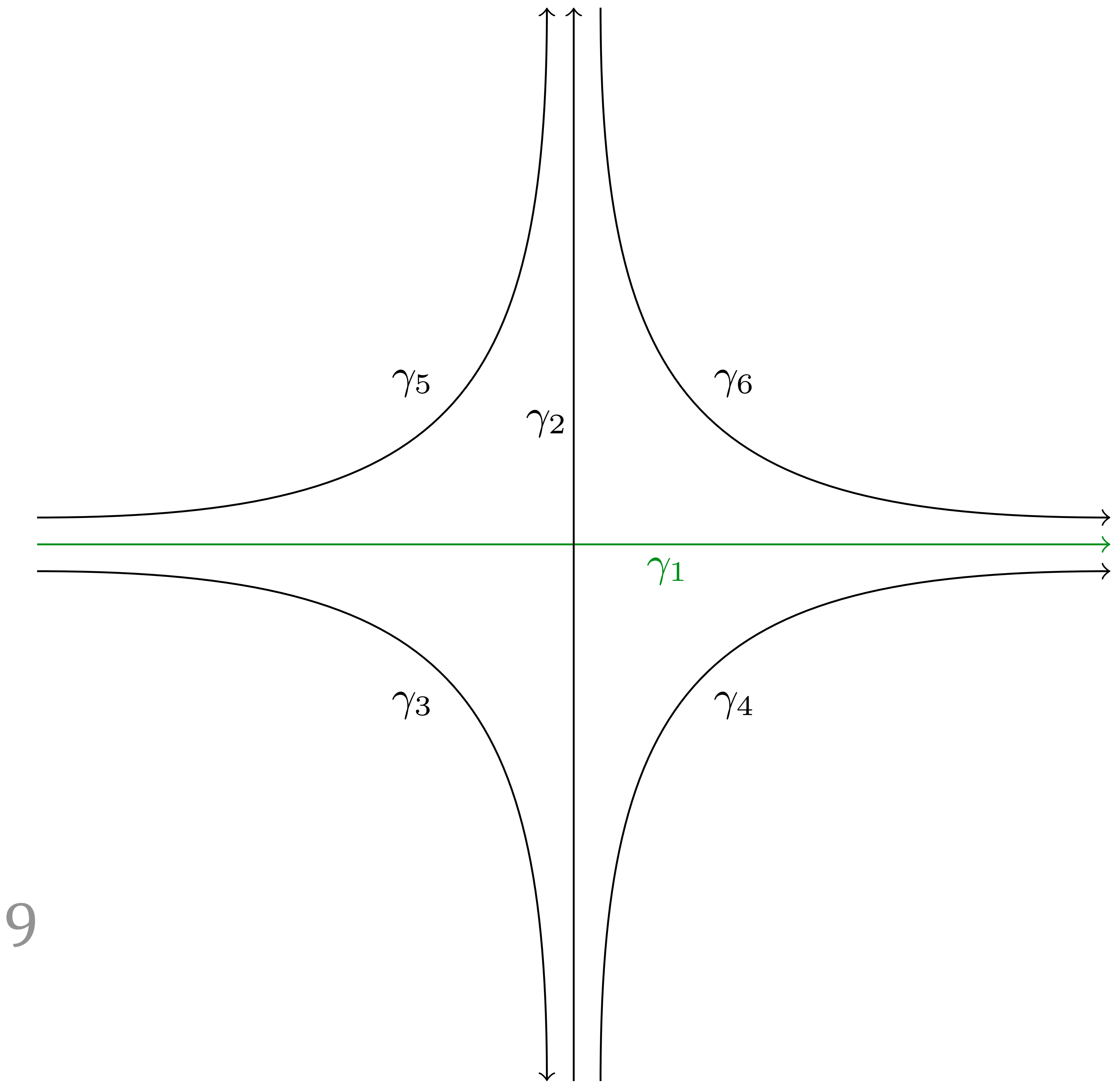
Integration cycles

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:

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

Salcedo, Seiler '19



Integration cycles*

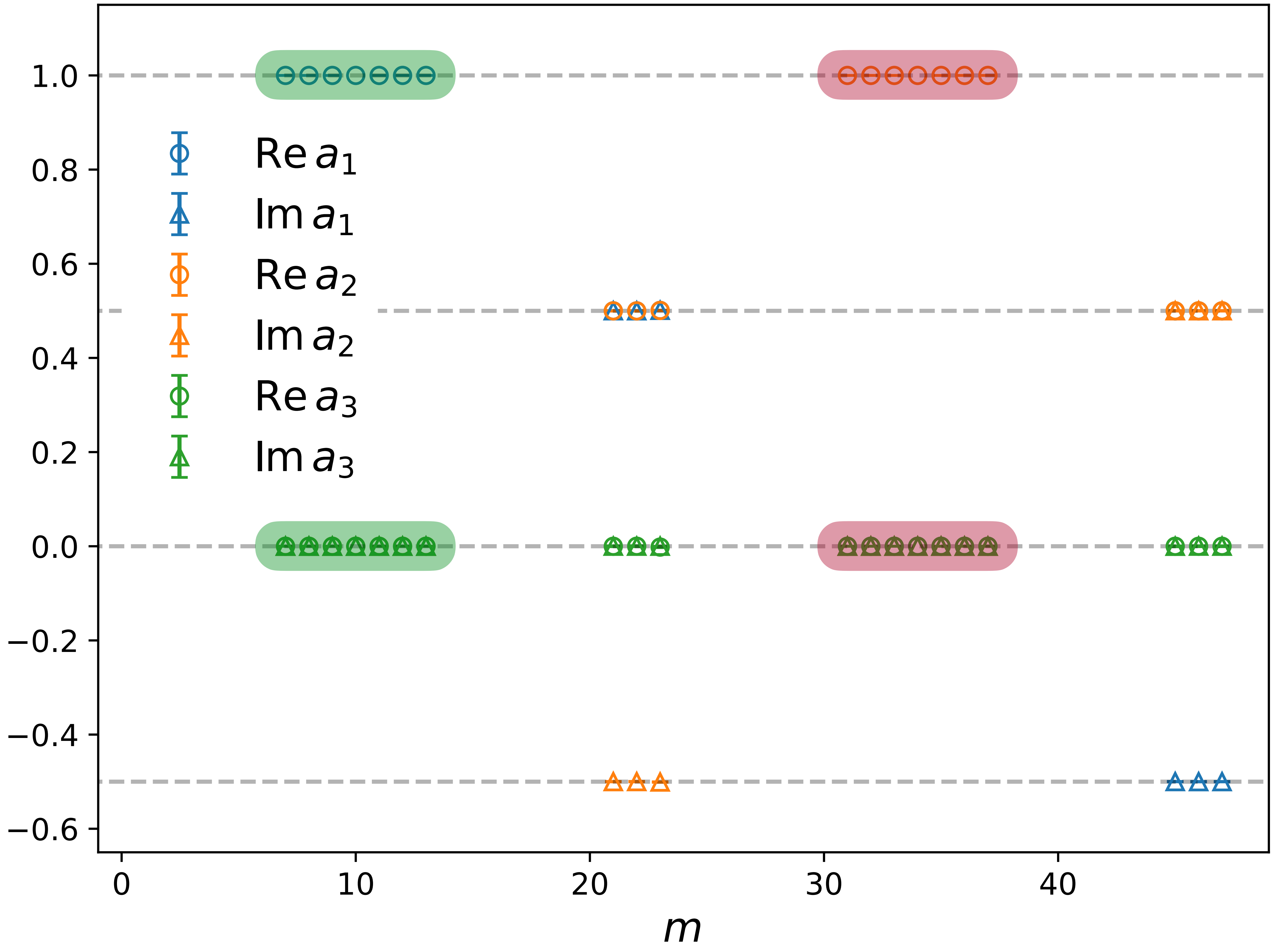
- The fact that the complex Langevin evolution can produce incorrect results despite vanishing boundary terms can be explained by a theorem by L. Salcedo and E. Seiler:
- Vanishing boundary terms only guarantee that the complex Langevin results are a (complex) linear combination of observables computed along the independent integration cycles of the theory.
- In general, of course, neither the integration cycles nor the observables are known. For our simple model, however, we can compute the coefficients via a least-squares fit and study their dependence on the kernel (see next slide).

Kernels and integration cycles

Hansen, M.M., Seiler, Sexty '25

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

- Kernel can favor certain cycles.
  Salcedo '93
- Fits are unreliable in the presence of boundary terms.
- Proven only for a single degree of freedom.



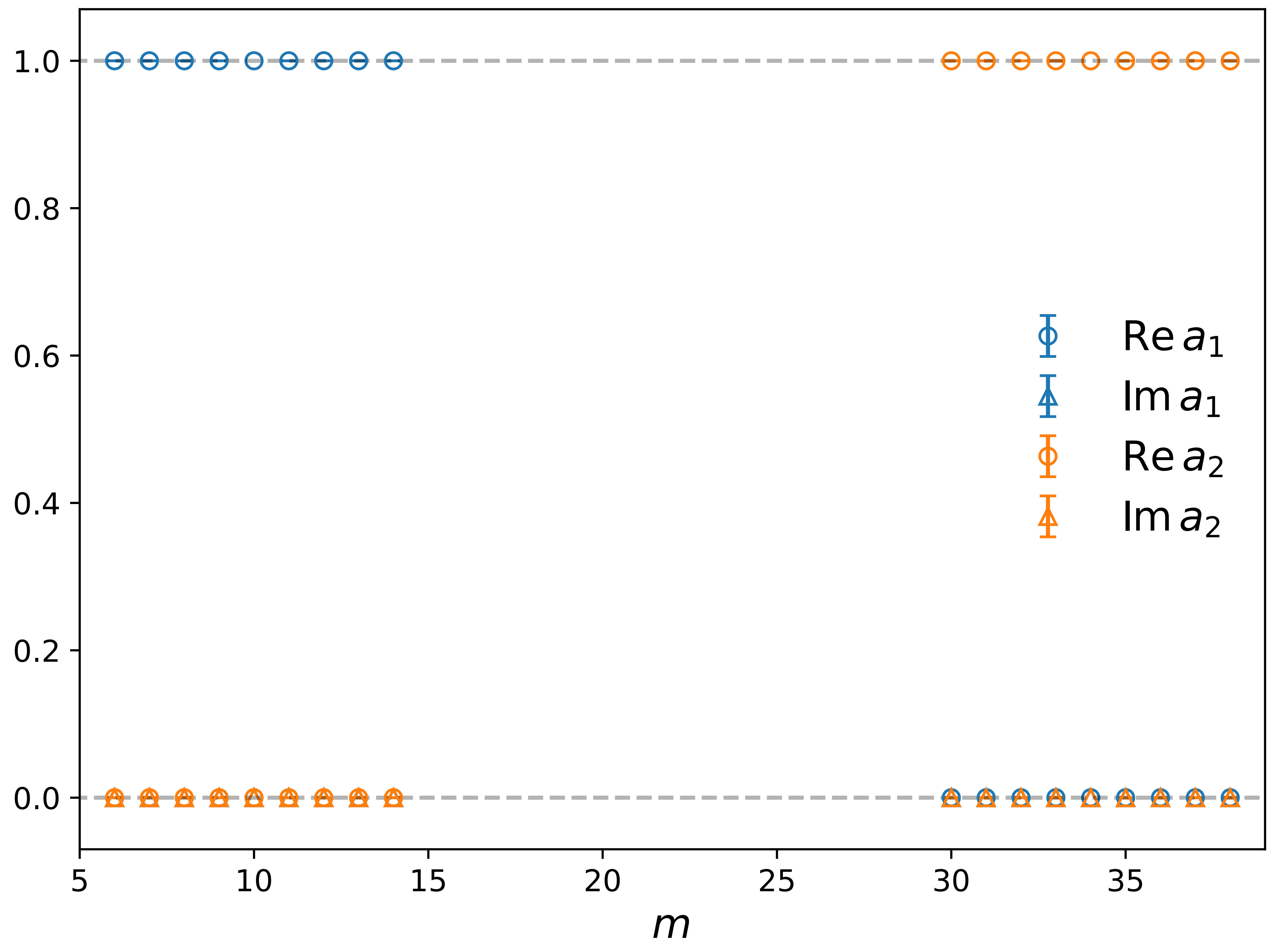
Kernels and integration cycles*

- A kernel — in some sense — gives rise to rotations in the space of integration cycles: for a proper choice of kernel we can project out the contributions from the (desired) real integration cycle γ_1. Other choices of kernel result in different linear combinations of cycles.
- We obtain reasonable fit results only for those kernels for which there are no boundary terms. This is in perfect agreement with the Salcedo—Seiler theorem.
- Since the theorem was proven only for a single degree of freedom, we have performed a numerical study of its validity in two dimensions (see the next slide).

Integration cycles in higher dimensions

Hansen, M.M., Seiler, Sexty '25

- $S(z_1, z_2) = \frac{\lambda}{4}(z_1^2 + z_2^2)^2.$
- $e^{-S(z_1,z_2)}$ has 8 zeros but there are only 2 independent integration cycles.
- Example: $\lambda = e^{\frac{5i\pi}{6}}, K = e^{-\frac{i\pi m}{24}}.$
- $\boxed{\langle \mathcal{O} \rangle_{\mathrm{CL}} = a_1 \langle \mathcal{O} \rangle_{\gamma_1} + a_2 \langle \mathcal{O} \rangle_{\gamma_2}}$



Integration cycles in higher dimensions*

- Our results provide striking evidence for the validity of the Salcedo—Seiler theorem beyond one dimension as all our two-dimensional results are in perfect agreement with its predictions.
- Note that the situation on the previous slide even appears to be somewhat simpler than in one dimension as there are only two independent integration cycles now. The number of cycles, however, depends on the coupling between the degrees of freedom in a non-trivial way (see next slide).

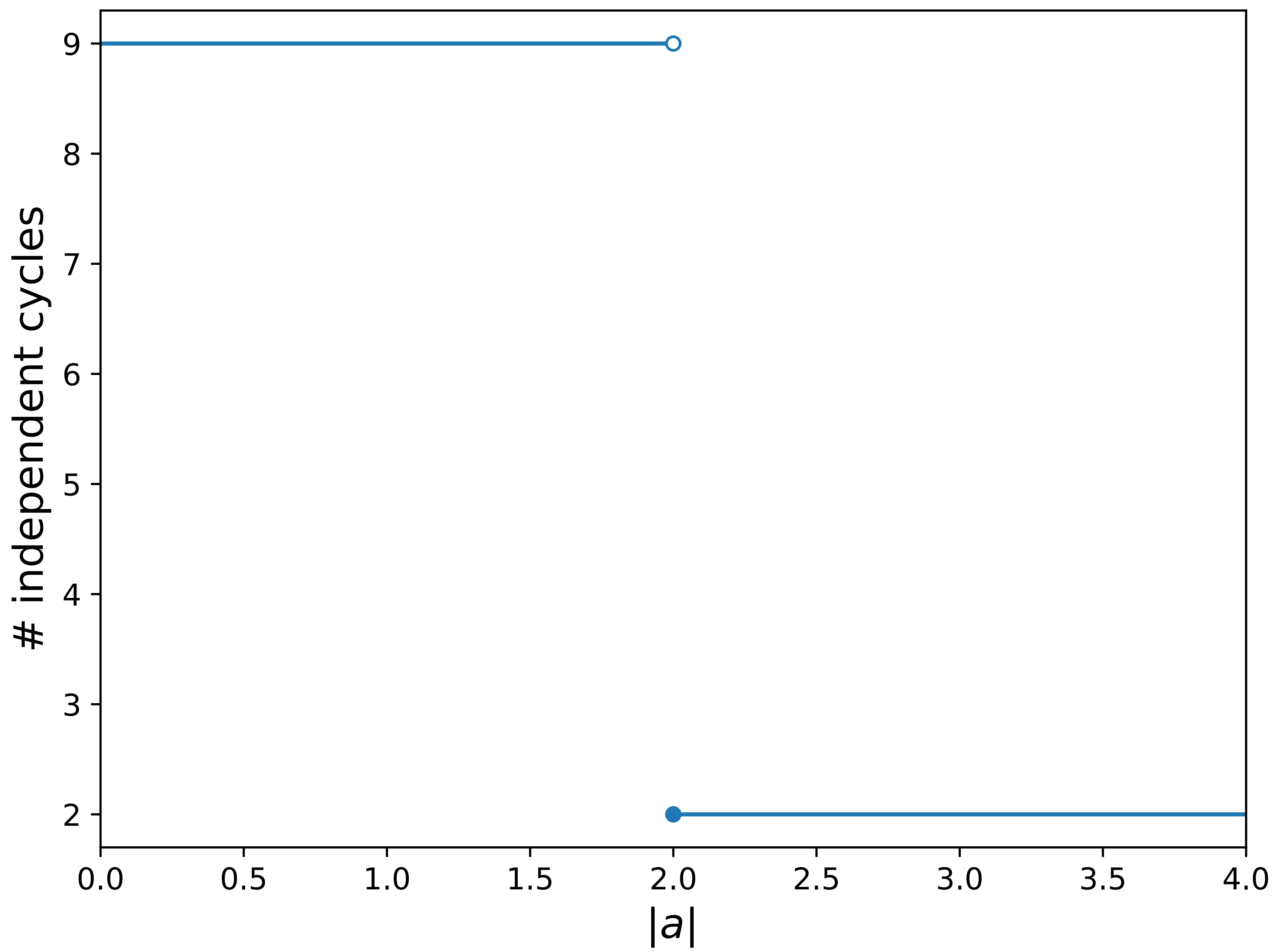
Breaking O(2) symmetry

Hansen, M.M., Seiler, Sexty '25

- Consider more general interactions:

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

- Number of independent integration cycles depends on a.



A new correctness criterion

- In addition to vanishing boundary terms, one should also require

$$\boxed{\left|\langle p(z)\rangle_{\mathrm{CL}}\right| \leq \mathscr{B}(p)}$$

- for all polynomials $p(z)$.
- This ensures correct convergence.

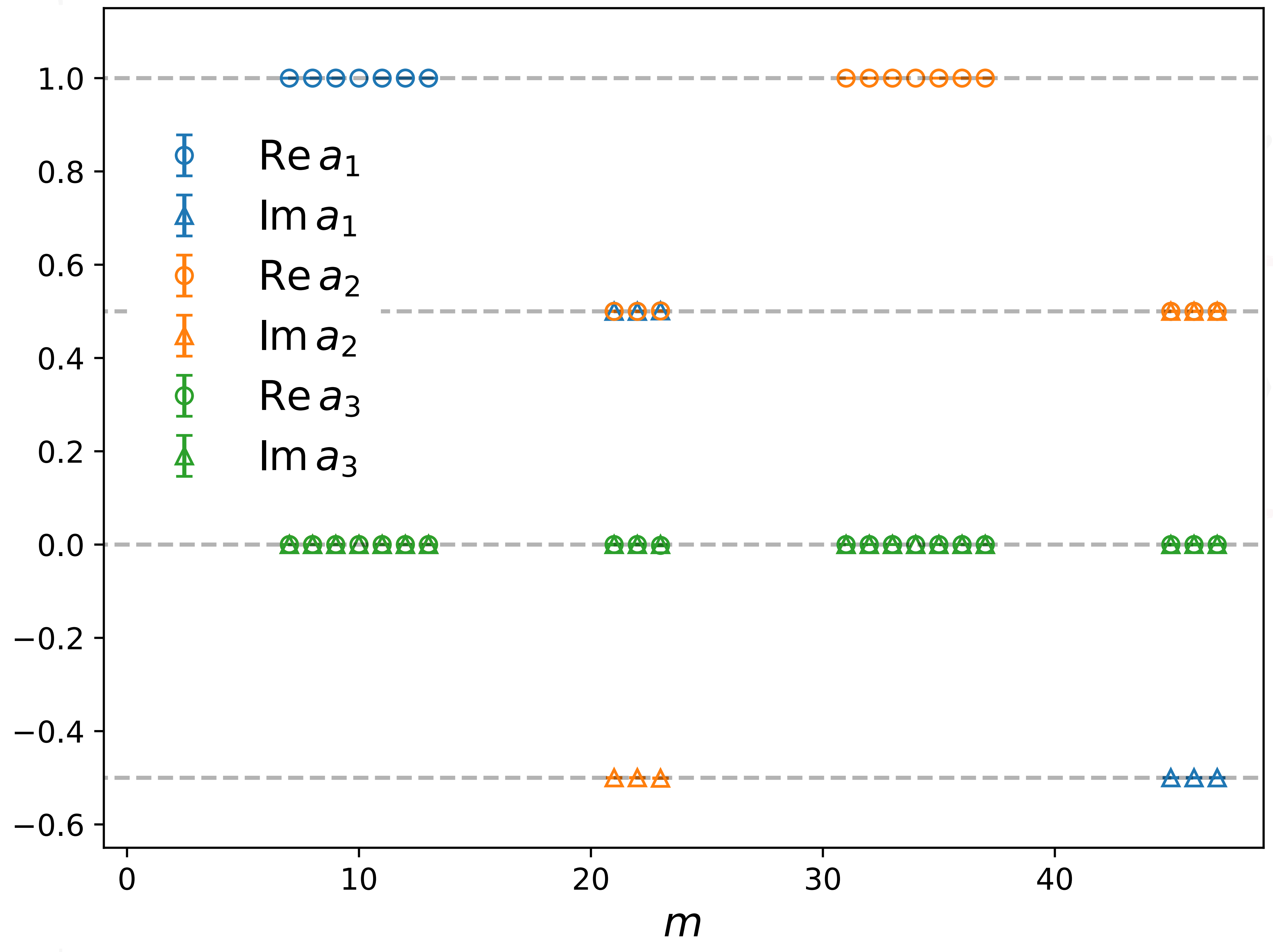
$$\mathscr{B}(p) := C\|p\|_S = \frac{\int_{-\infty}^{\infty} dz \left| e^{-\frac{S(z)}{2}} \right|}{\left| \int_{-\infty}^{\infty} dz\, e^{-S(z)} \right|} \sup_{z\in\mathbb{R}} \left| p(z)\, e^{-\frac{S(z)}{2}} \right|$$

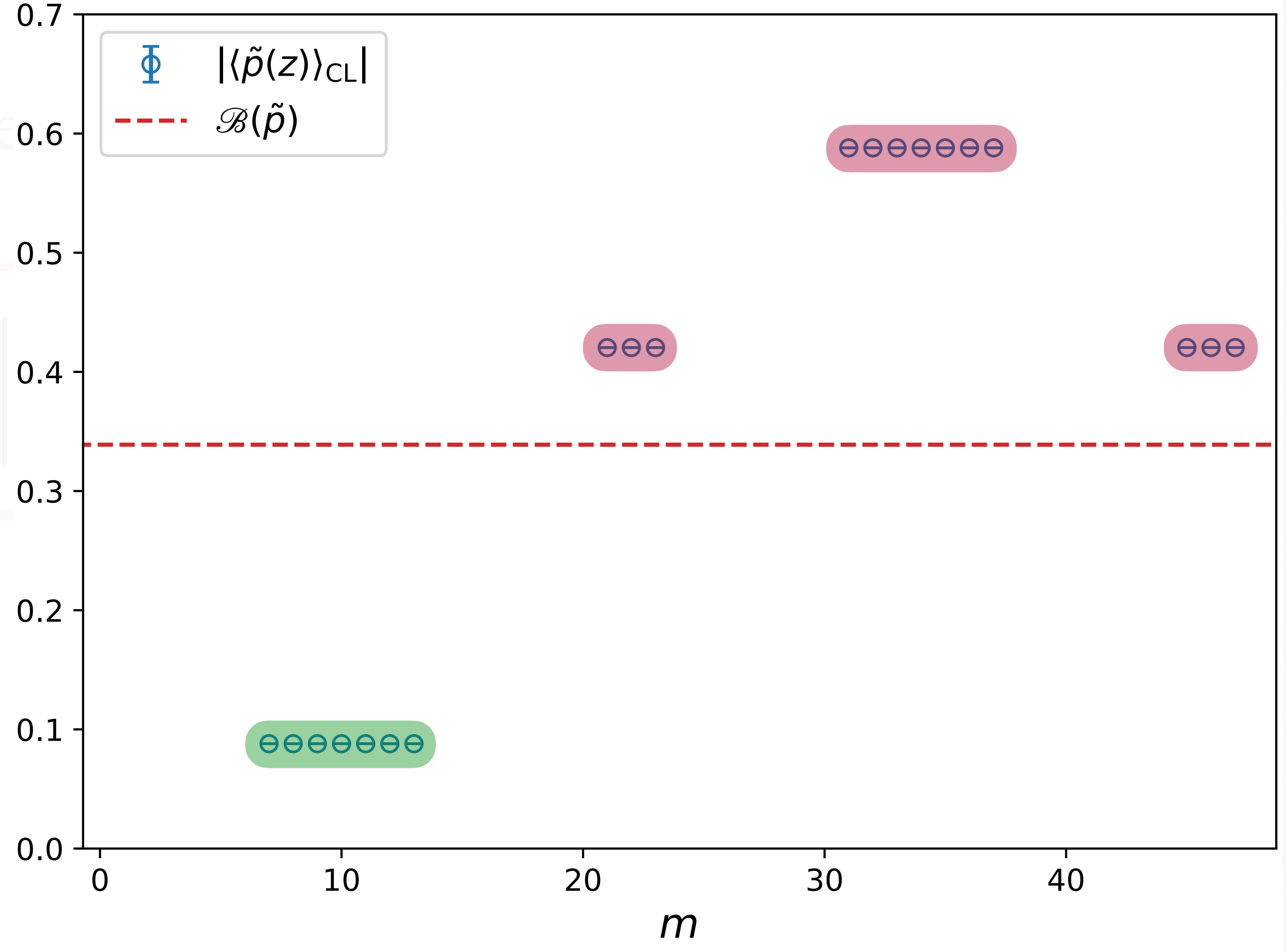
A new correctness criterion

$$S(z) = \frac{\lambda}{4} z^4, \ \lambda = e^{\frac{5i\pi}{6}}, \ K = e^{-\frac{i\pi m}{24}}$$

$$\boxed{\left| \langle \tilde{p}(z) \rangle_{\mathrm{CL}} \right| \overset{!}{\leq} \mathscr{B}(\tilde{p})}$$

$$\tilde{p}(z) = \frac{\lambda}{4} z^4 - \frac{\sqrt{\lambda}}{2} z^2$$





A new correctness criterion*

- As boundary terms are insufficient to detect unwanted integration cycles, one would like to establish a stronger correctness criterion.
- A candidate for such a criterion is given by the bounds shown on the previous slide. Of course, they are only of limited practical use as one cannot check the bounds for *all* polynomials. However, as we also show, one can use the criterion and a certain educated guess $\tilde{p}(z)$ for a polynomial in order to exclude certain results. While this does not yet guarantee the results on the plateau around $m = 10$ to be correct, it proves that the results on all other plateaus are necessarily wrong, without having to compute the coefficients a_i or exact results for all observables.

Summary & Outlook

- CL promising approach for systems with a complex-action problem.

- Wrong convergence due to boundary terms or unwanted integration cycles.

- Can in principle be fixed by kernels.
  - How to construct them?
  - How to verify convergence? New criterion might be helpful.

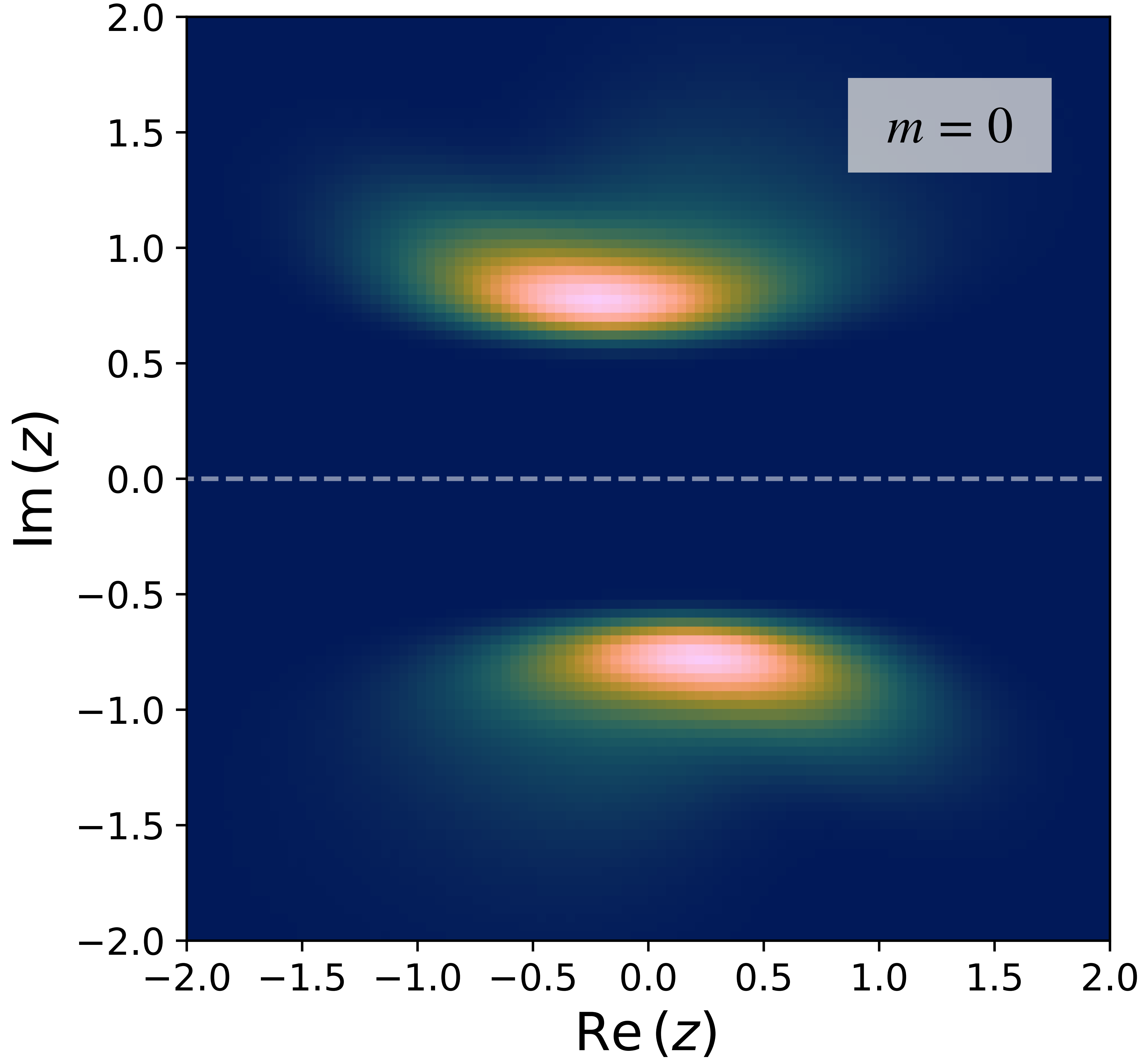
- Outlook: Kernels and role of integration cycles in realistic theories?

Backup

Complex Langevin evolution with a kernel*

- Example: $S(z) = \dfrac{\lambda}{4} z^4\,,\ \lambda = e^{\frac{5i\pi}{6}}\,,\ K = e^{-\frac{i\pi m}{24}}\,.$

- Here, we show histograms of z in the complex plane for different values of the kernel parameter m.



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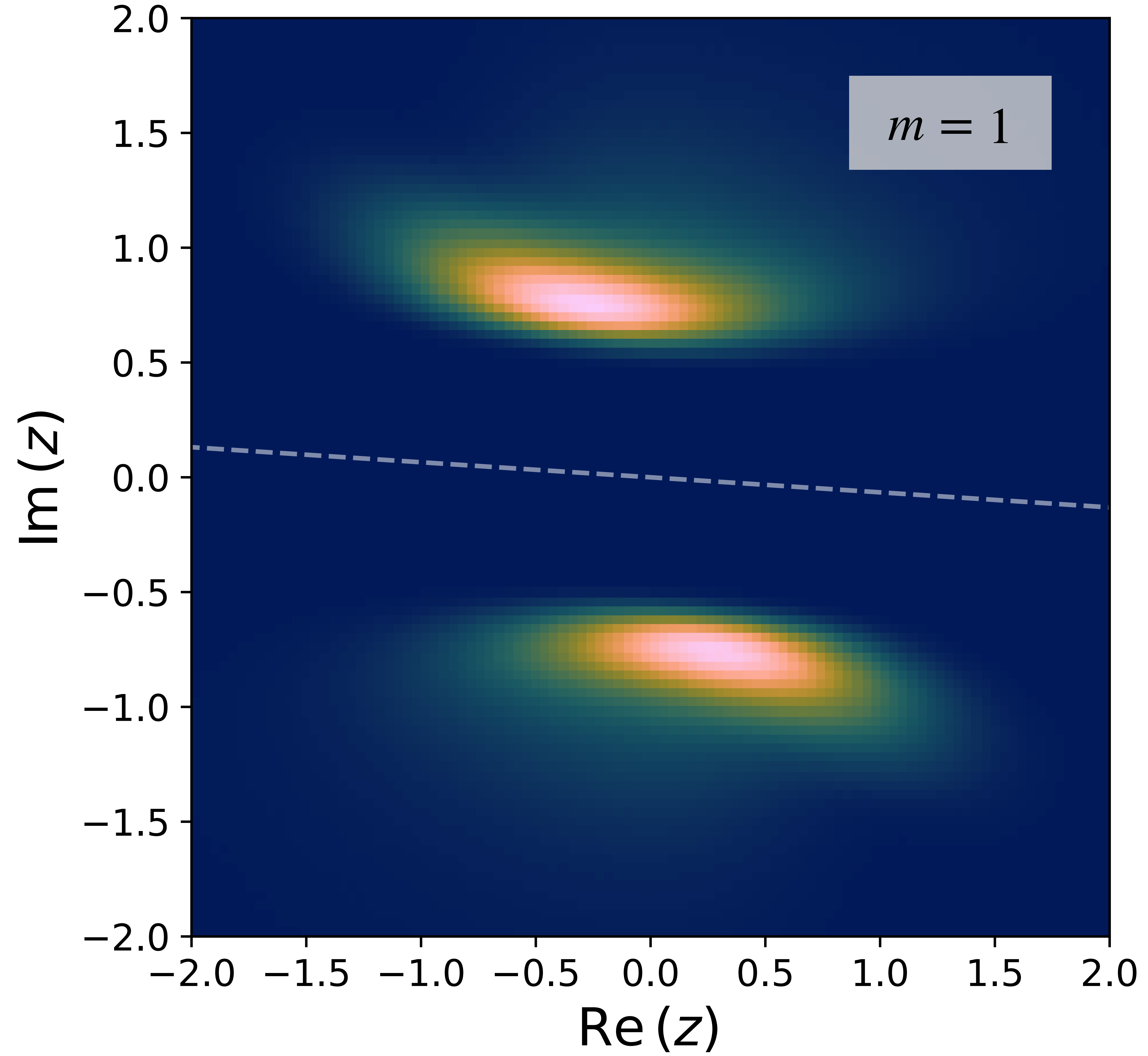

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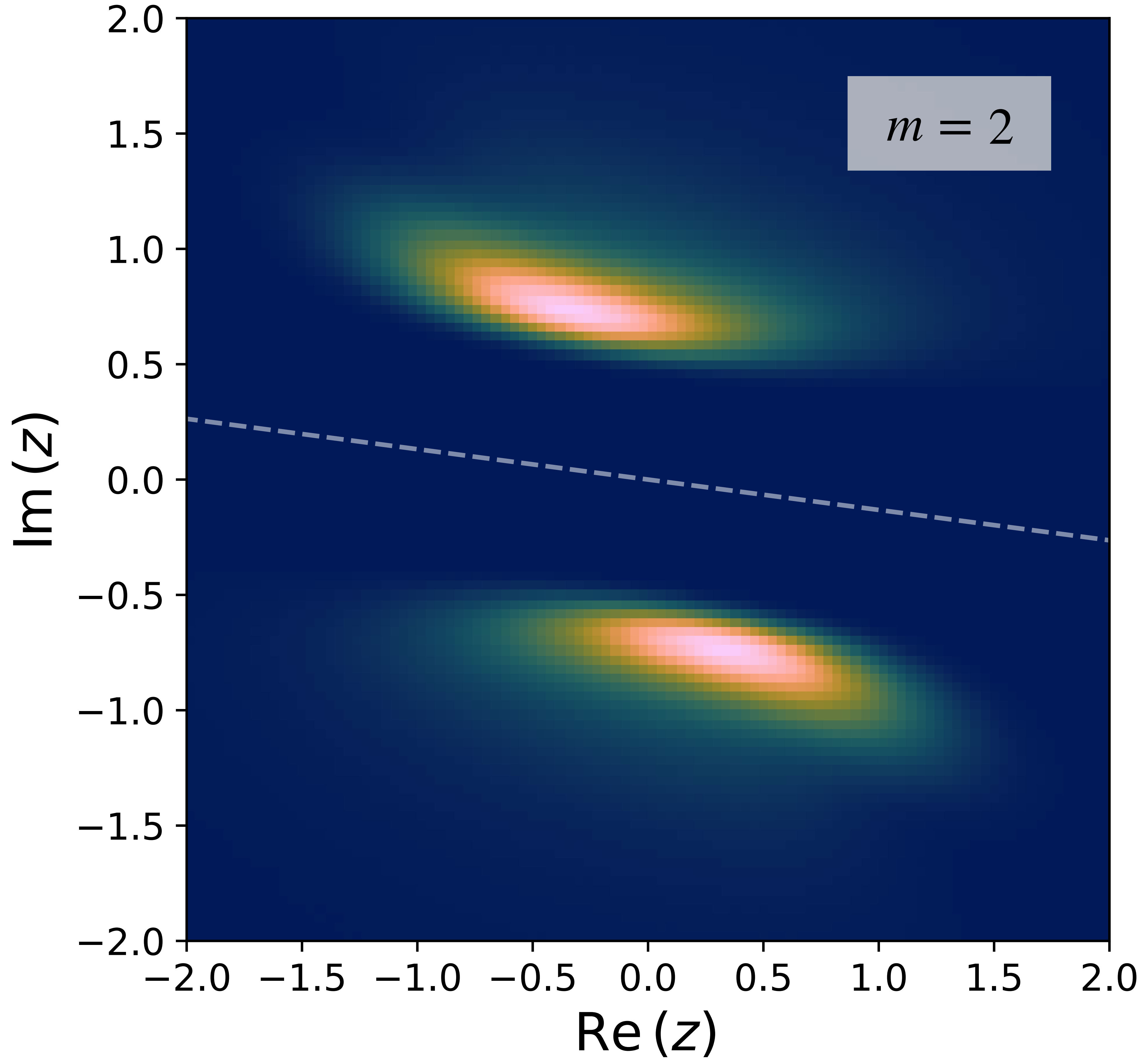

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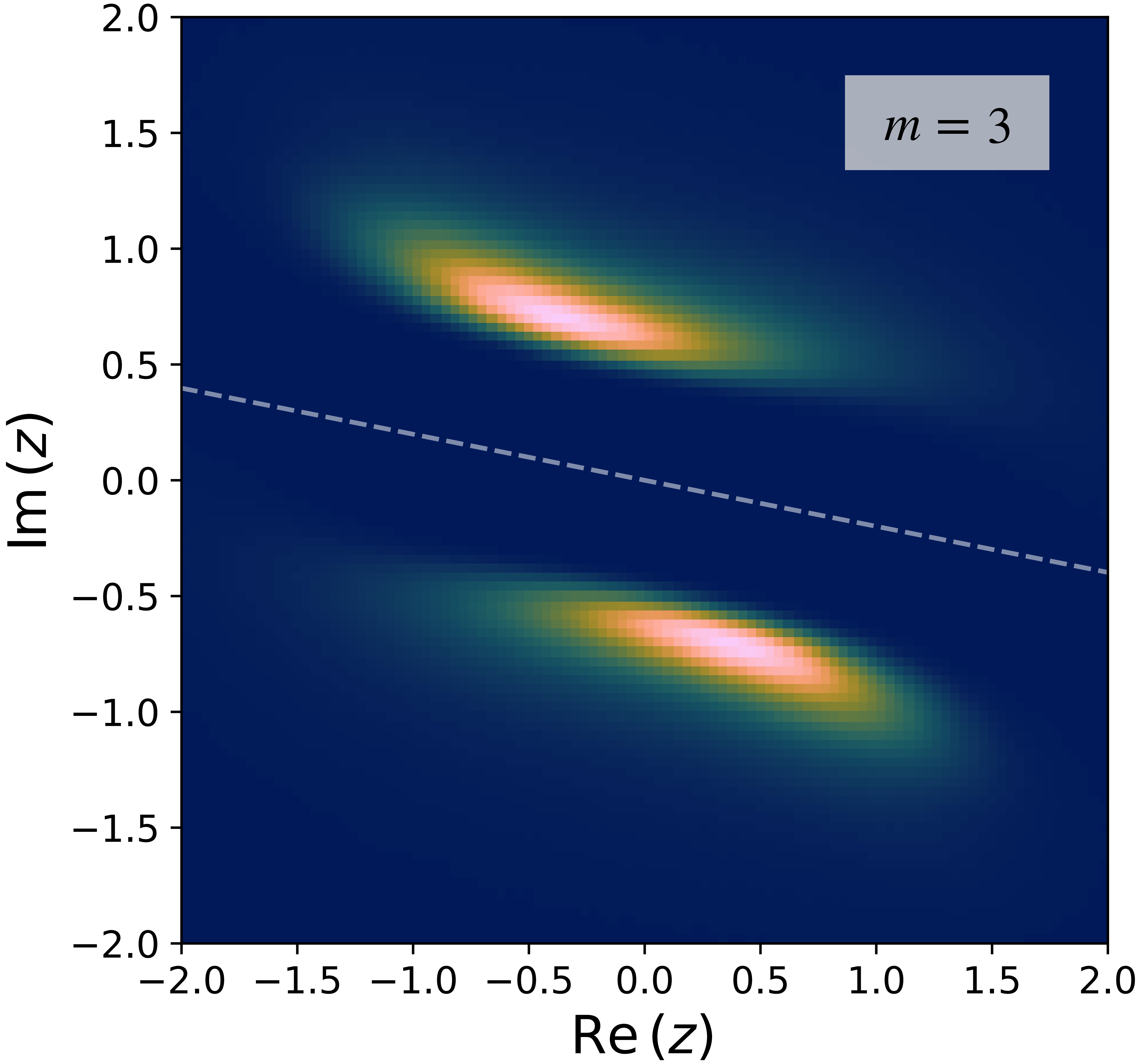

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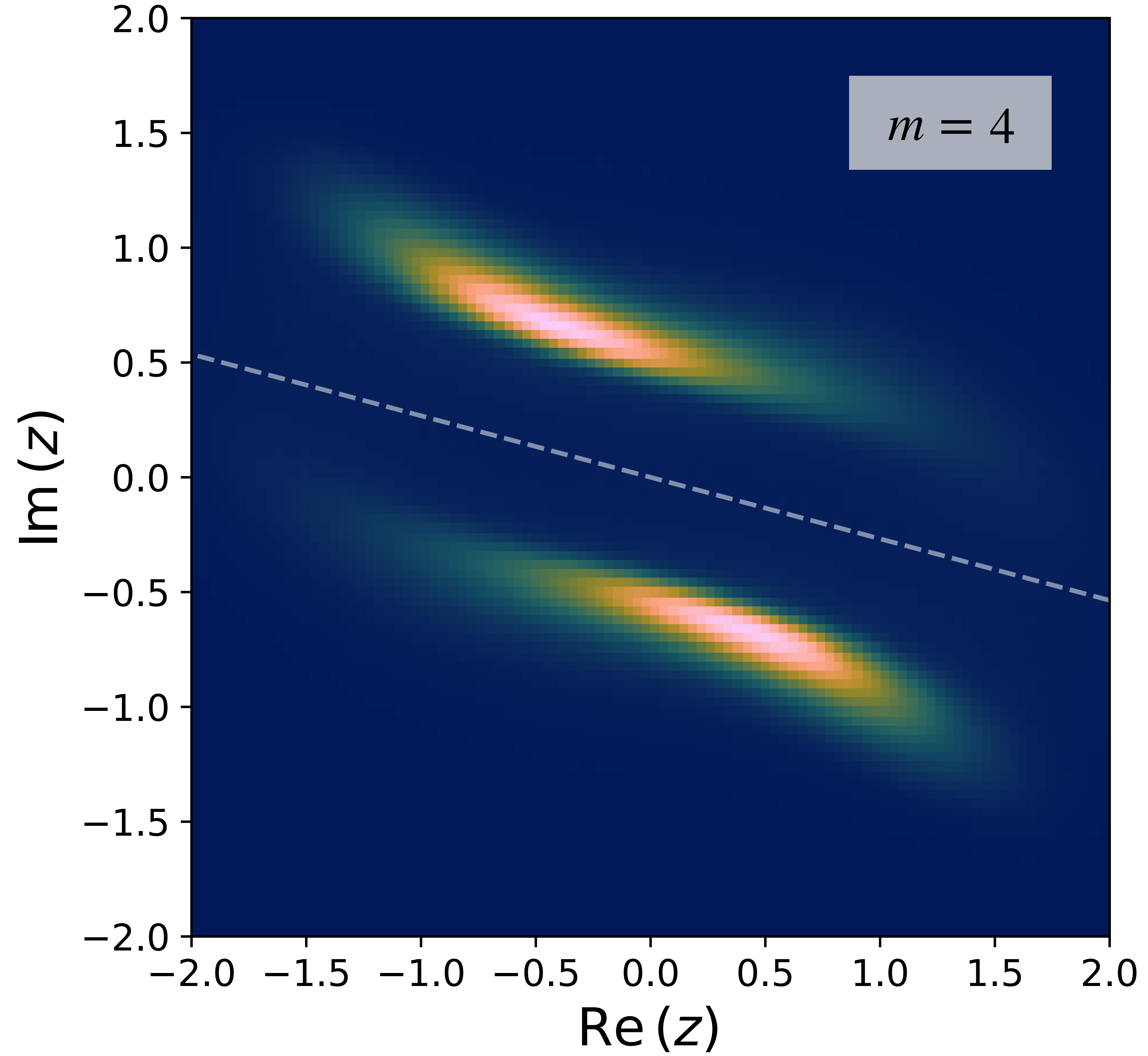

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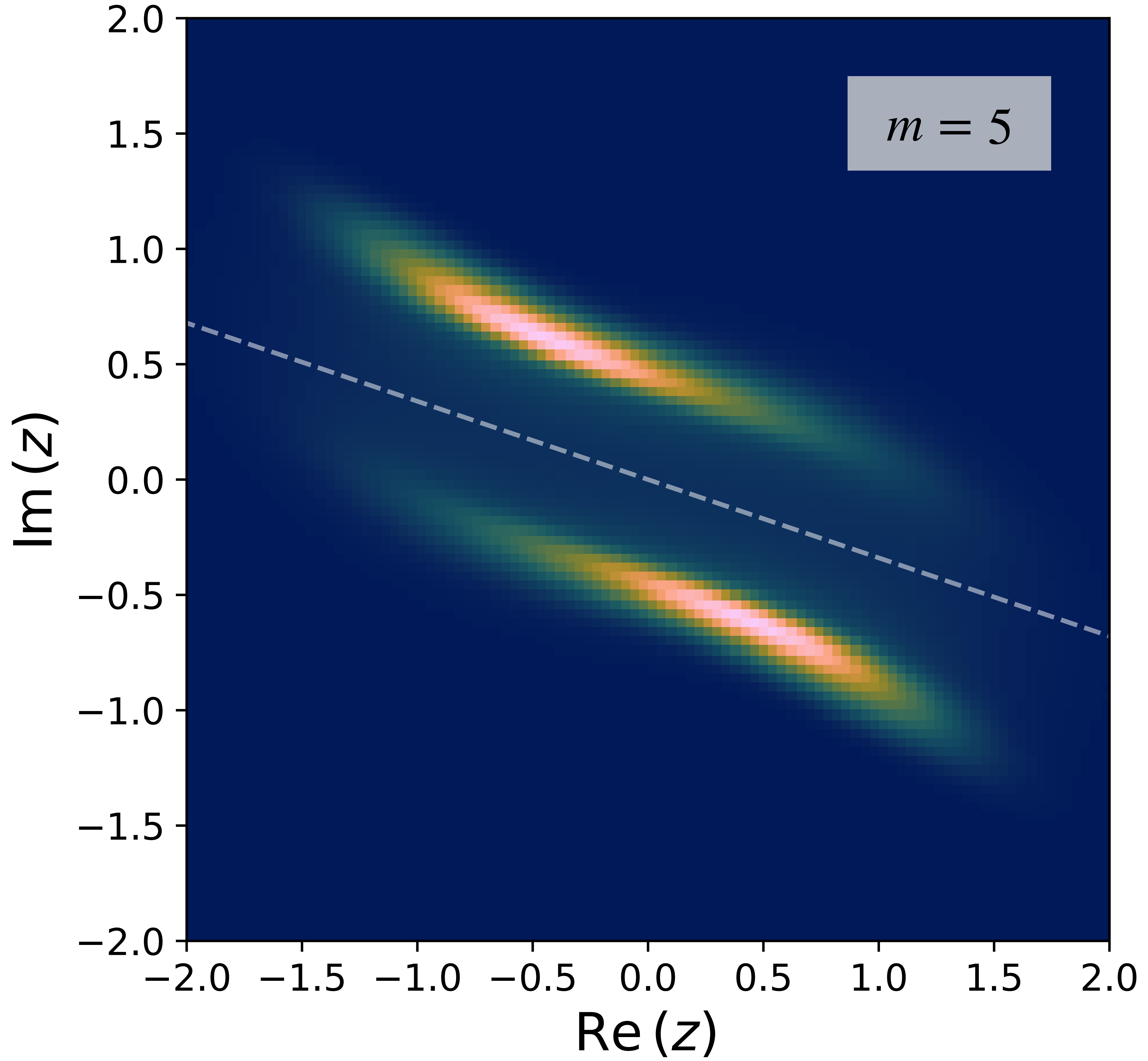

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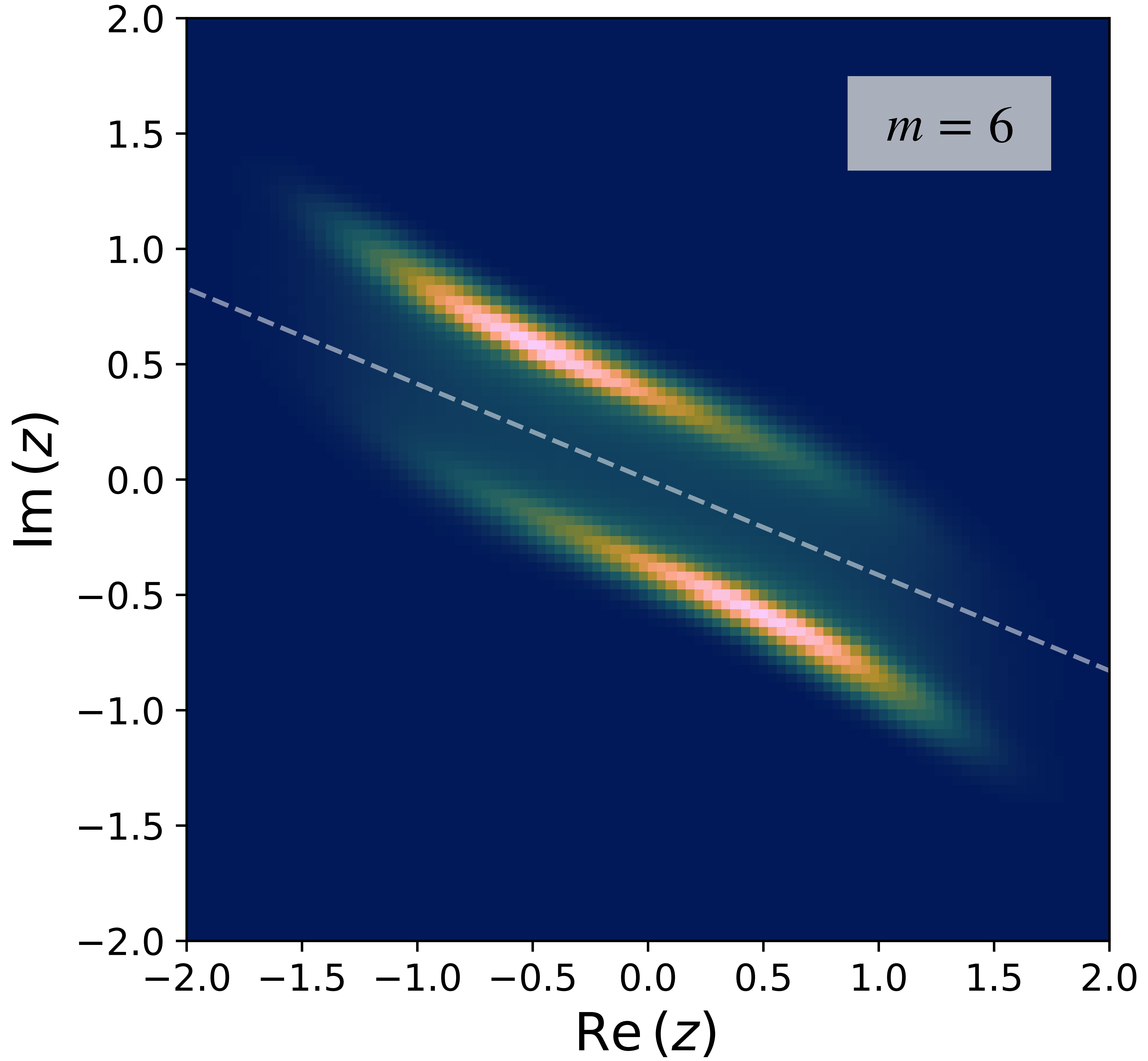

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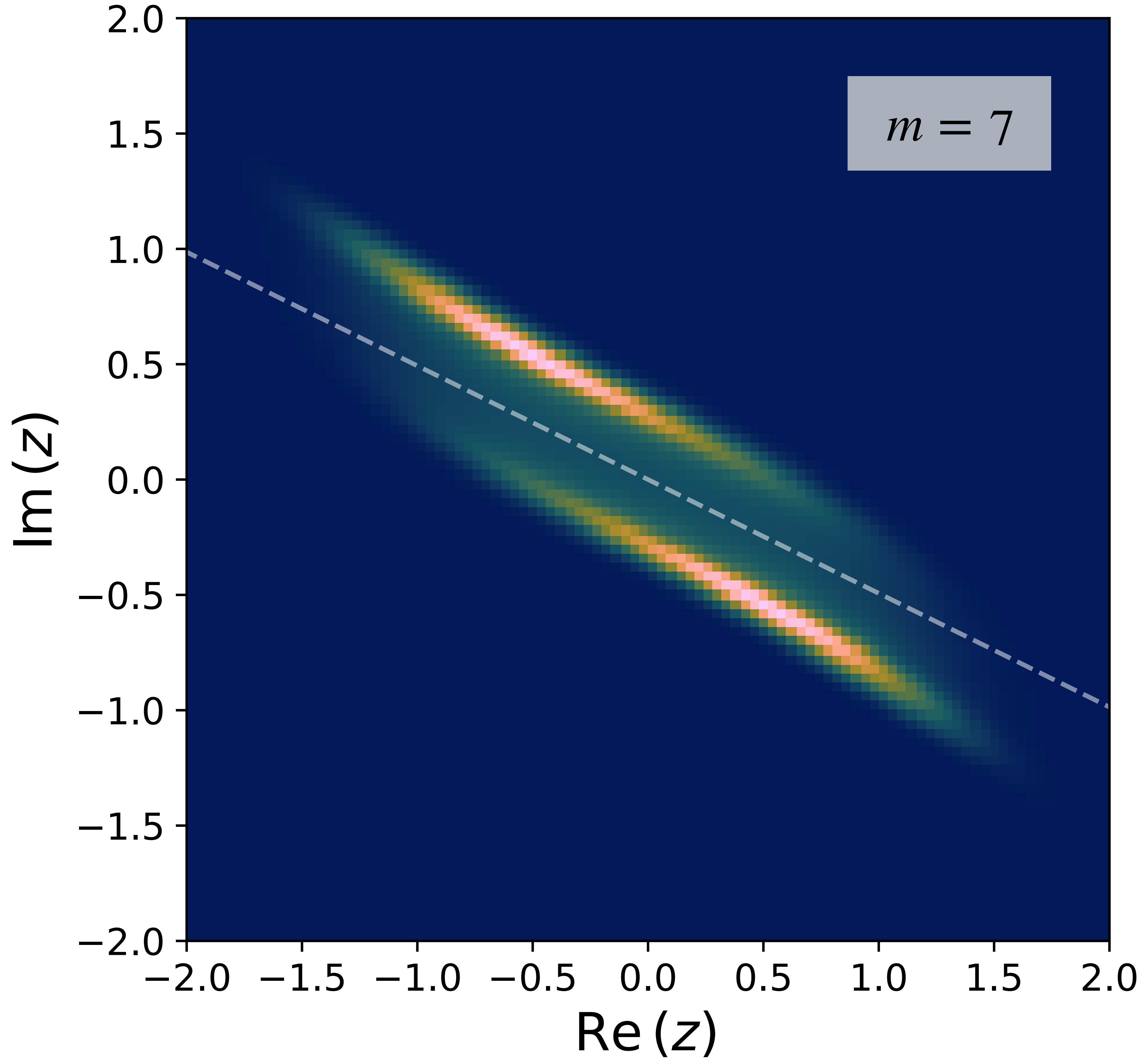

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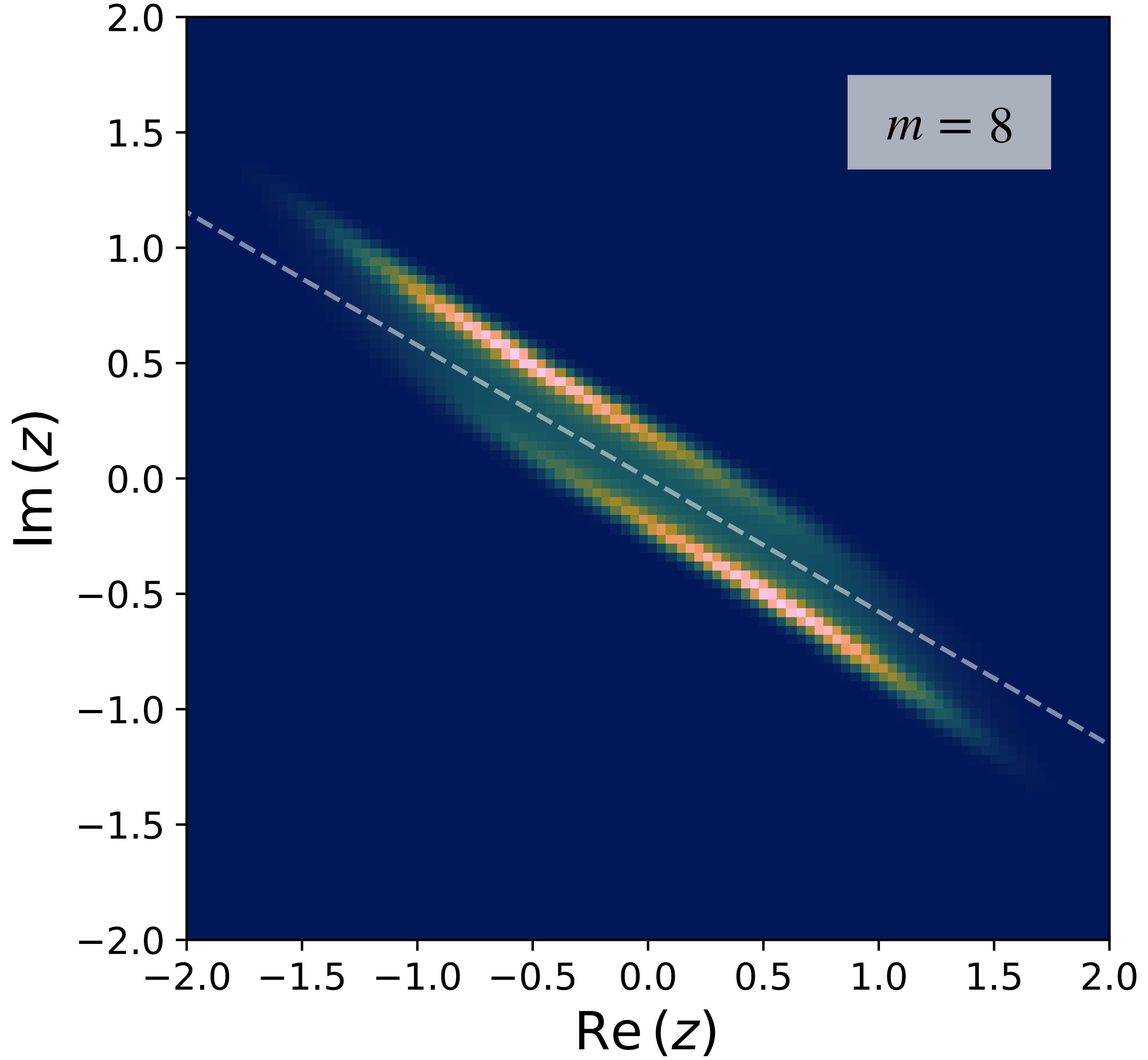

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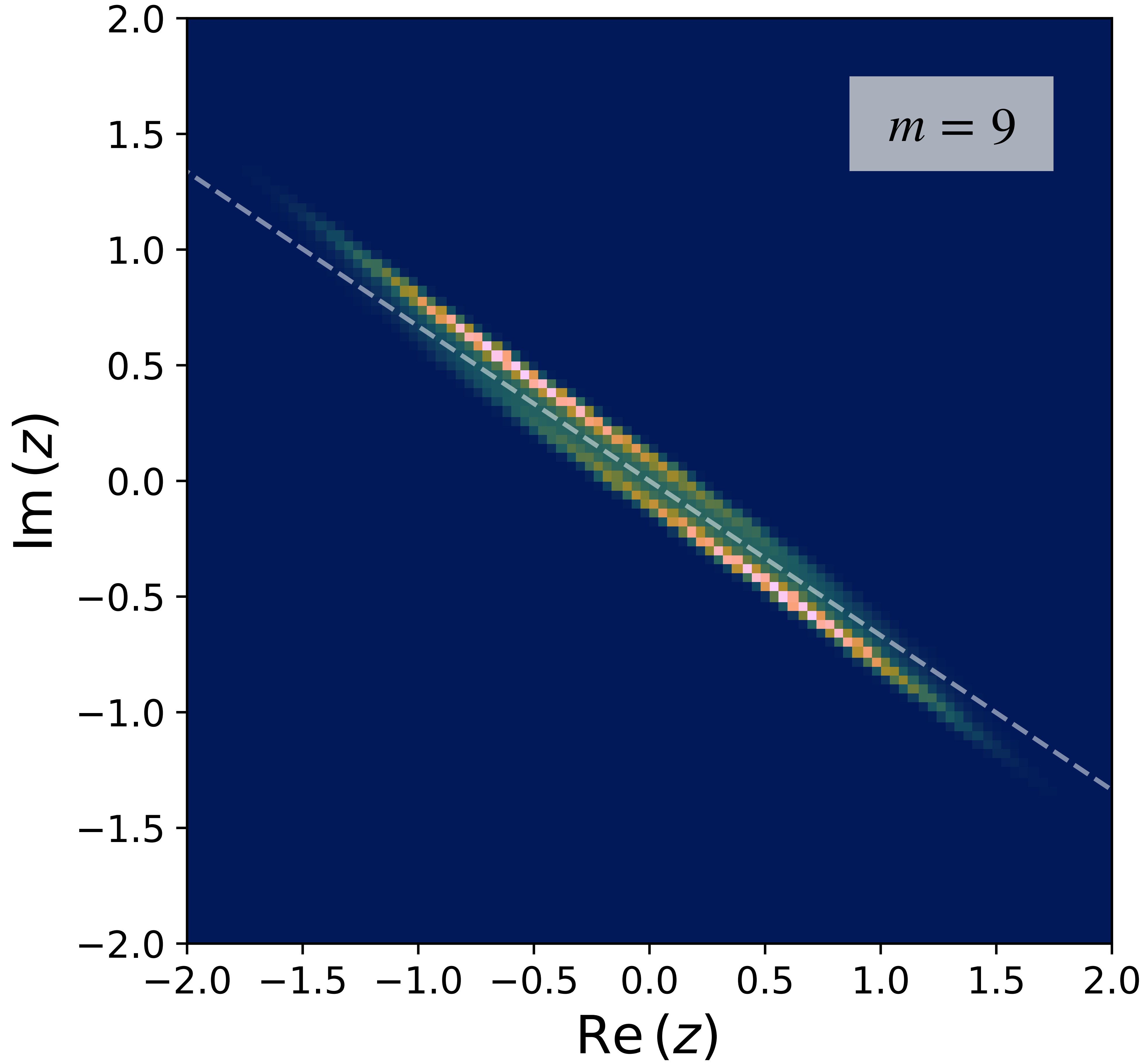

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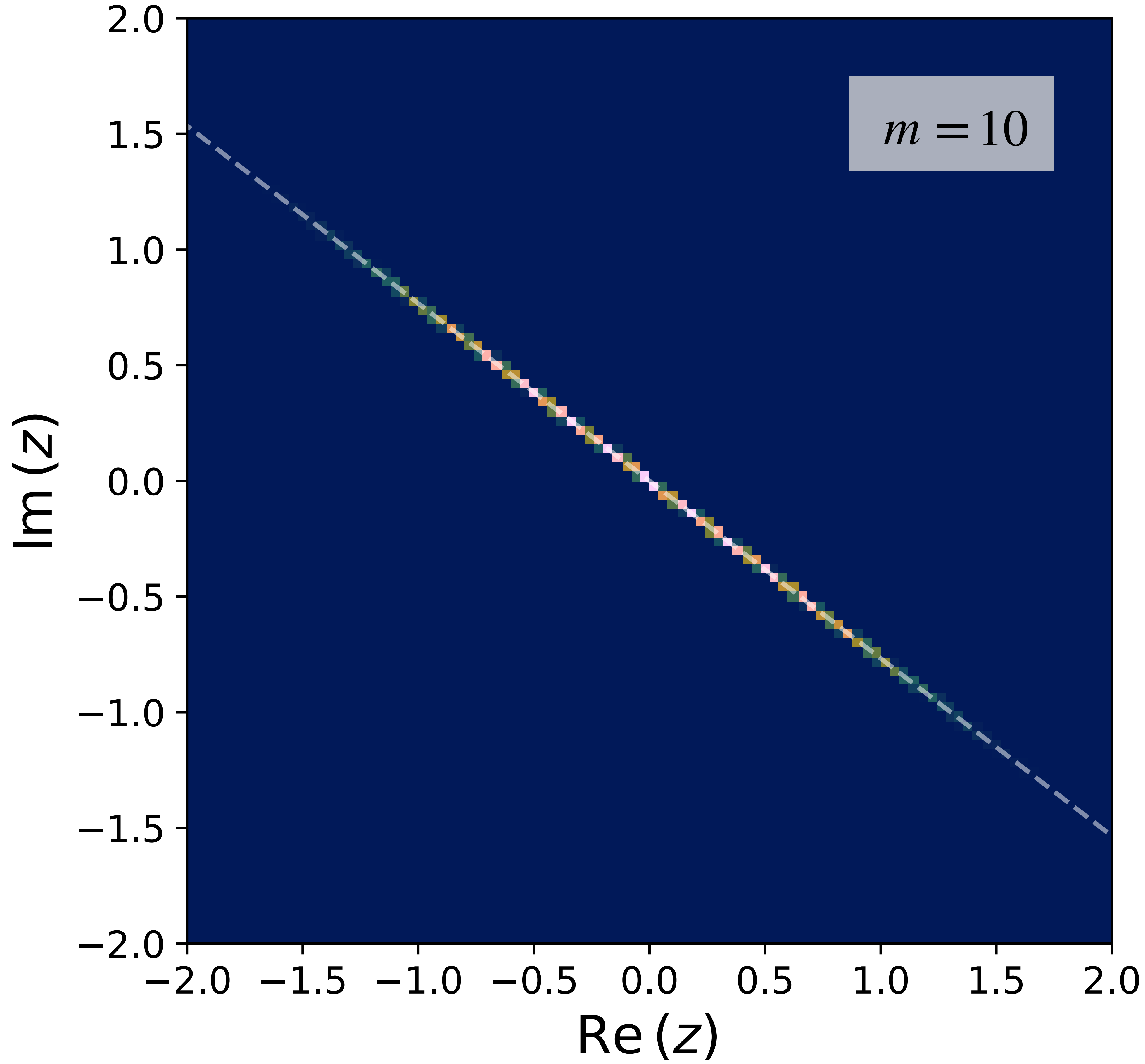

Contact*

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