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The Lefschetz thimbles and the sign problems

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Thanks to: M.Cristoforetti, F.Di Renzo,
G.Eruzzi, A.Mukherjee, C.Schmidt, C.Torrero.

See also poster by A.Mukherjee.

I. Introducing the Lefschetz thimble

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Saddle-point integration

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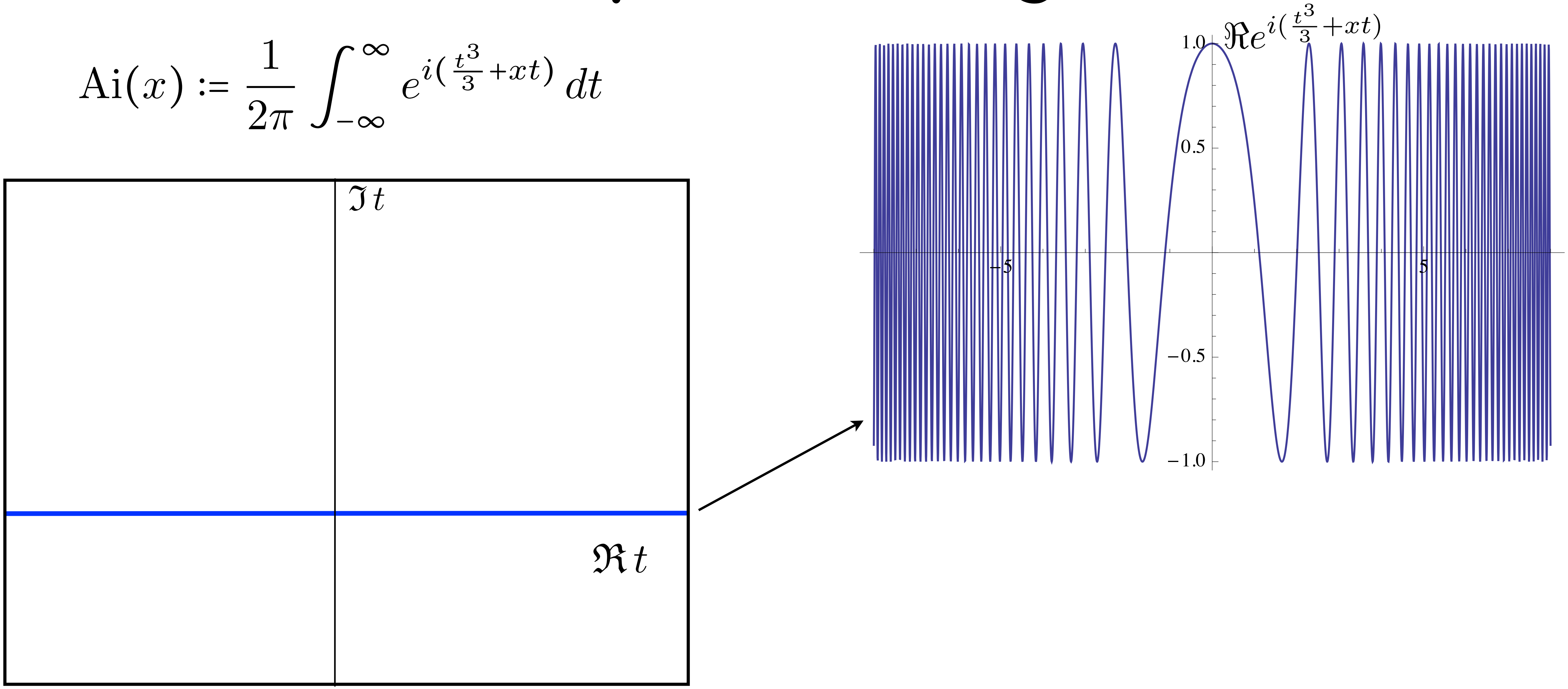

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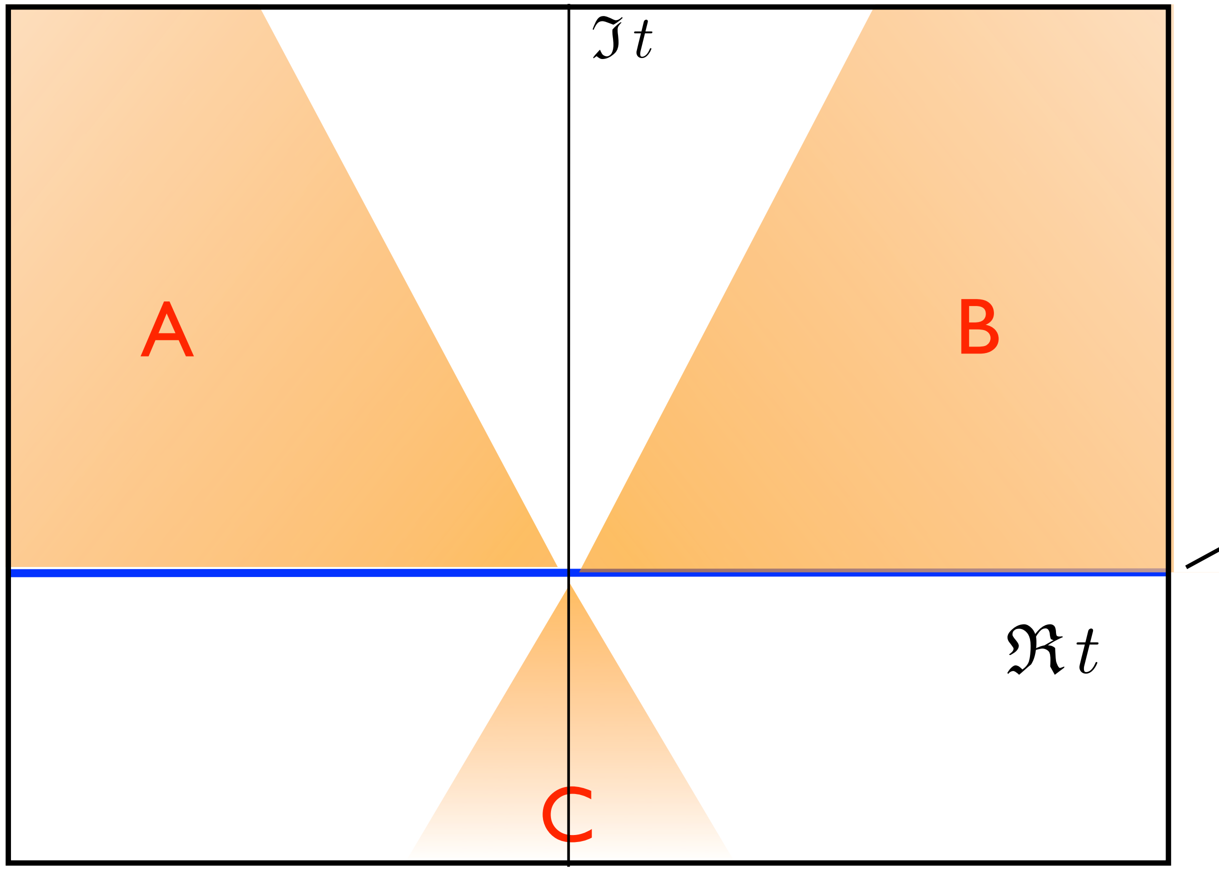

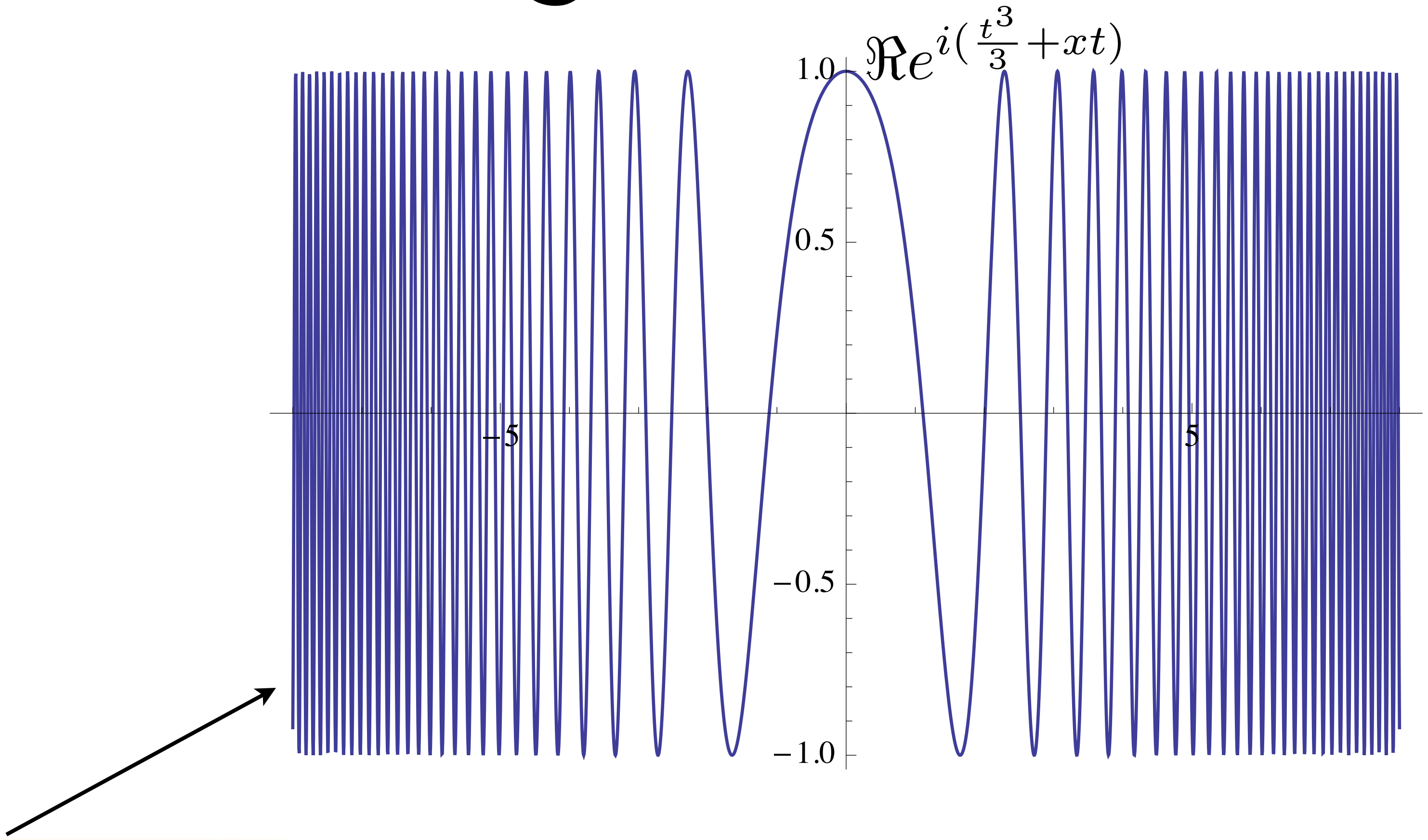

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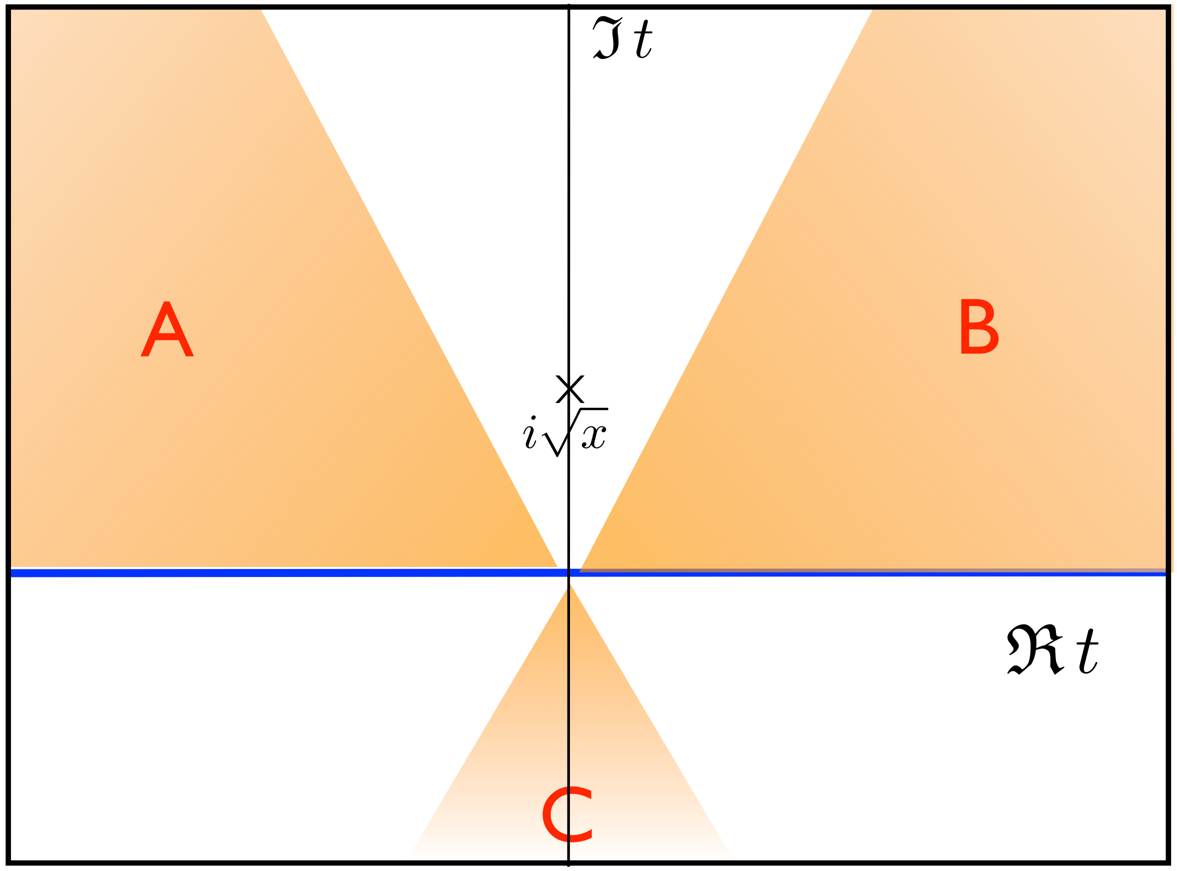

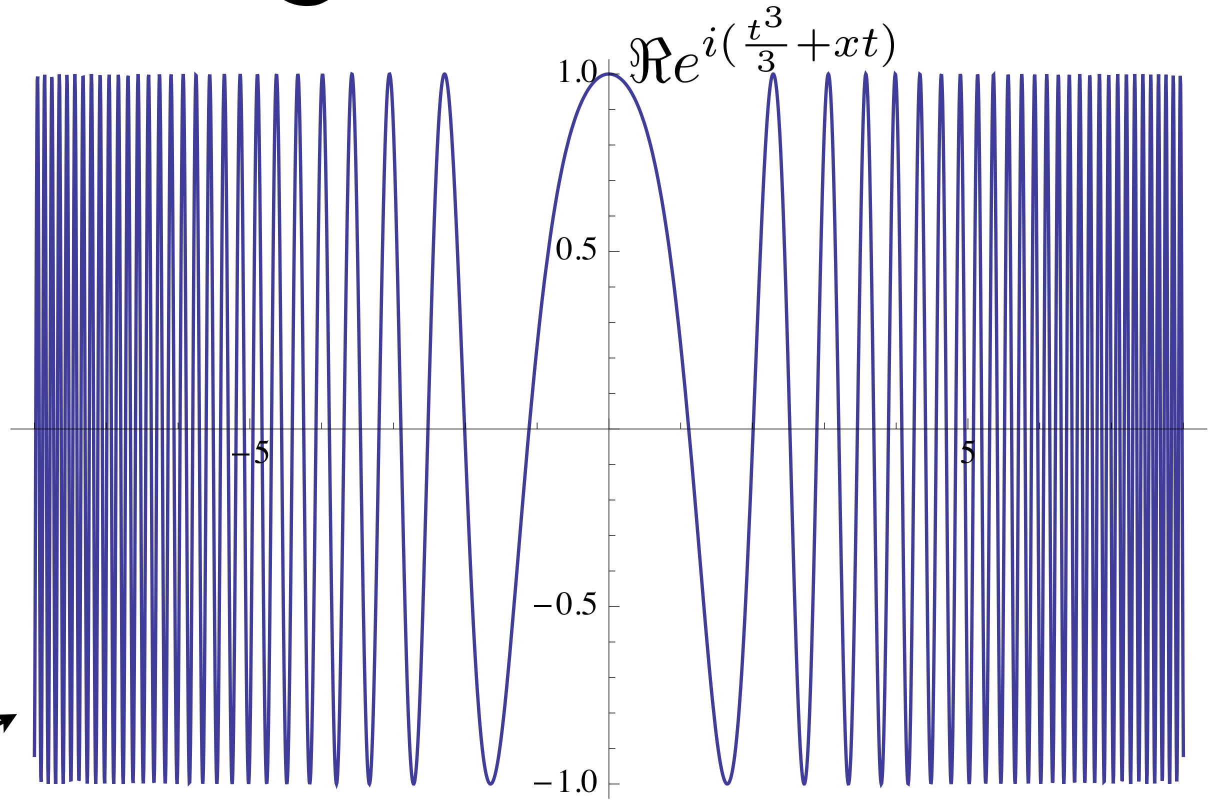

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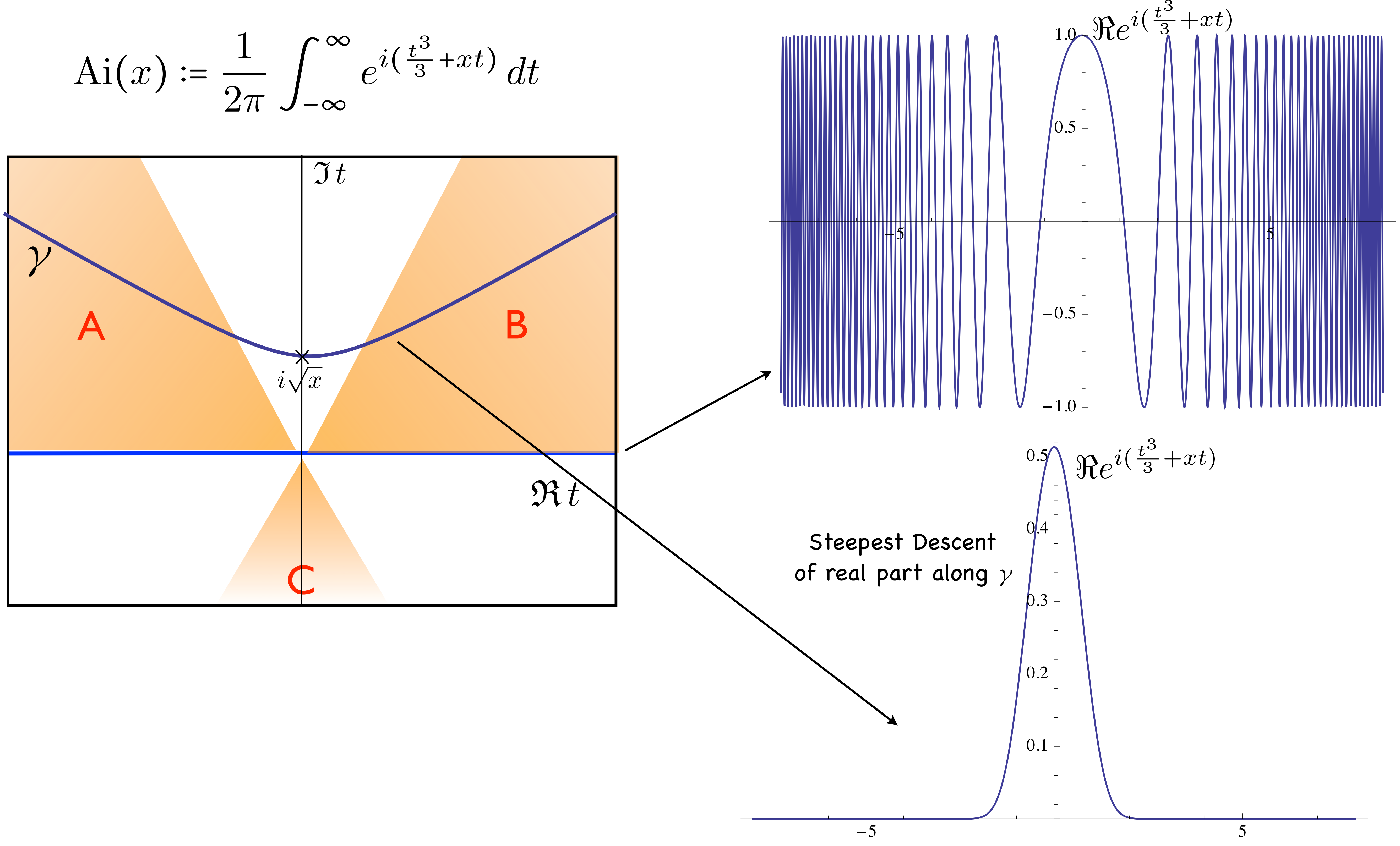

Steepest Descent
of real part along γ

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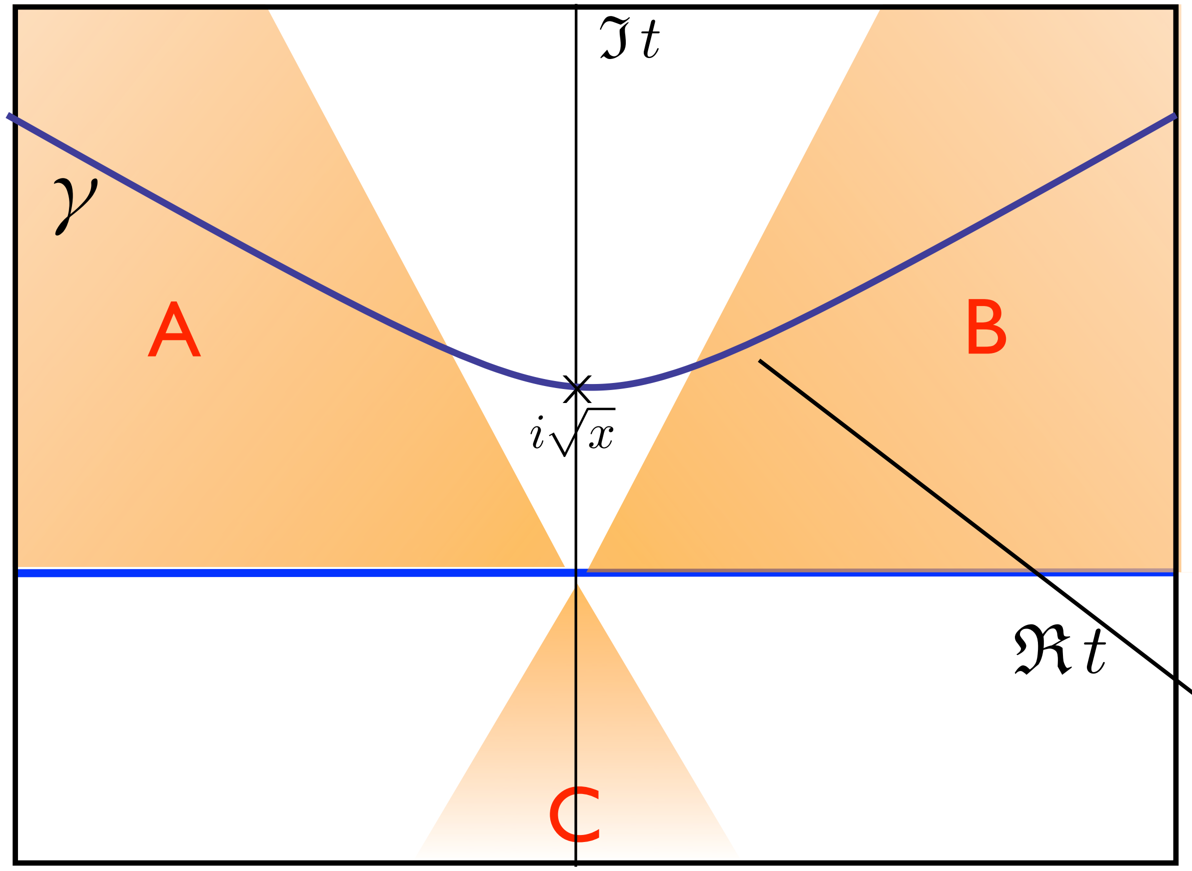
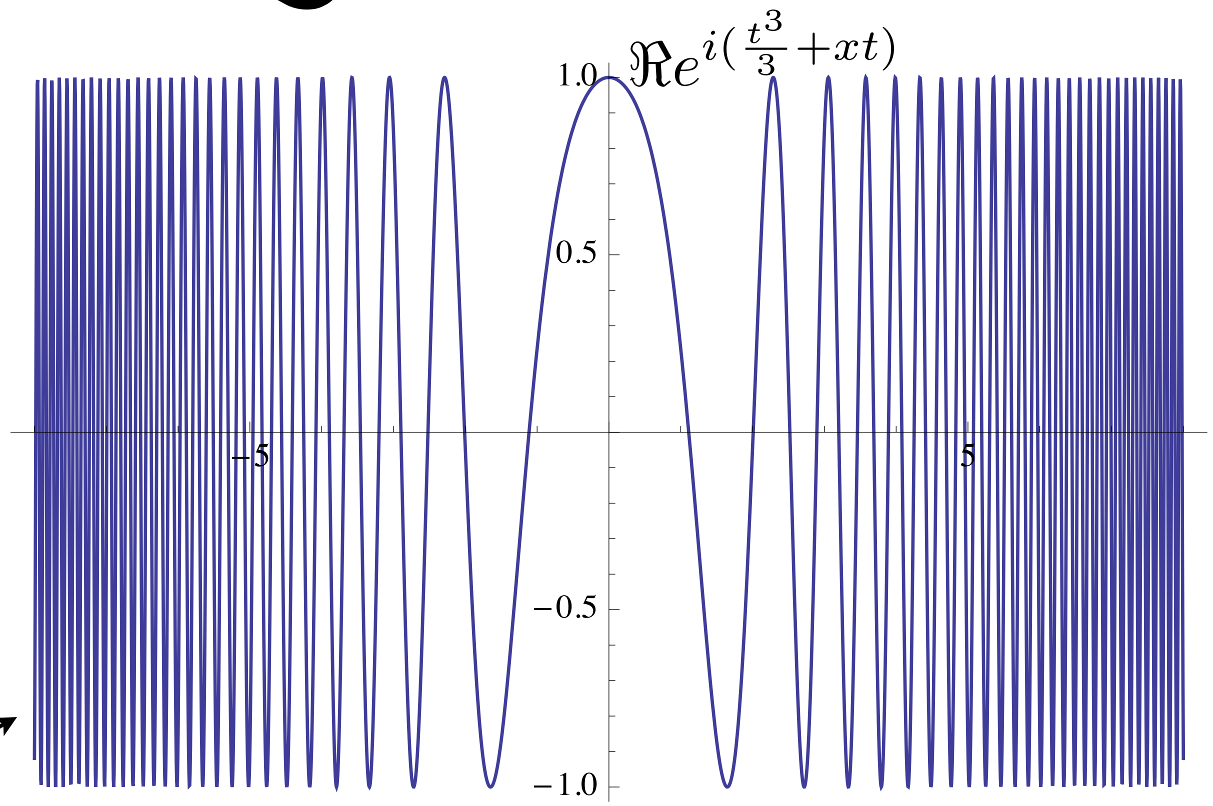
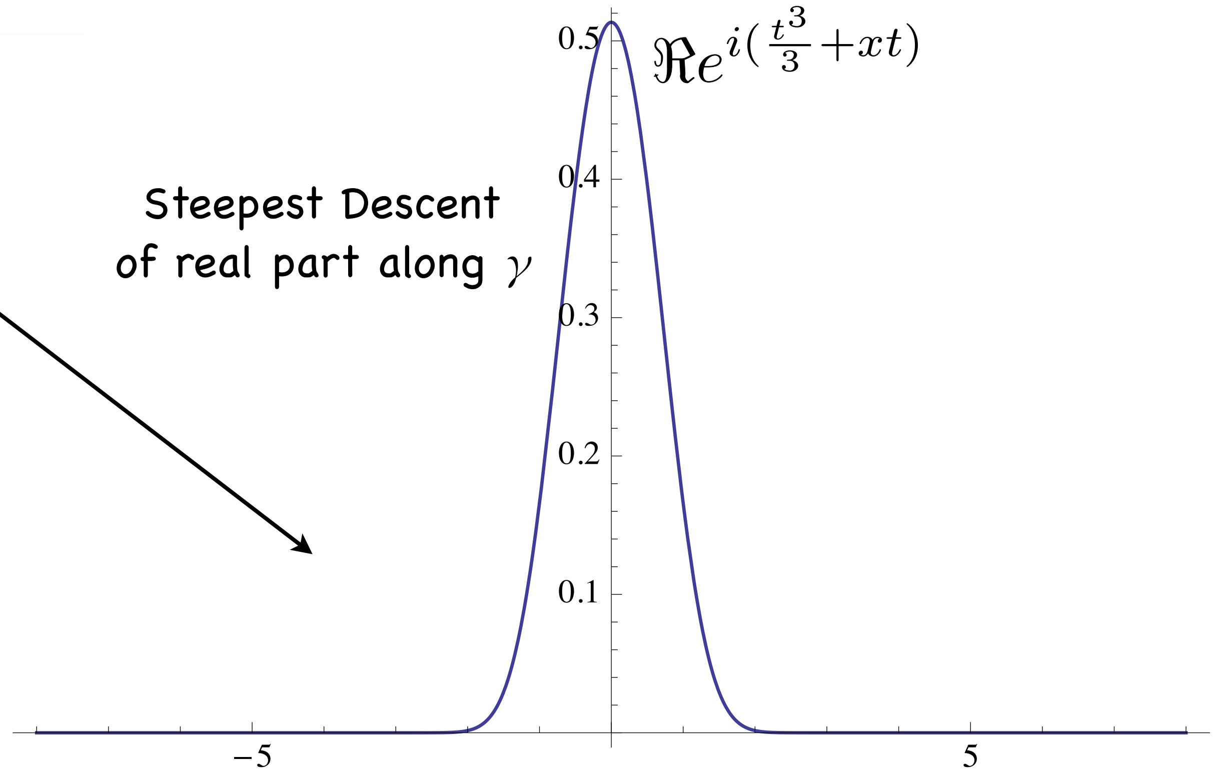


Stationary phase along γ

$$\frac{1}{2\pi}\int_\gamma e^{i(\frac{z^3}{3}+xz)}\,dz \to \frac{1}{2\pi}e^{i\phi}\int_\gamma e^{\mathfrak{R}[i(\frac{z^3}{3}+xz)]}\,dz$$





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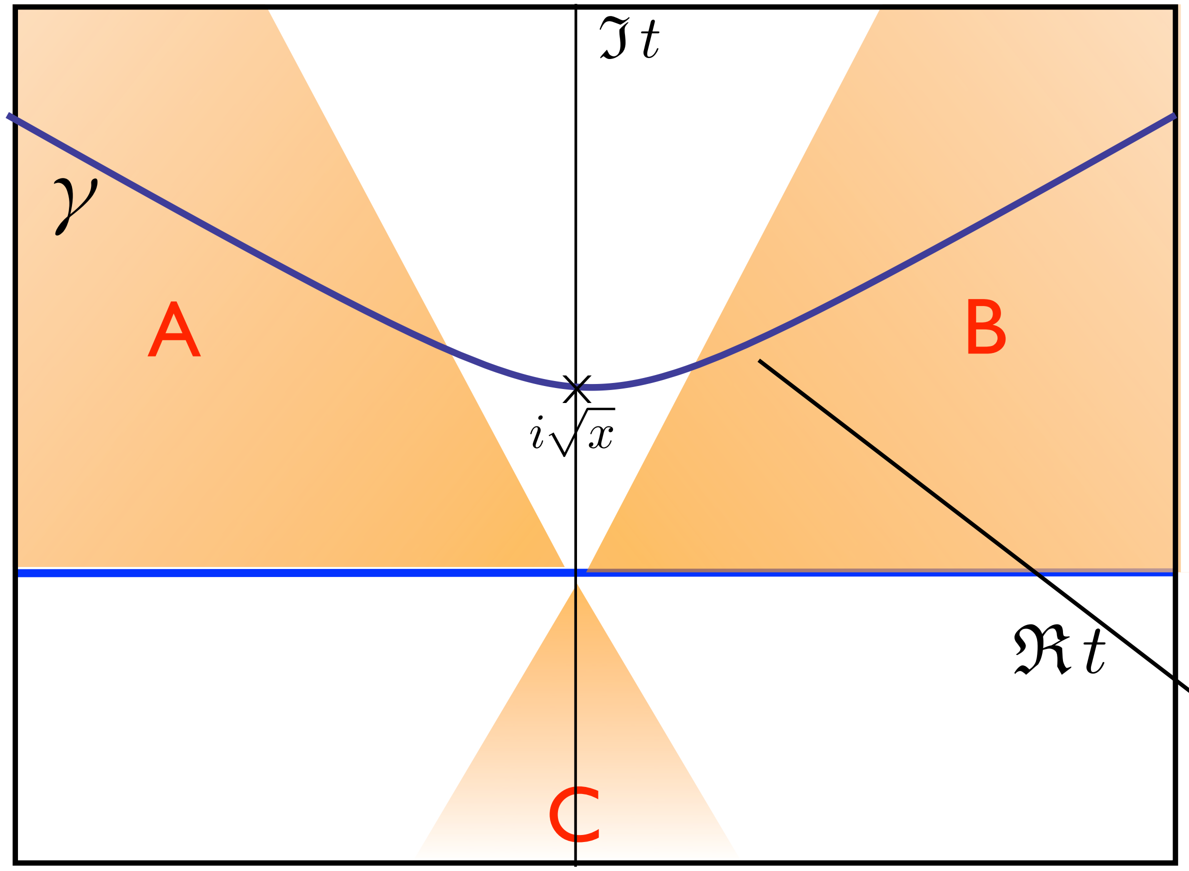

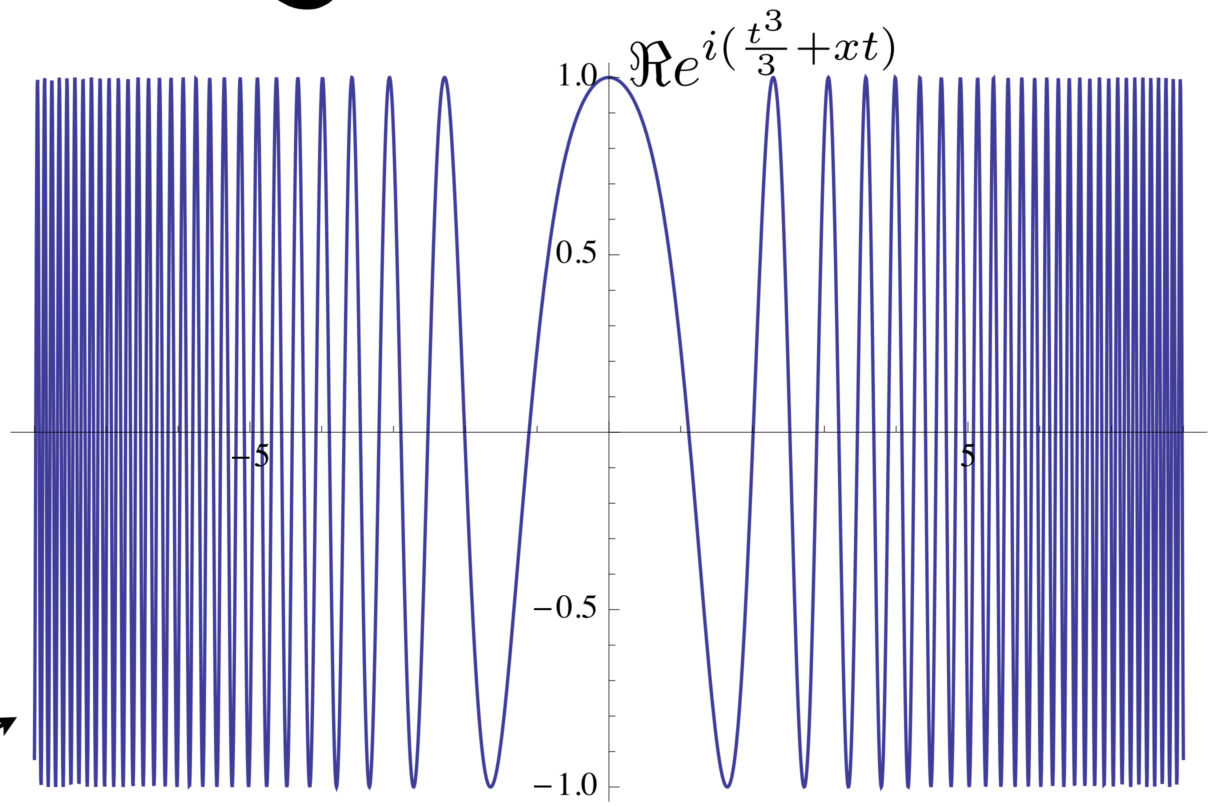

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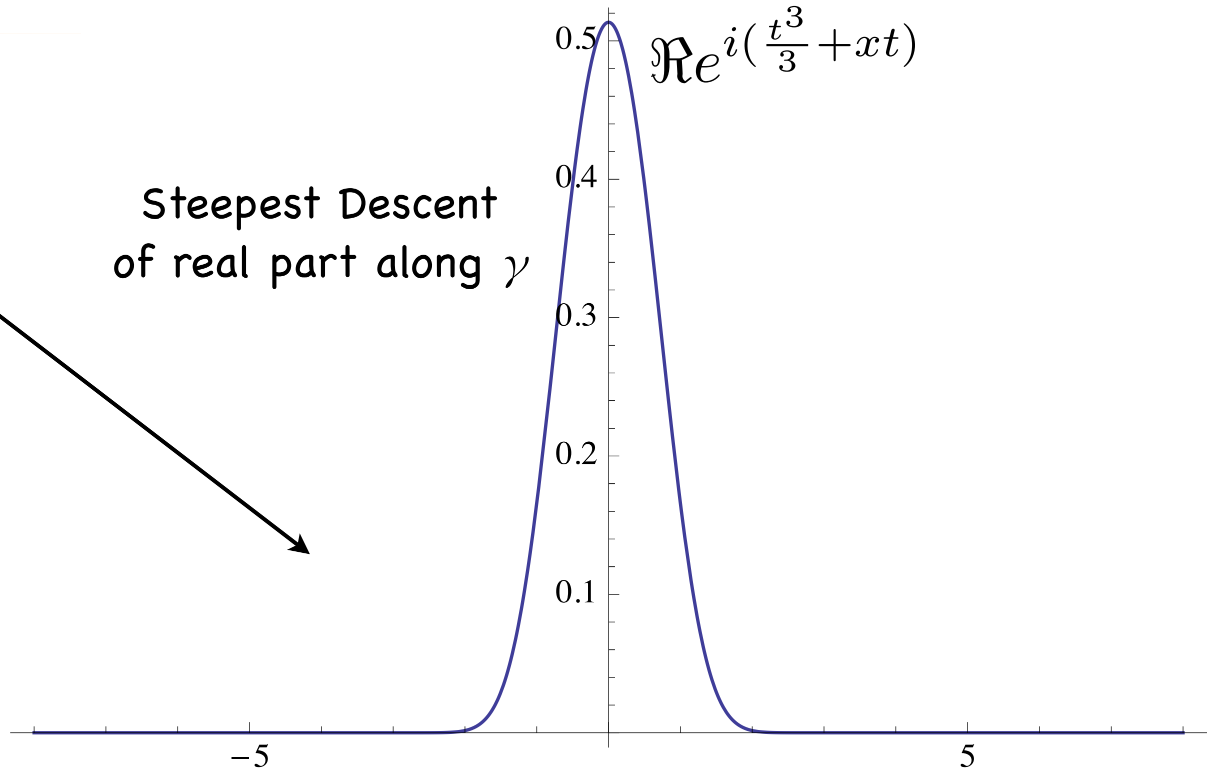

Stationary phase along γ

$$\frac{1}{2\pi}\int_{\gamma} e^{i(\frac{z^3}{3}+xz)}\,dz \rightarrow \frac{1}{2\pi}e^{i\phi}\int_{\gamma} e^{\Re[i(\frac{z^3}{3}+xz)]}\,dz$$

NOTE γ' is not constant, but changes smoothly!

Saddle-point integration

comments

- It is a classic and elementary tool that works extremely well for low dimensional oscillating integrals.

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- However, the idea of **deforming the path** is independent of the **series expansion**. And a path where the phase is stationary and the important contributions are more localized is very attractive from the point of view of the sign problem.
  - What about a Monte Carlo integral along the curves of steepest descent (SD)?

Higher dimensions

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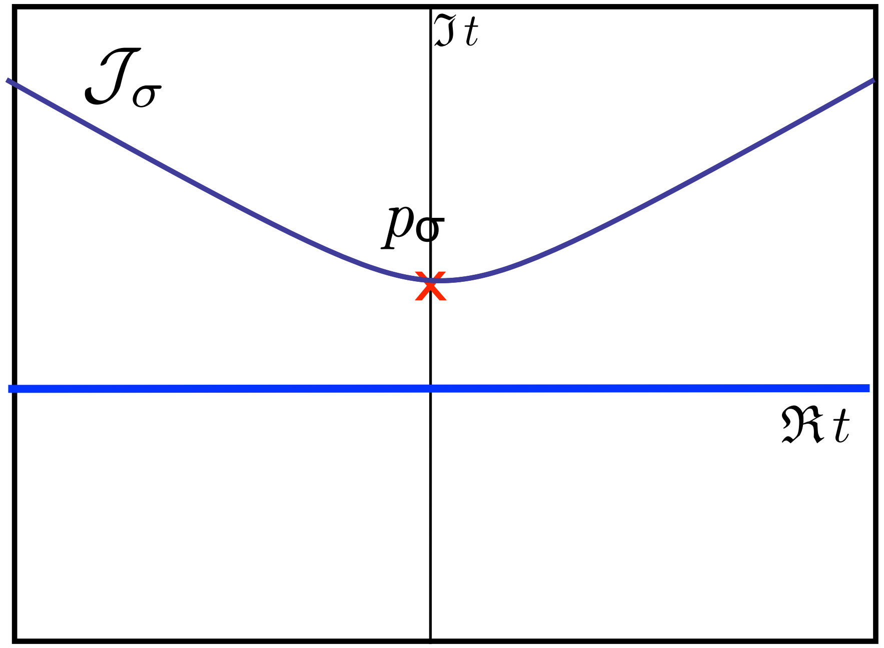

The generalization of the paths of SD are called Lefschetz thimbles $\mathcal{J}_\sigma$,

For each stationary point p_σ of the complexified $f(z)$,

$\mathcal{J}_\sigma$ is the union of the paths

of SD that fall in p_σ at ∞.

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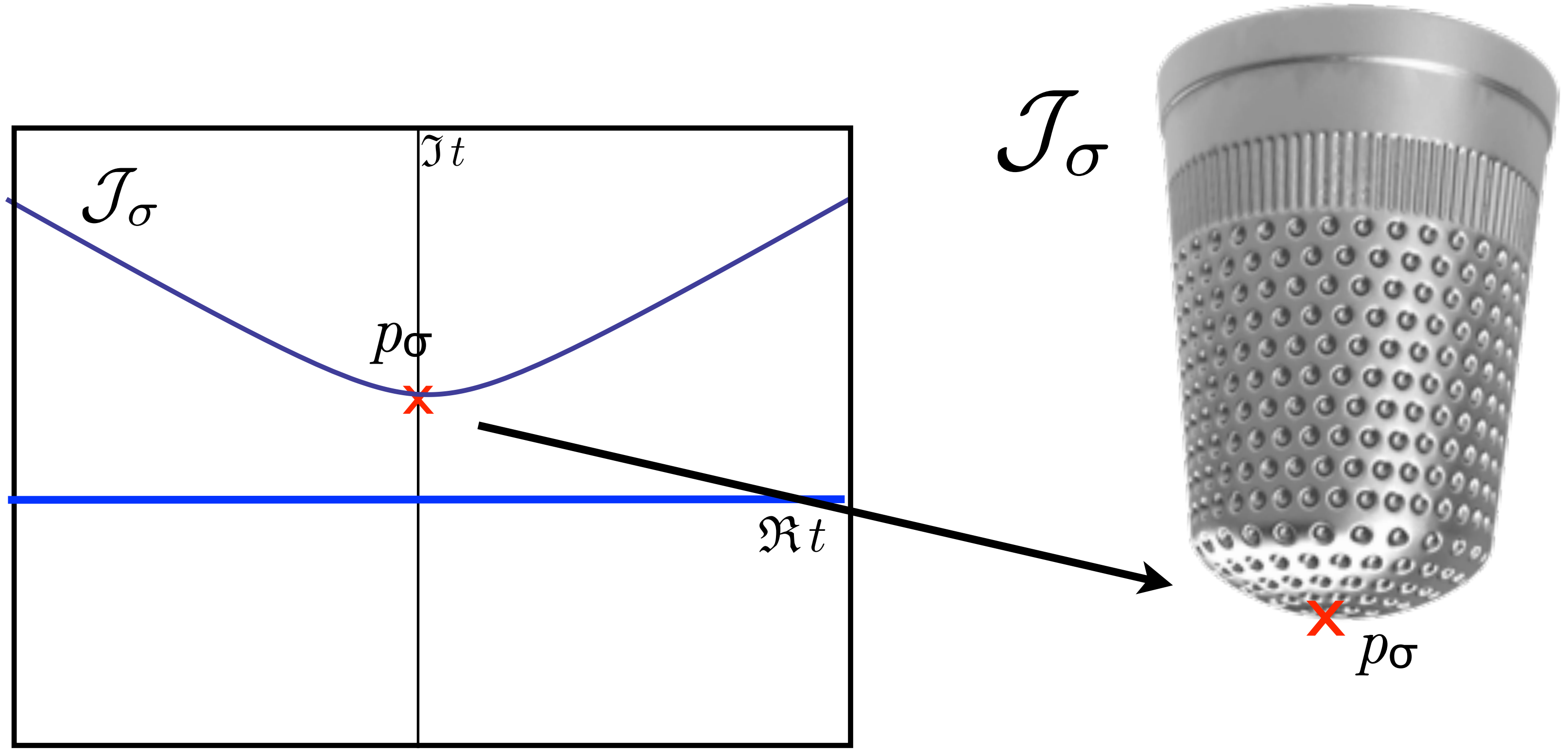

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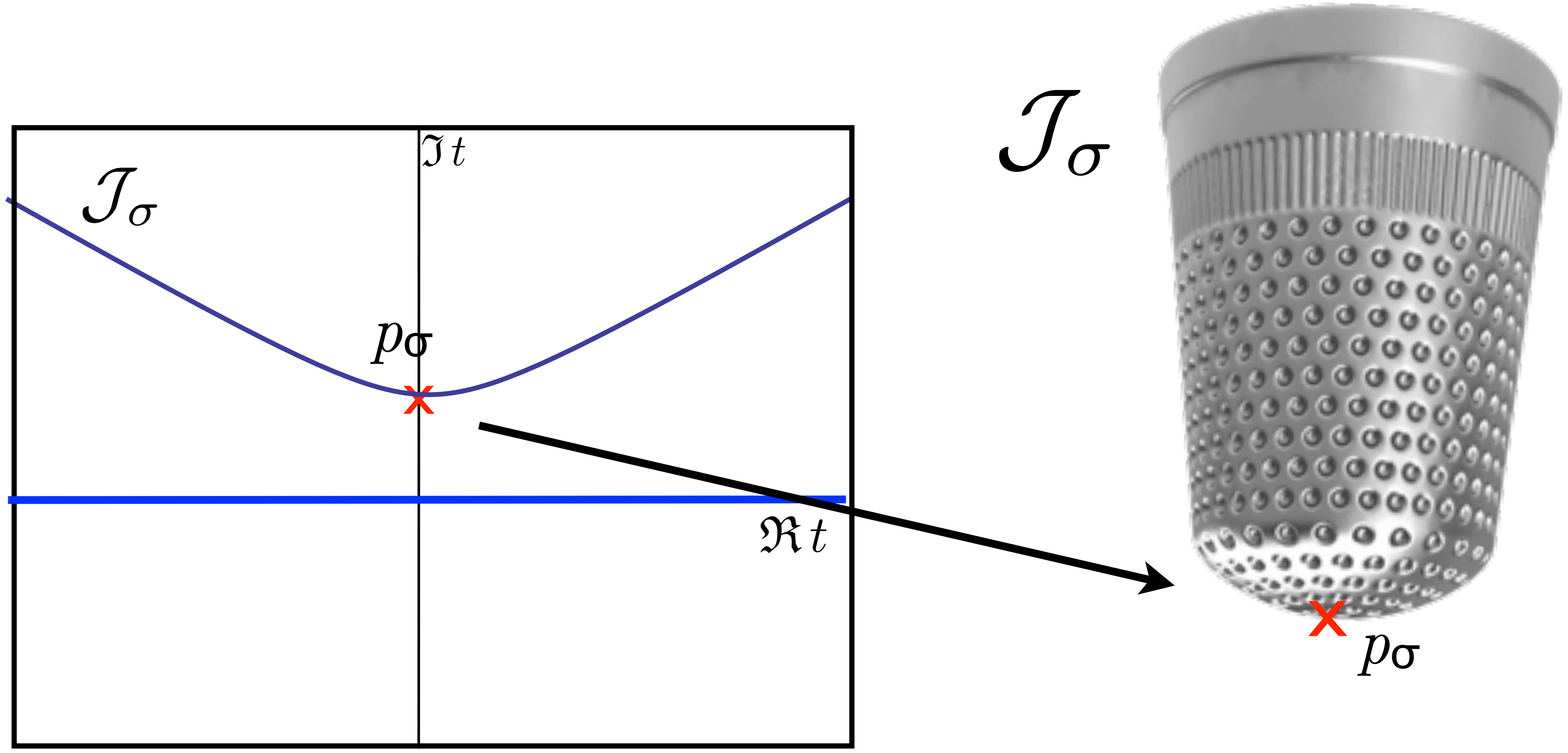

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Under suitable conditions on $f(x)$ and $g(x)$, **Morse theory** (Pham '83, Vassiliev '02, Nicolaescu '11, Witten '10) tells us that the timbles $\mathcal{J}_\sigma$ are smooth manifolds of real dimension n immersed in $\mathbb{C}^n$, and, for each cycle C, where the integral converges:

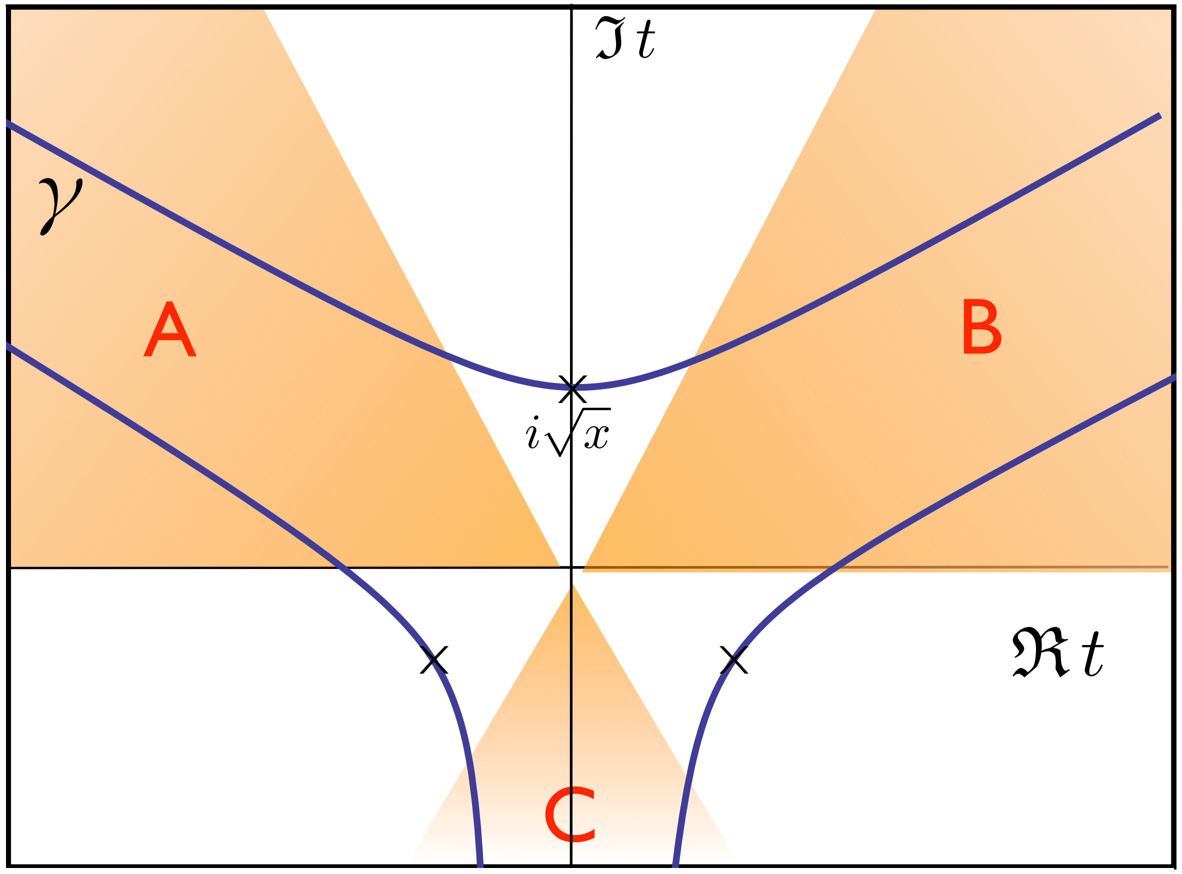
$$\int_{\mathcal{C}} dx\; g(x) e^{f(x)} = \sum_\sigma n_\sigma \int_{\mathcal{J}_\sigma} dz\; g(z) e^{f(z)}$$

i.e. the thimbles provide a **basis** of the relevant homology group, with integer coefficients.

$$\mathcal{C} = \sum_\sigma n_\sigma \mathcal{J}_\sigma$$

(in the homological sense)

E.g. The basis of 3 thimbles for the Airy integral.



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Any domain of integration for the Airy integral corresponds to a combination of these three with integer coefficients.

The path integral of a QFT?

Can we use the thimble basis to compute the path integral of a QFT?

$$\langle \mathcal{O} \rangle = \frac{\int_{\mathcal{C}} \prod_x d\phi_x \; e^{-S[\phi]} \mathcal{O}[\phi]}{\int_{\mathcal{C}} \prod_x d\phi_x \; e^{-S[\phi]}}$$

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In principle yes:

$$\langle \mathcal{O} \rangle = \frac{\sum_\sigma n_\sigma \int_{\mathcal{J}_\sigma} \, \prod_x d\phi_x \; e^{-S[\phi]} \mathcal{O}[\phi]}{\sum_\sigma n_\sigma \int_{\mathcal{J}_\sigma} \, \prod_x d\phi_x \; e^{-S[\phi]}}$$

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...but computing the contribution from all the thimbles is not realistic.

However, including all the thimbles corresponds to reproduce the original integral exactly.

Can we simplify it by choosing a **different regularization**?

Three arguments supporting this idea:

1. universality
2. thermodynamic limit
3. resurgence

1. Universality

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→ regularize the QFT on that single $\mathcal{J}_0$ attached to $\phi_{\text{glob-min}}$.

$$\mathcal{C} = \xcancel{\sum_{\sigma}} n_\sigma \mathcal{J}_\sigma \longrightarrow \mathcal{J}_0$$

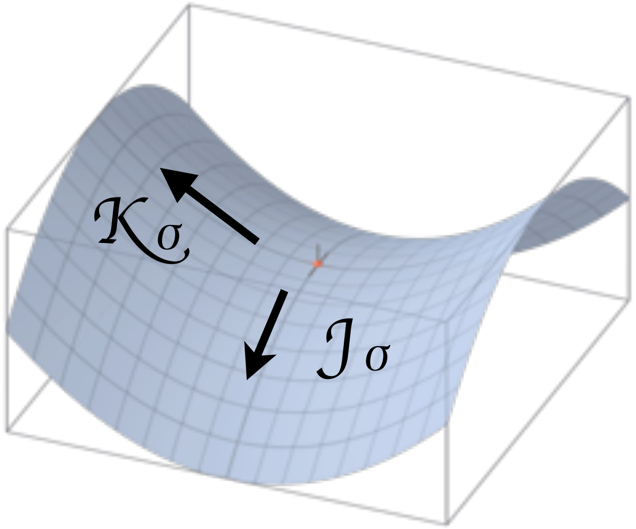
thimble attached to the global minimum of S_R

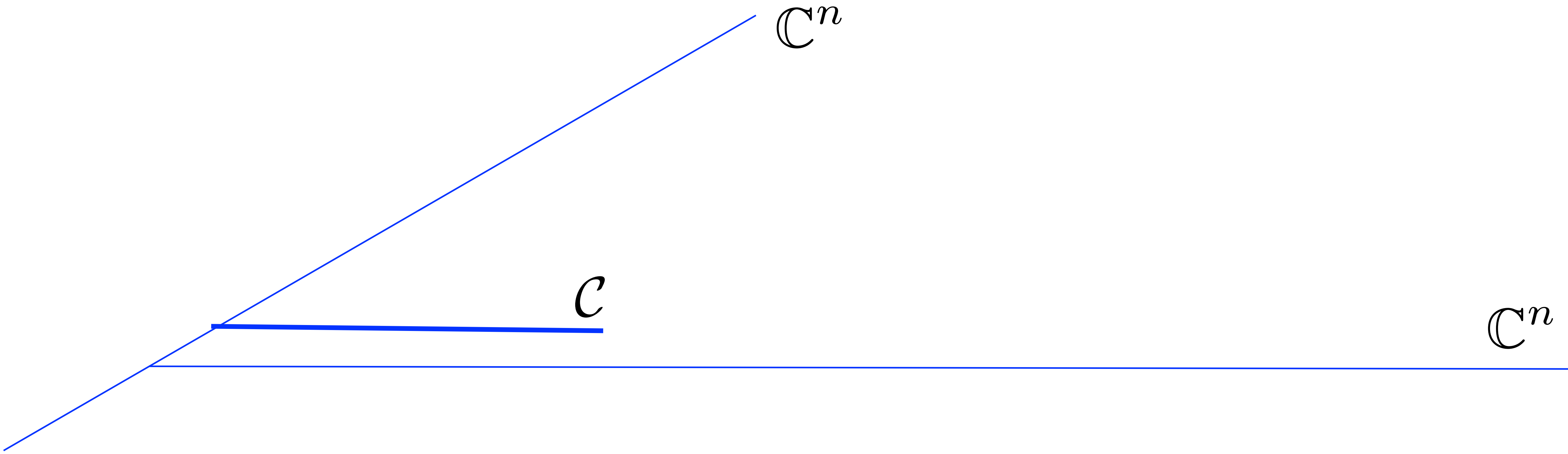
2. Thermodynamic argument and Morse Theory

(see Witten **arXiv:1001.2933**)

Remember the decomposition: $$\mathcal{C} = \sum_\sigma n_\sigma \mathcal{J}_\sigma$$

where $n_\sigma = \langle\, C, \mathcal{K}_\sigma \,\rangle$ are the intersection numbers between the original integration domain C and the dual thimbles $\mathcal{K}_\sigma$, defined as the union of the curves of steepest ascent.

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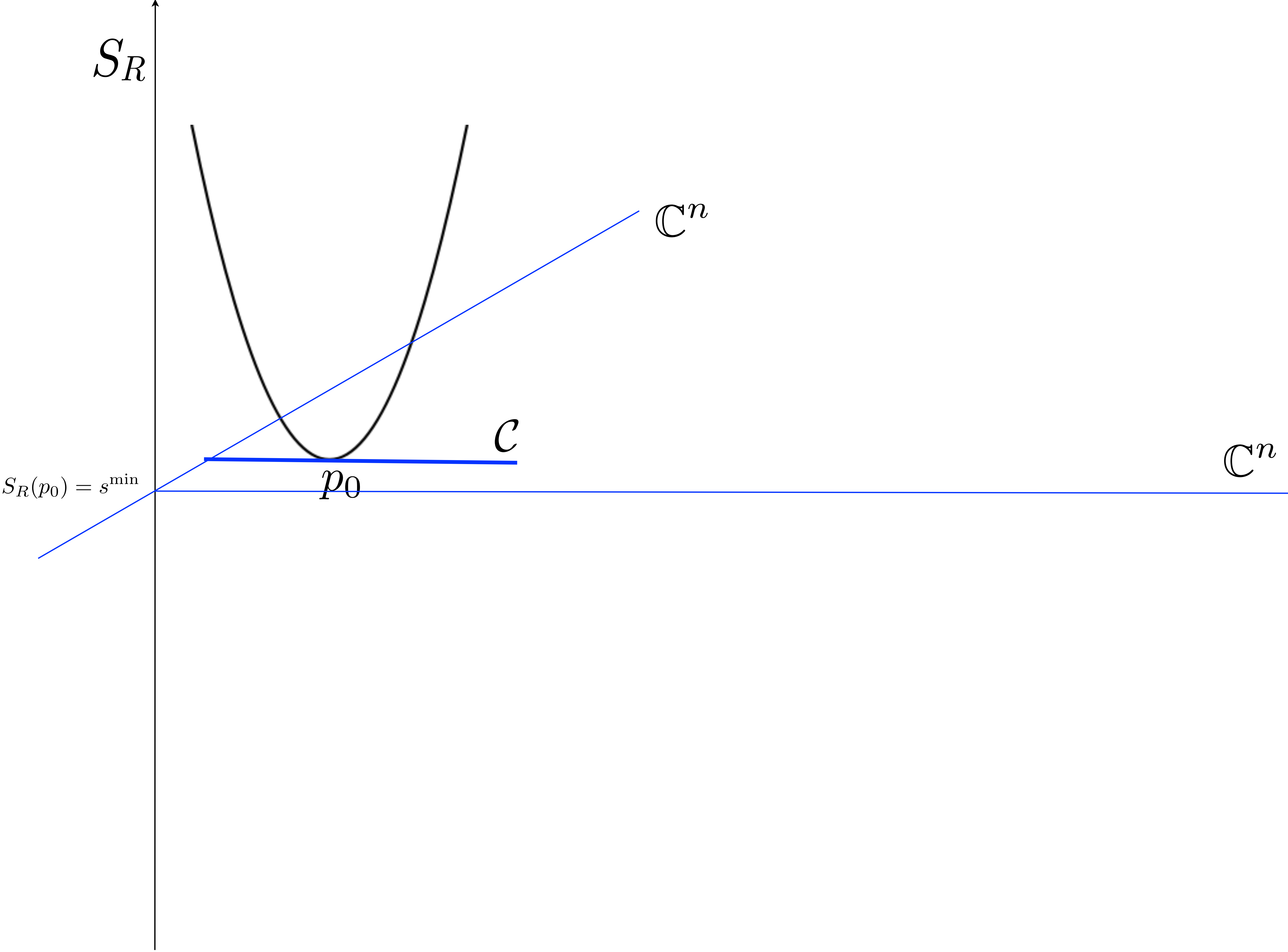
S_R
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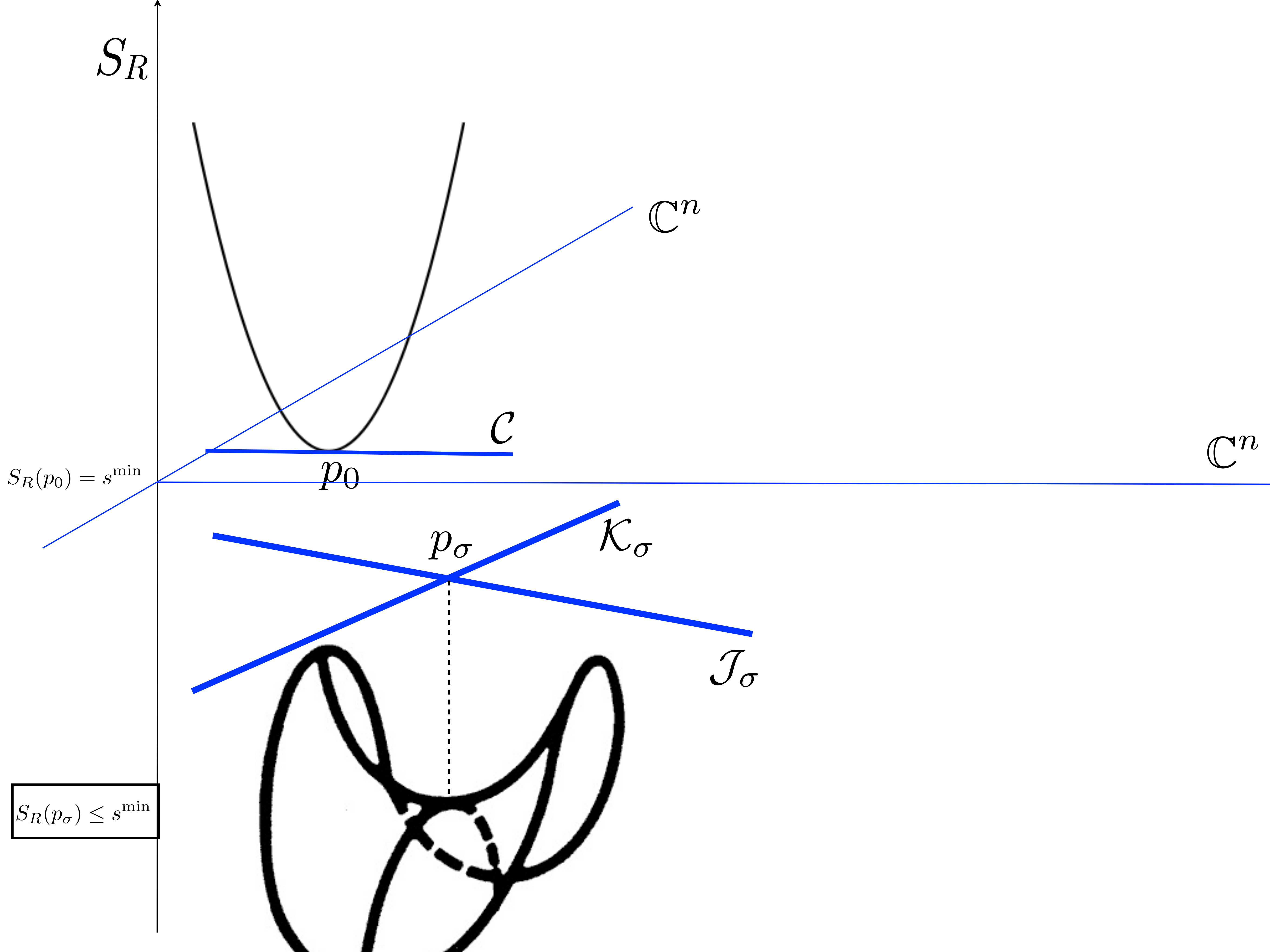
p_0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$\mathcal{K}_\sigma$
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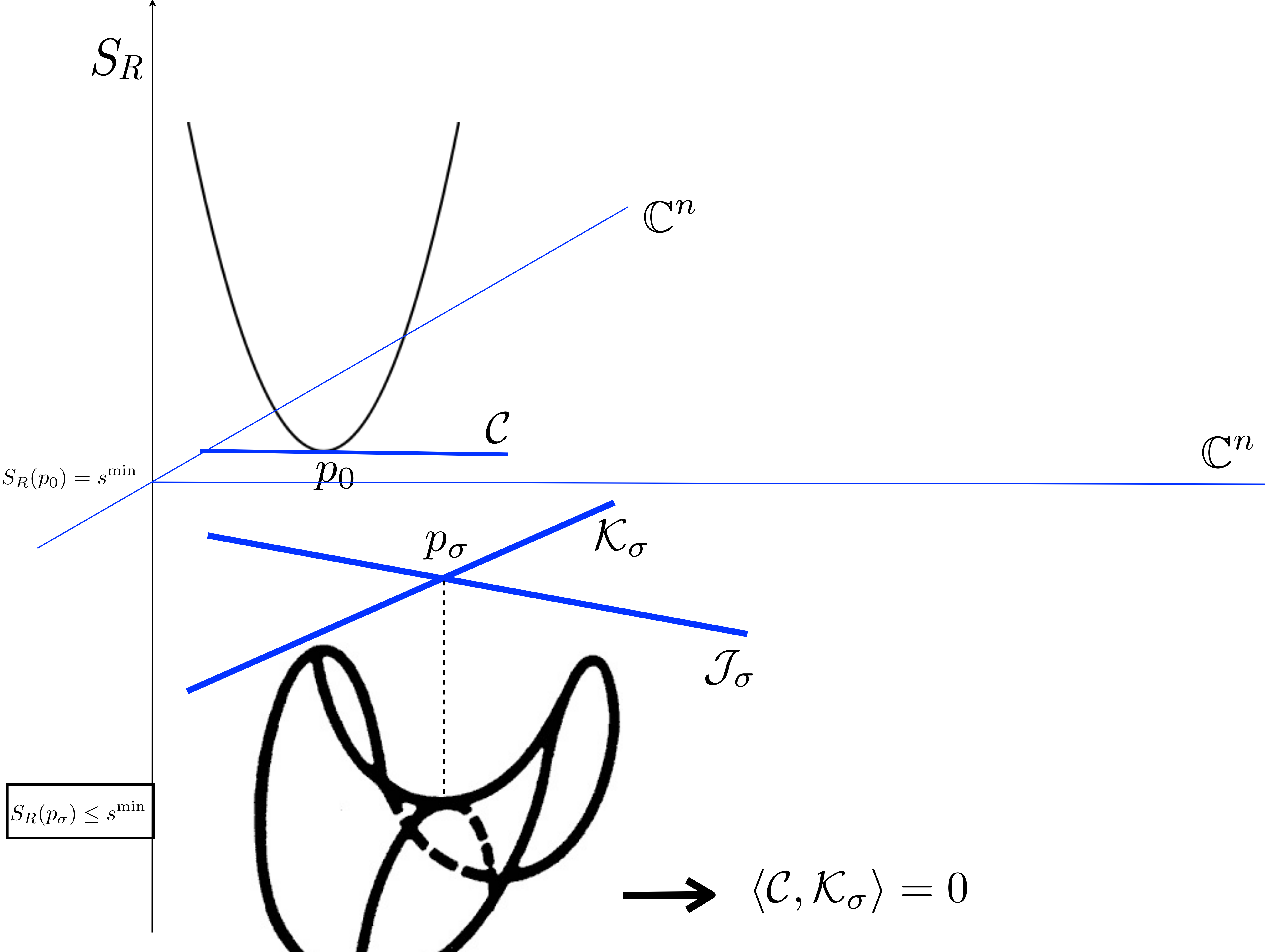
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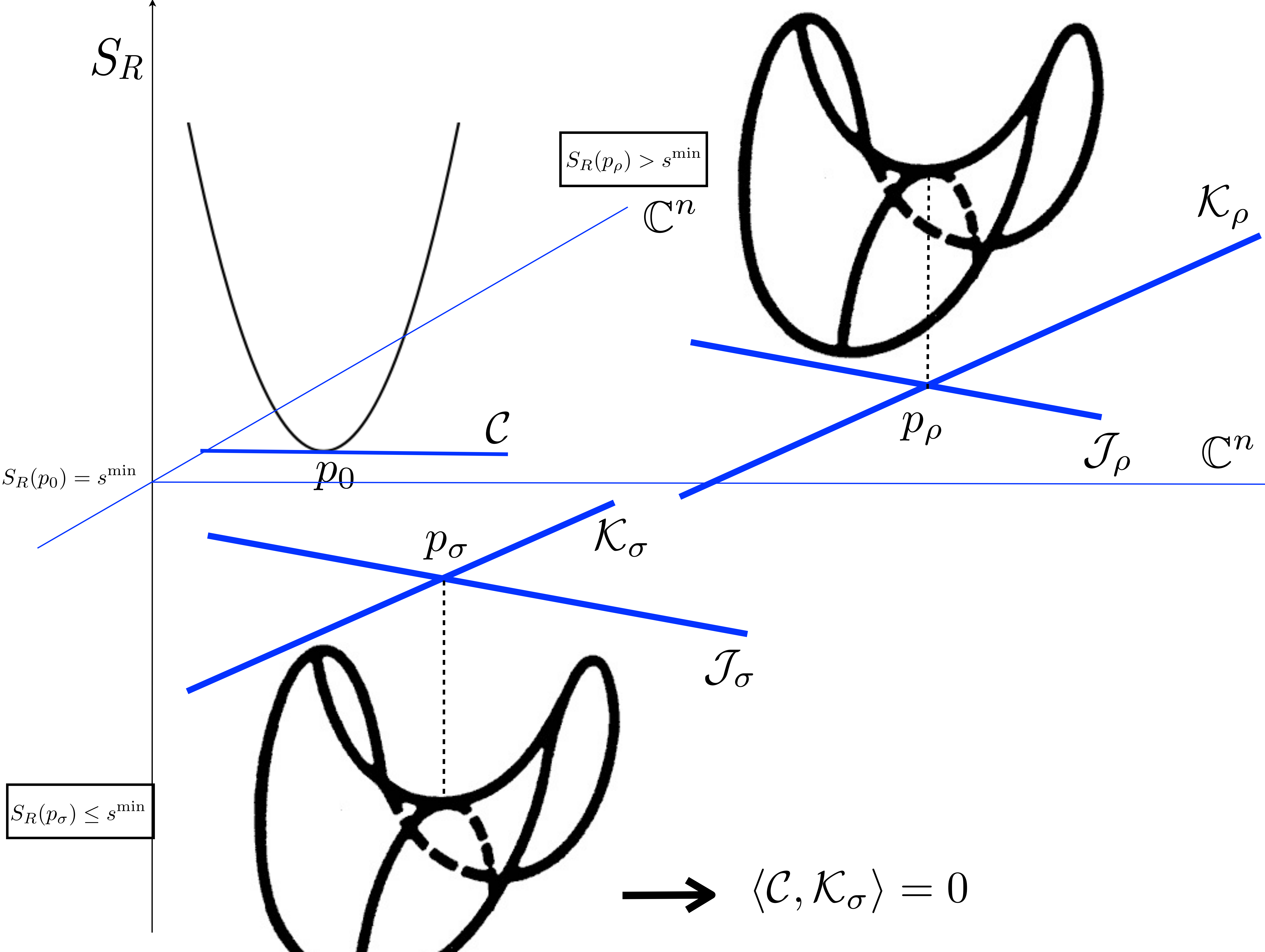
$\longrightarrow \langle \mathcal{C}, \mathcal{K}_\sigma \rangle = 0$


S_R
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p_ρ
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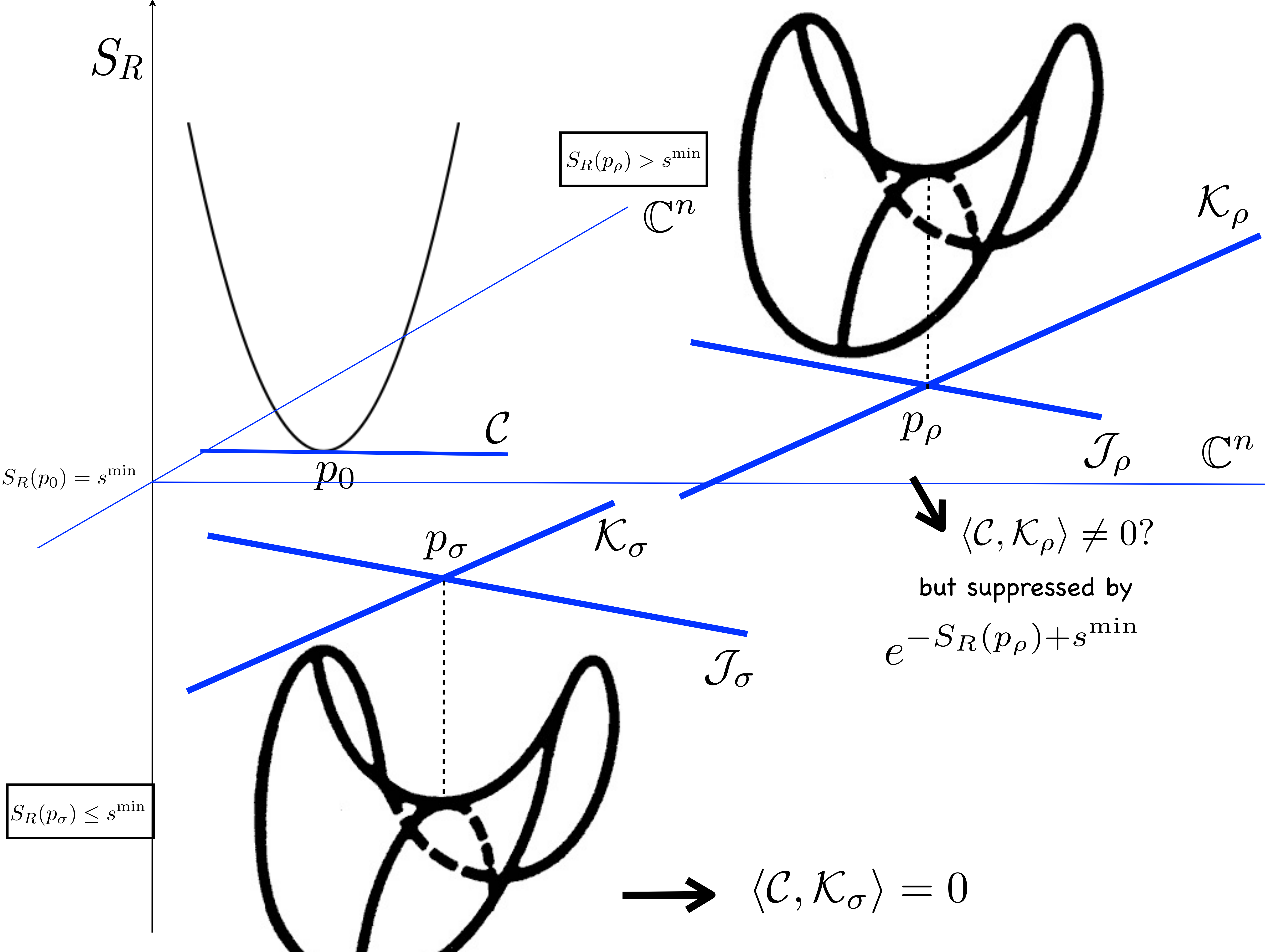
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$\langle \mathcal{C}, \mathcal{K}_\rho \rangle \neq 0?$
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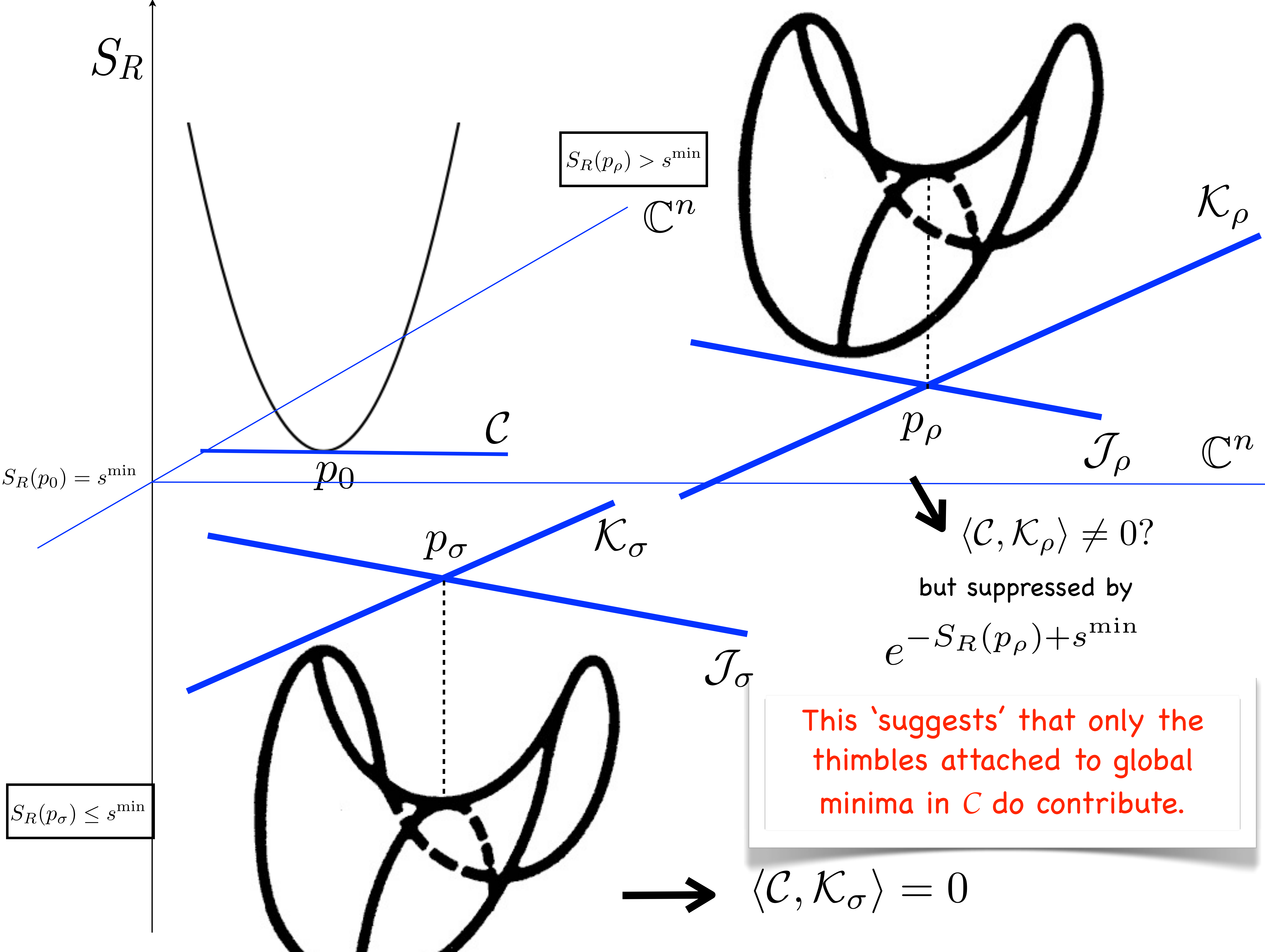

$\langle \mathcal{C}, \mathcal{K}_\rho \rangle \neq 0?$

but suppressed by

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This 'suggests' that only the thimbles attached to global minima in C do contribute.

$\langle \mathcal{C}, \mathcal{K}_\sigma \rangle = 0$

3. Resurgence

See Guralnik et al (hep-th/9612079, 0710.1256, 1301.4233) and Basar Dunne Unsal - 1308.1108

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(Open question: how to formulate Reflection Positivity here?)

II. A Monte Carlo algorithm for a Lefschetz thimble?

Langevin Algorithm on a thimble

I want to compute:

$$\frac{1}{Z_0}\int_{\mathcal{J}_0}\prod_x d\phi_x\; e^{-S[\phi]}\mathcal{O}[\phi]$$

Langevin Algorithm on a thimble

Constant on $\mathcal{J}_0$!

I want to compute:

$$\frac{1}{Z_0}e^{\boxed{-iS_I}}\int_{\mathcal{J}_0}\prod_x d\phi_x \; e^{-S_R[\phi]}\mathcal{O}[\phi]$$

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Constant on $\mathcal{J}_0$!

Bounded from below on $\mathcal{J}_0$!

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Bounded, real action: use MC.
E.g. Langevin algorithm

$$\frac{d}{d\tau}\phi^{(R)}_{a,x} = -\frac{\delta S_R}{\delta \phi^{(R)}_{a,x}} + \eta^{(R)}_{a,x}$$

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Langevin Algorithm on a thimble

I want to compute:

$$\frac{1}{Z_0} e^{\overset{\text{Constant on } \mathcal{J}_0\,!}{\boxed{-iS_I}}} \int_{\mathcal{J}_0} \prod_x d\phi_x \; e^{\overset{\text{Bounded from below on } \mathcal{J}_0\,!}{\boxed{-S_R[\phi]}}} \mathcal{O}[\phi]$$

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How can I stay in $\mathcal{J}_0$?

Langevin Algorithm on a thimble

Constant on $\mathcal{J}_0$!

Bounded from below on $\mathcal{J}_0$!

I want to compute:

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action: use MC.
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... unless we think in 5D!!

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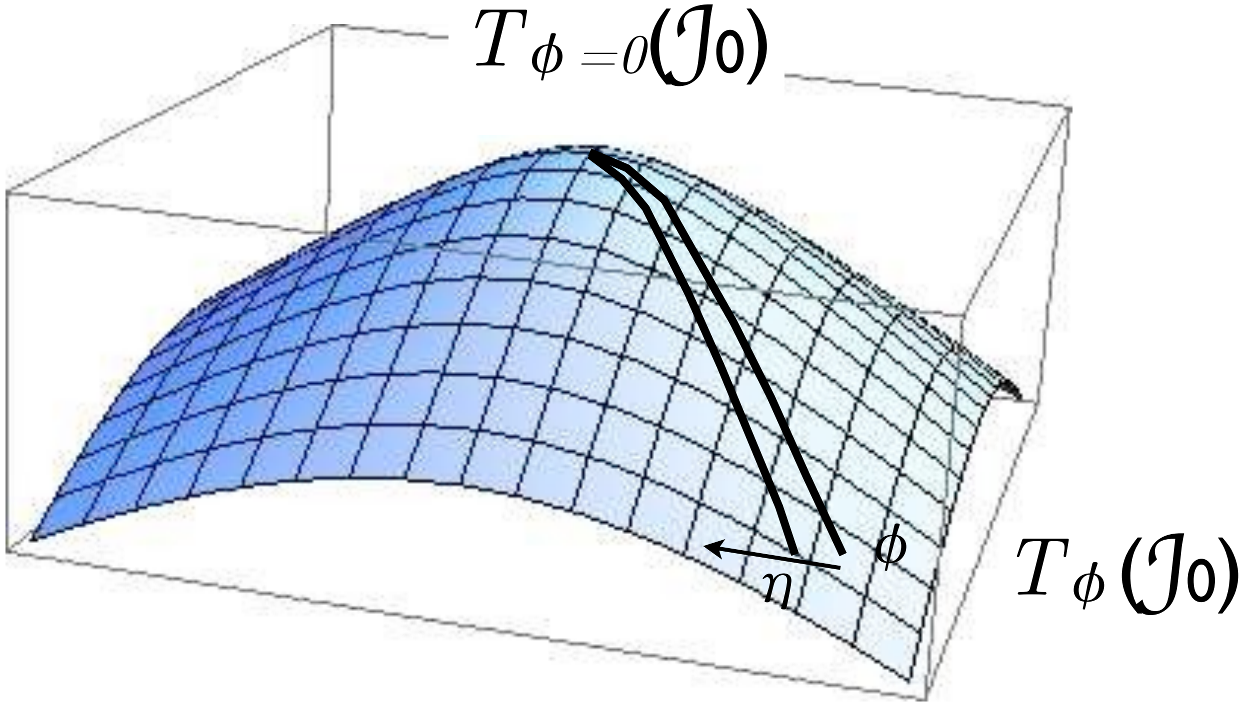

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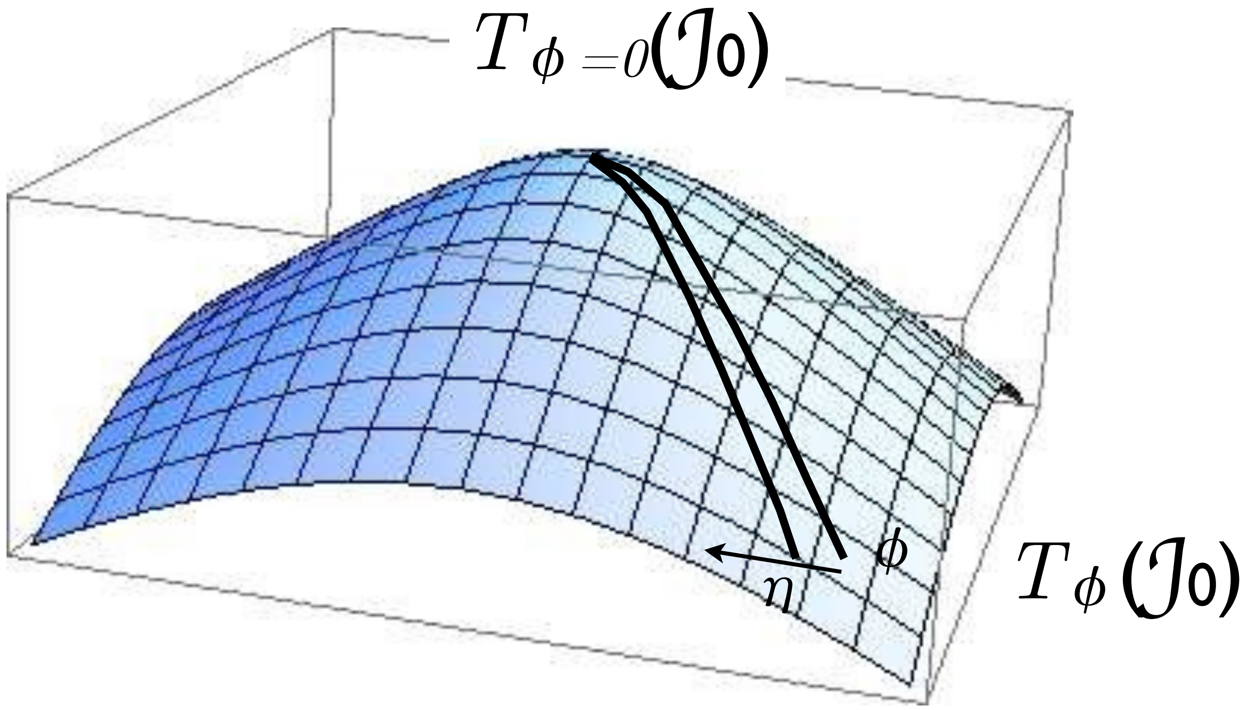

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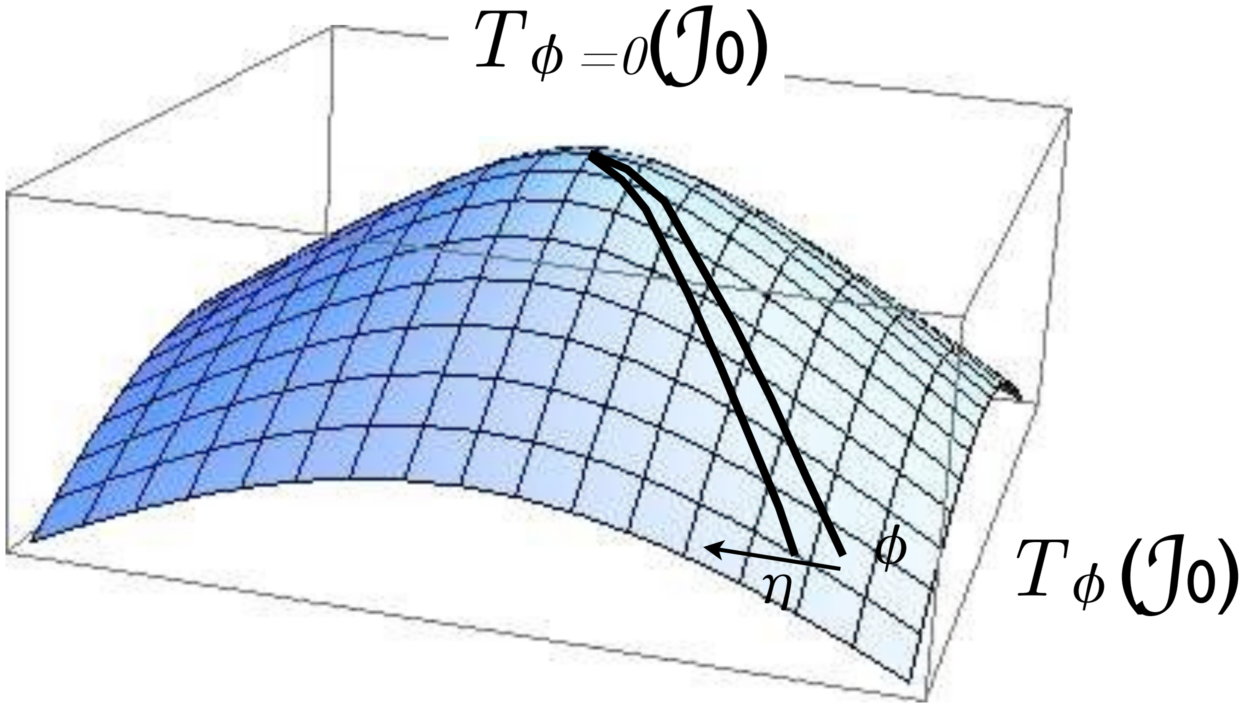

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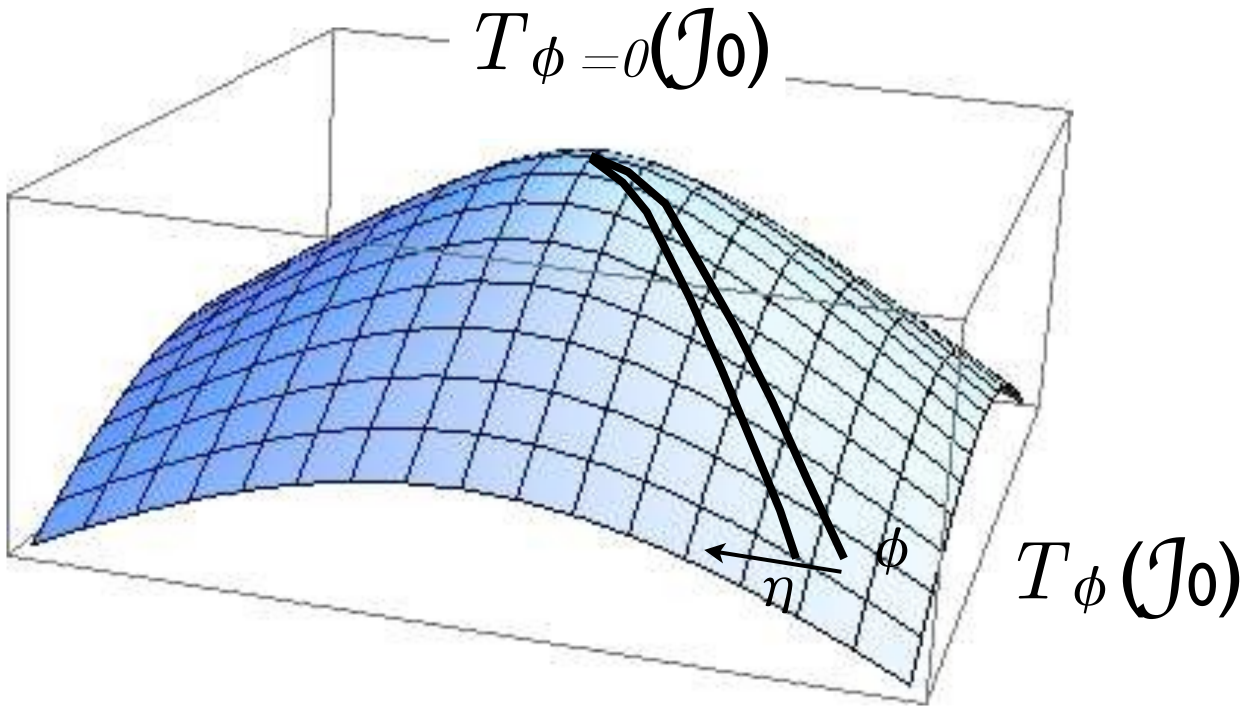

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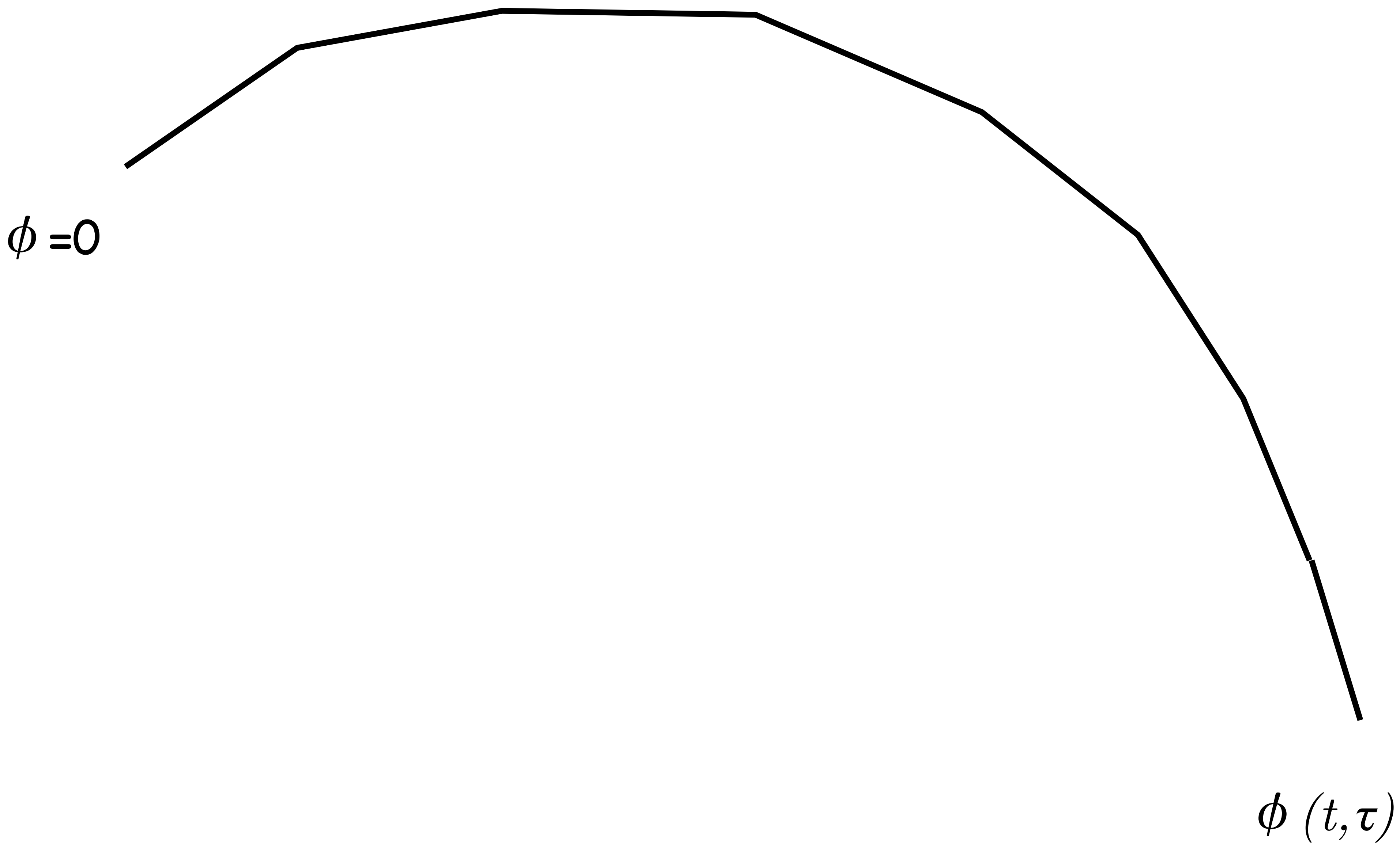
Which also leads to a simple prescription to compute η:

$$0 = [\partial S_R, \eta(\tau)]_k = \sum_j \partial_j S_R \partial_j \eta_k(\tau) - \sum_j \eta_j(\tau) \partial_j \partial_k S_R$$

$$\Leftrightarrow \boxed{\frac{d}{d\tau}\eta_j(\tau) = \sum_k \eta_k(\tau) \partial_k \partial_j S_R,}$$

Graphical summary of a Langevin step



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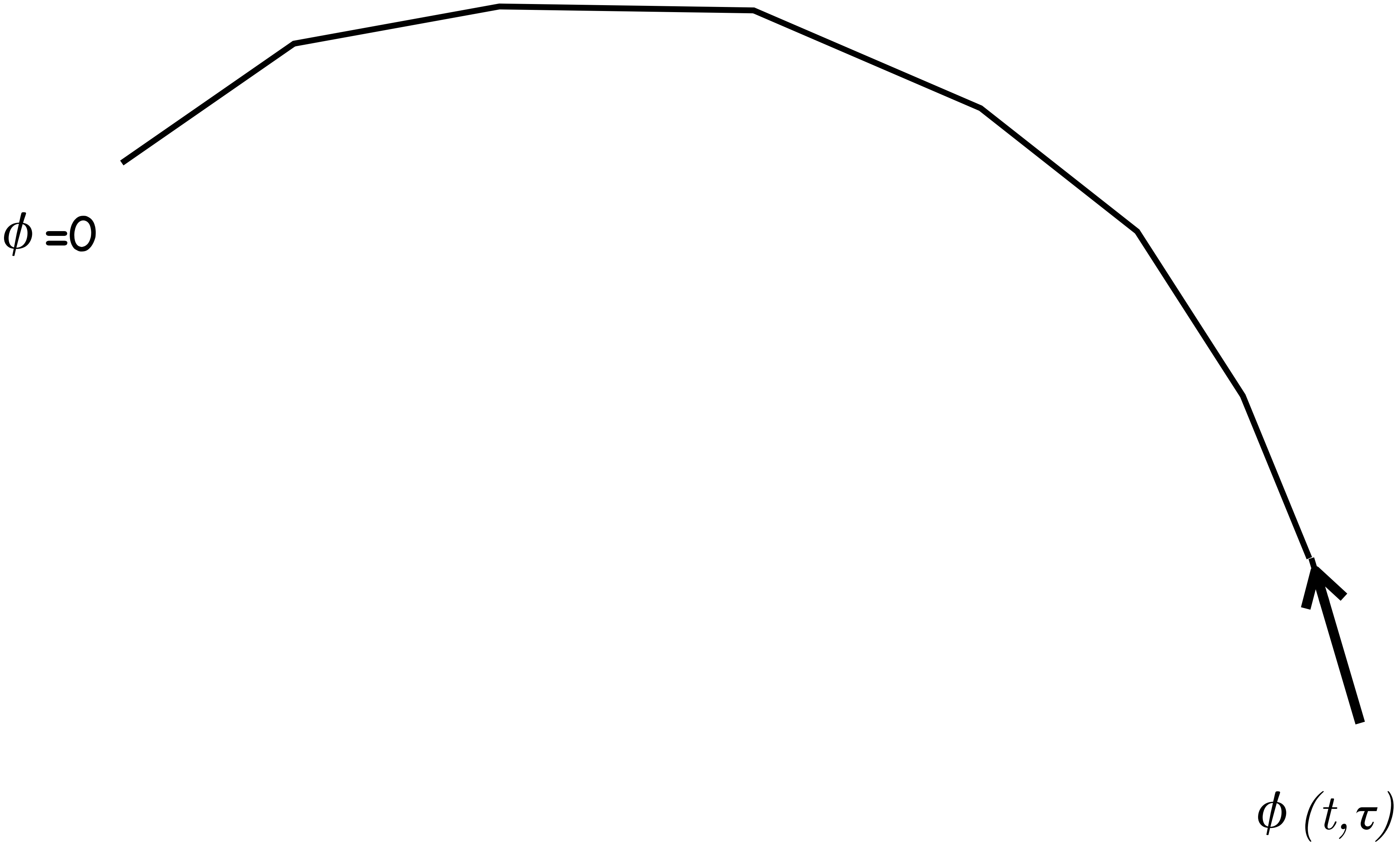

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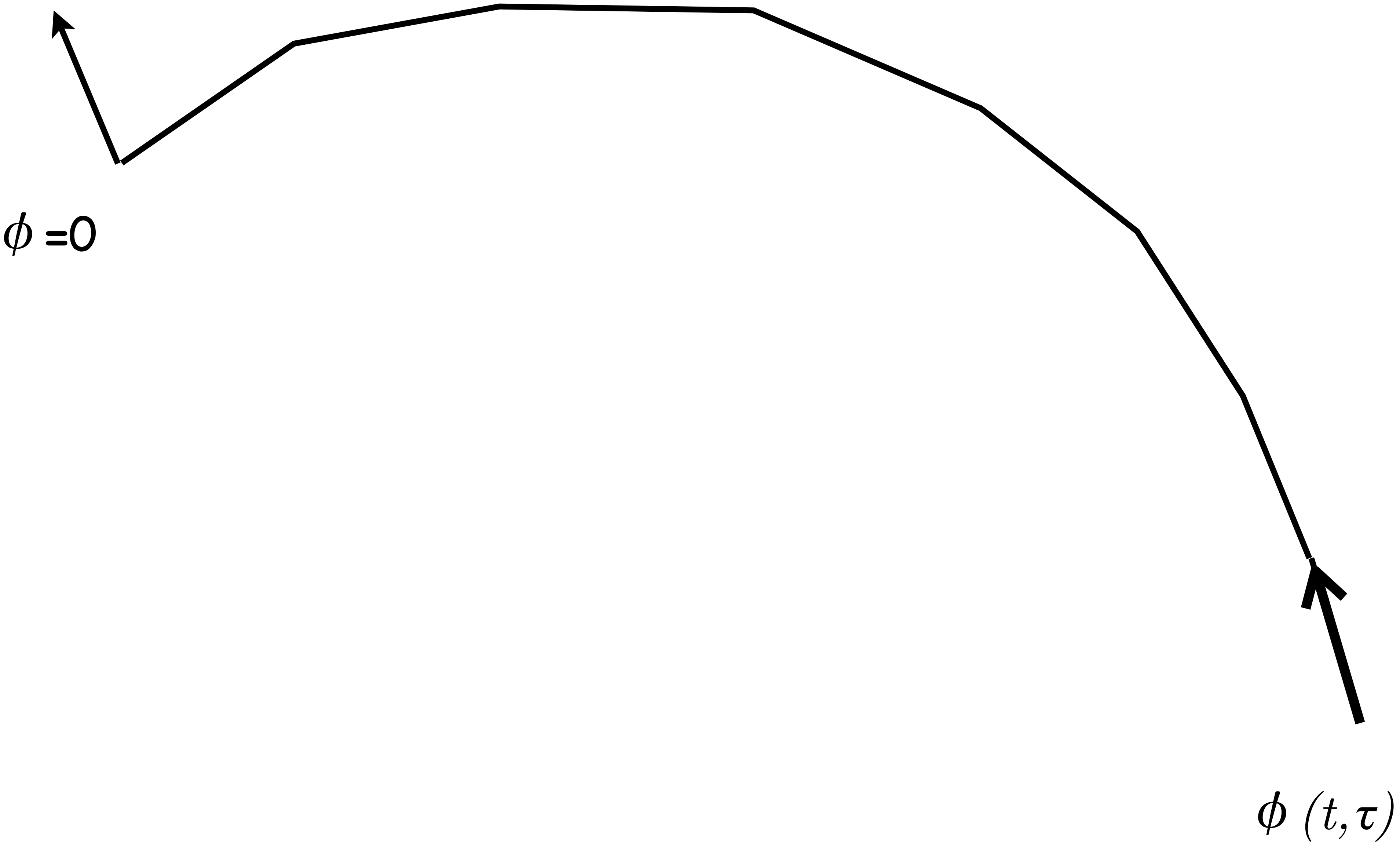

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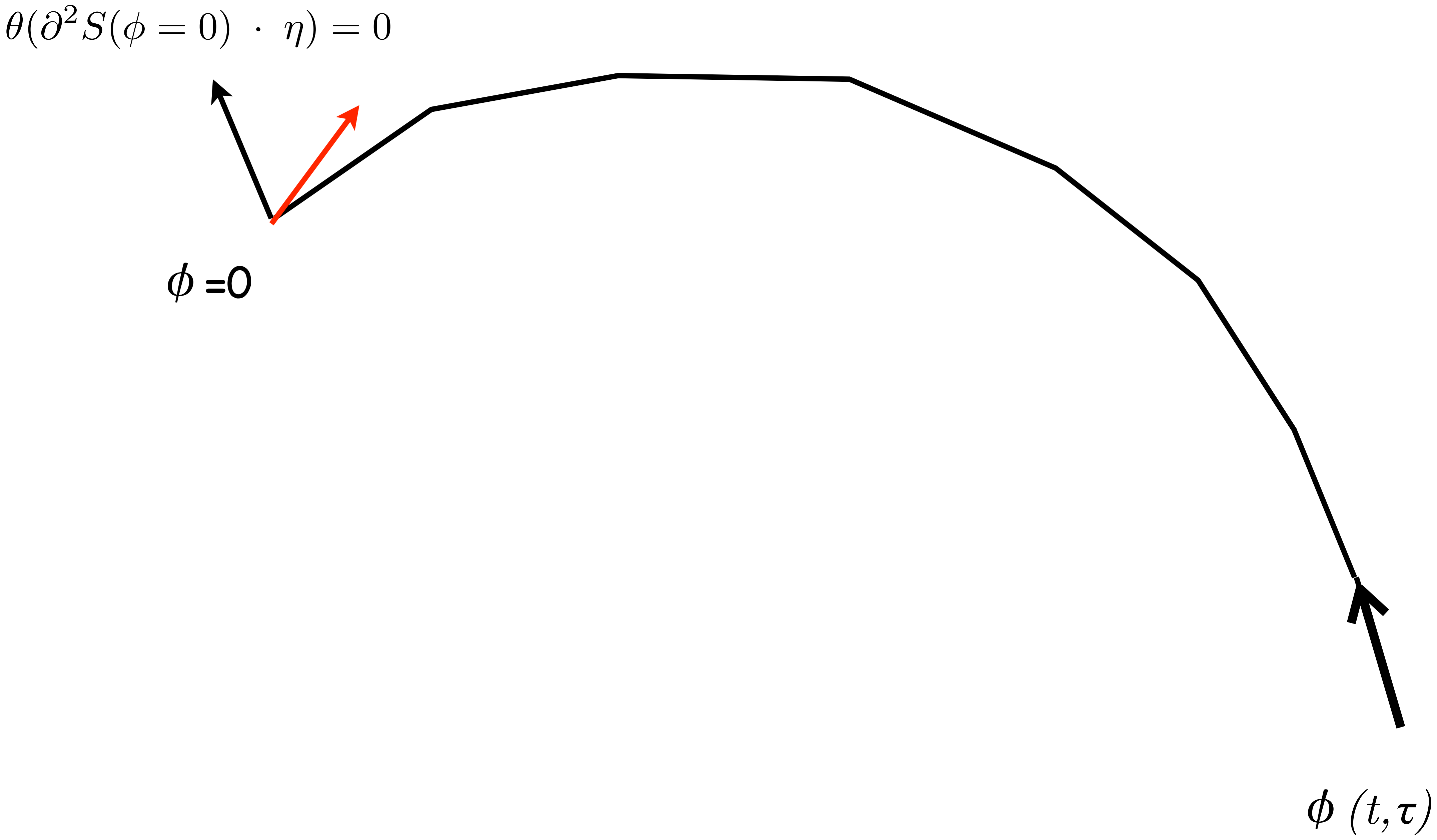

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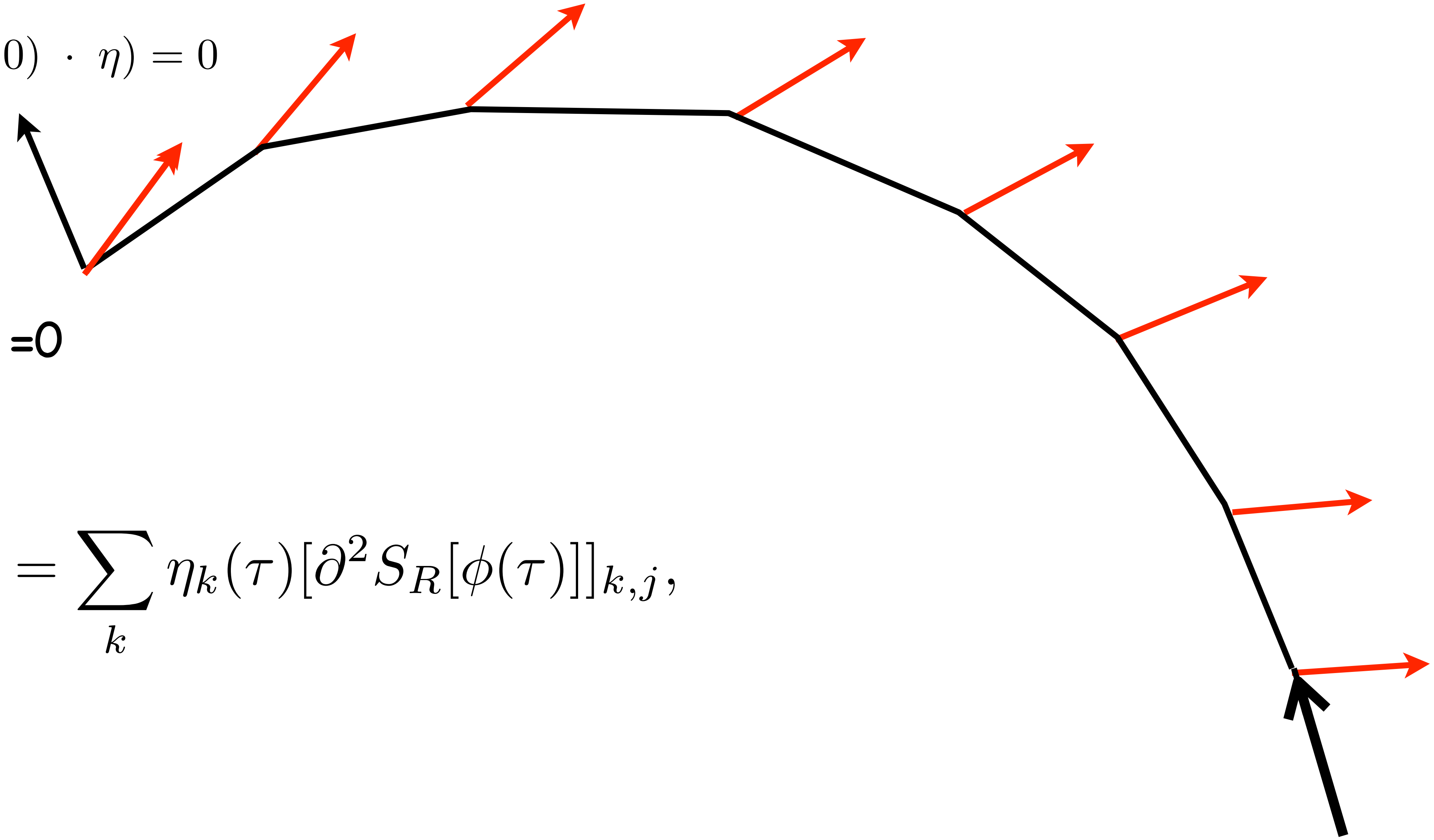

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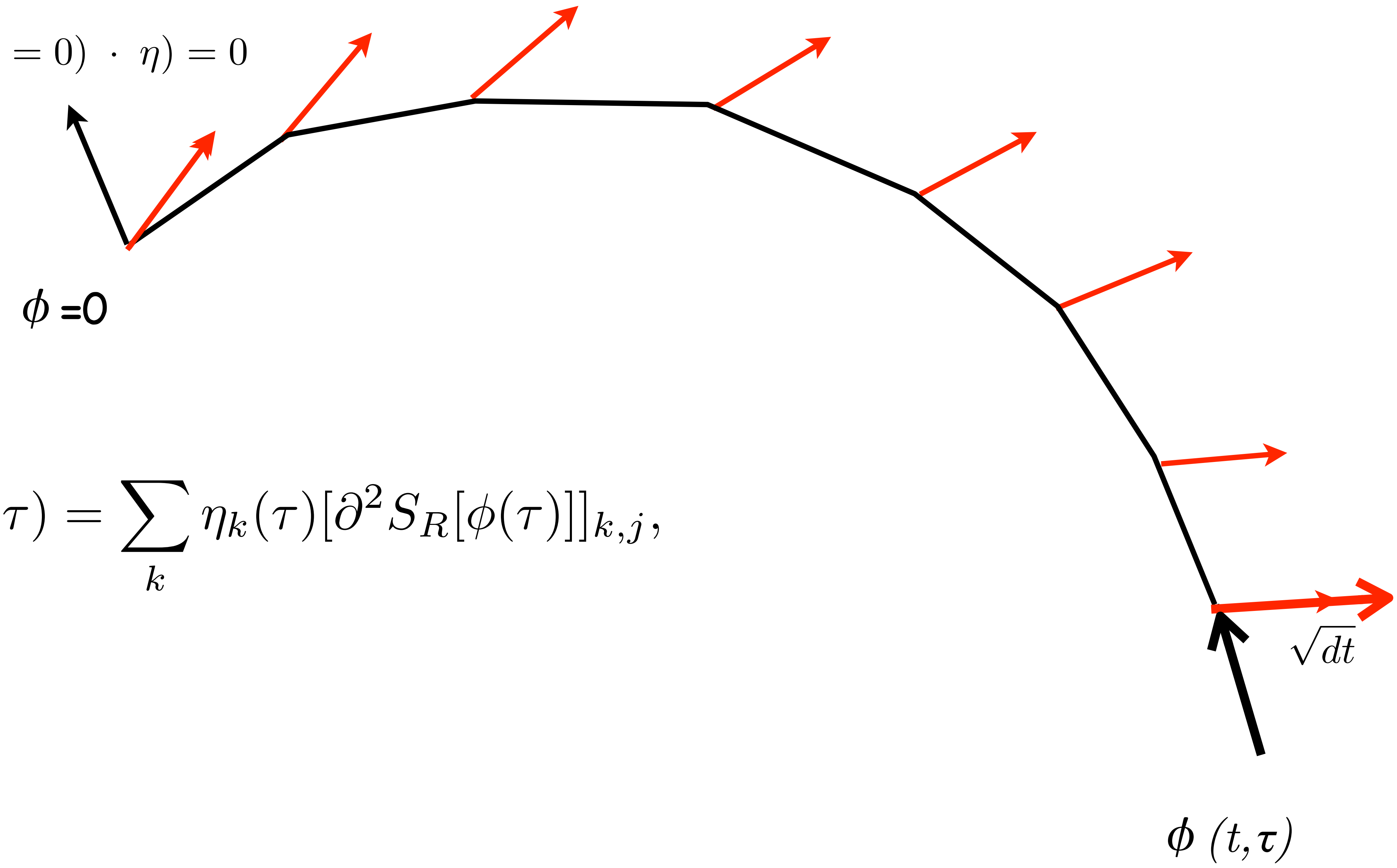

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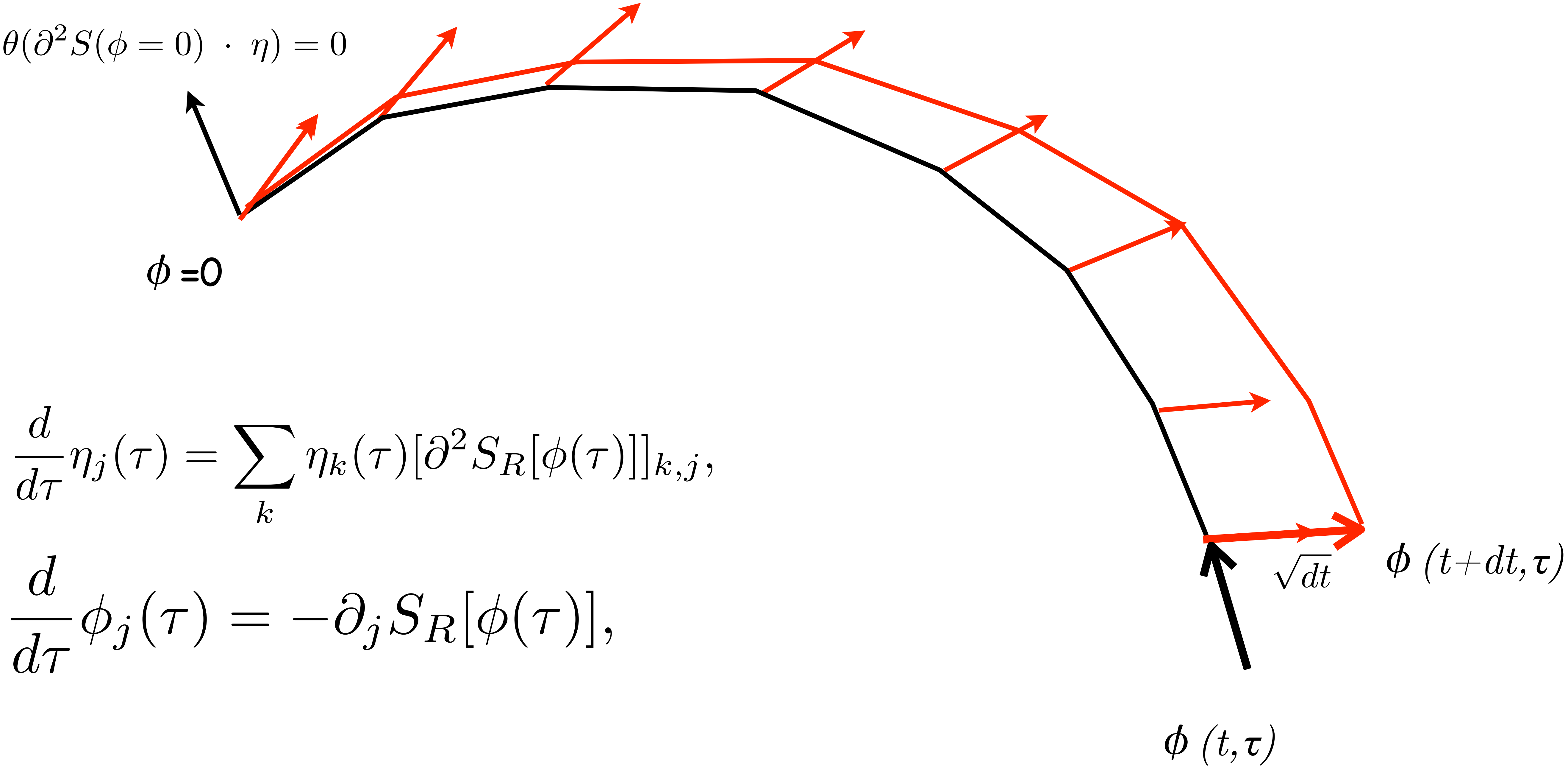

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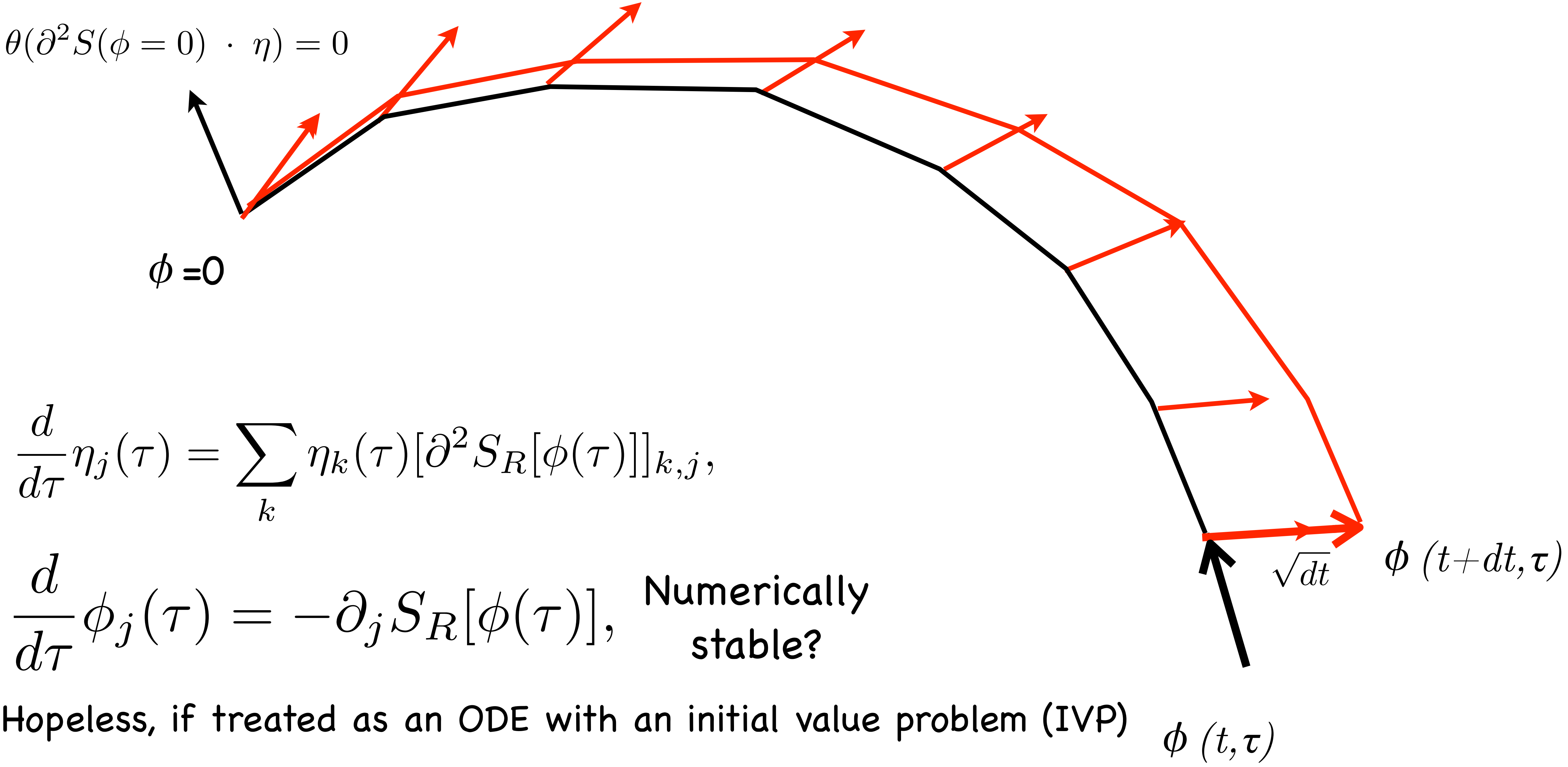

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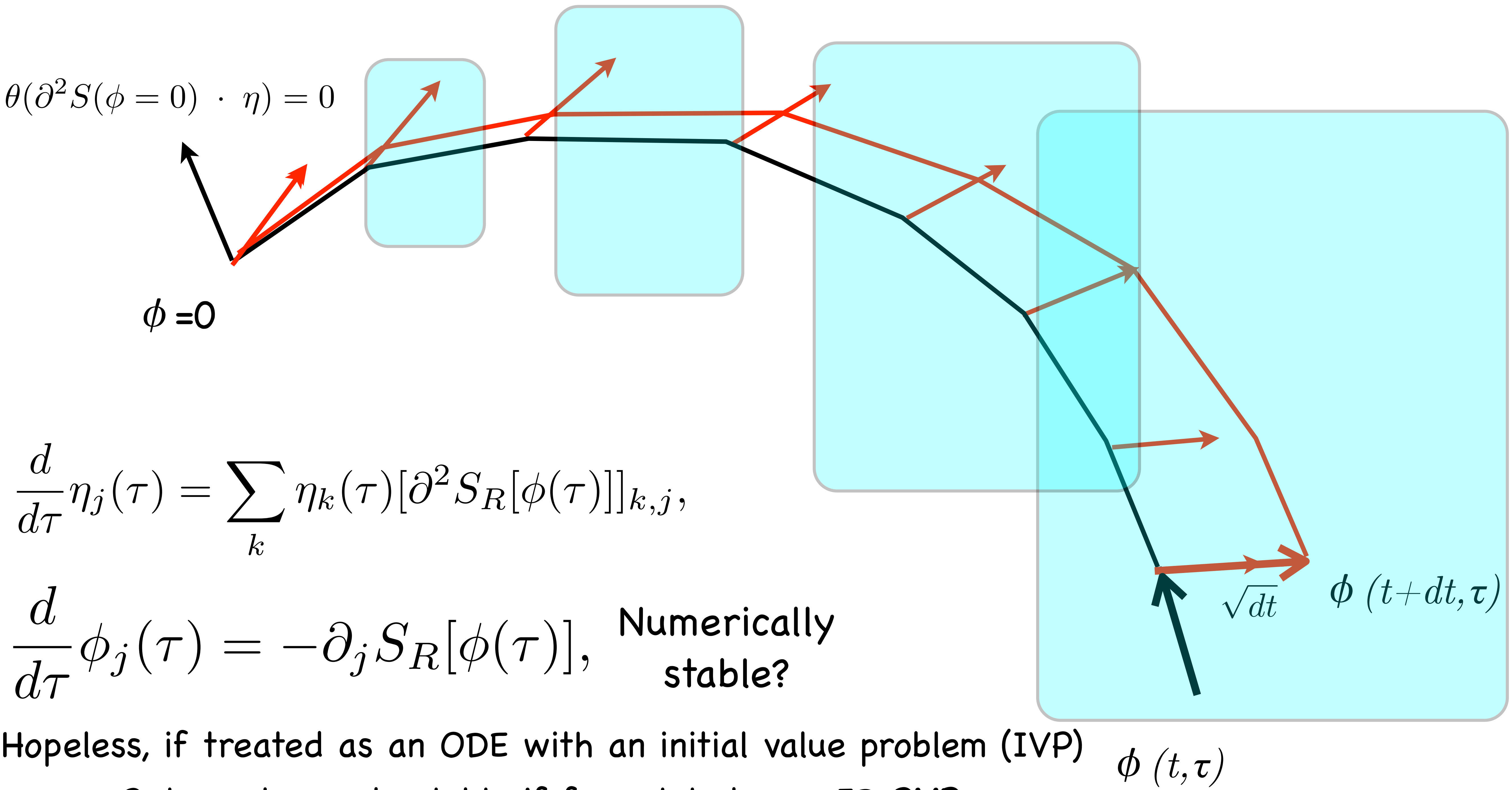

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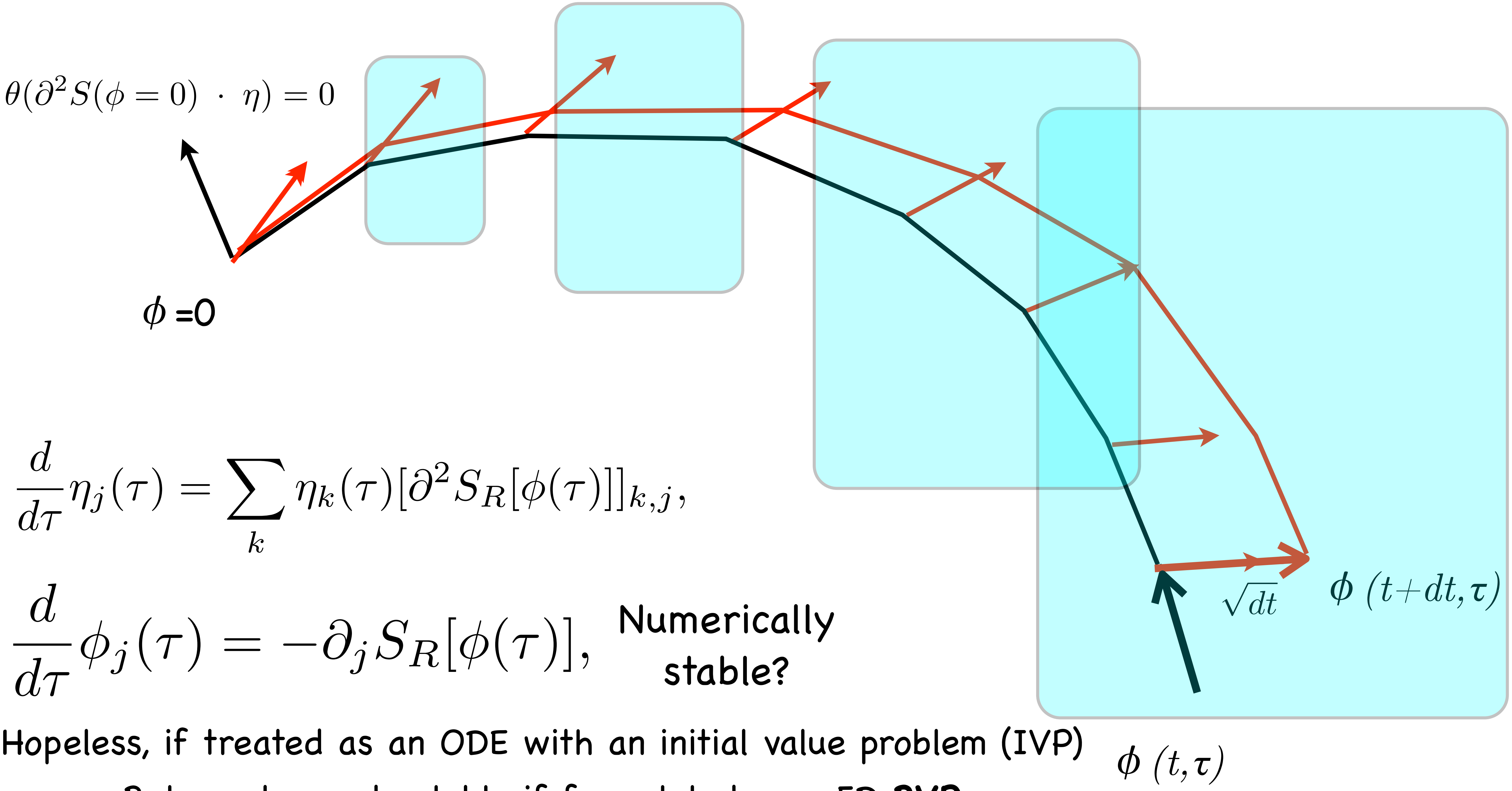

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How long needs the 5th dimension be? Test it!

Residual phase

As noticed at the beginning, there is still a phase

$$\frac{1}{Z_0}\int_{\mathcal{J}_0} \boxed{\prod_x d\phi_x}\, e^{-S_R[\phi]}\mathcal{O}[\phi]$$

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Is there an efficient way to compute it?

$$\log\det T_{\phi_s}\big|_{s=\tau_0}^{s=\tau} = i\int_{\tau_0}^{\tau} ds\,\frac{1}{N_R}\sum_{r=1}^{N_R}\eta^{(r)T}\,JH(s)\,\eta^{(r)}$$

Cost is linear in Volume and N_R (noisy estimators η). Quadratic in τ.

(Currently being tested)

III. The Bose gas

Let me discuss a simple model,
which already contains most of the interesting aspects

A complex scalar field with U(1) symmetry

$$S = \int d^4x[|\partial\phi|^2 + (m^2-\mu^2)|\phi|^2 + \boxed{\mu j_0} + \lambda|\phi|^4] \qquad j_\nu := \phi^* \overleftrightarrow{\partial_\nu} \phi$$

When μ≠0, the action is not real, Re[exp[-S]] is not positive and we have a sign problem.

E.g.: U(1) Symmetry

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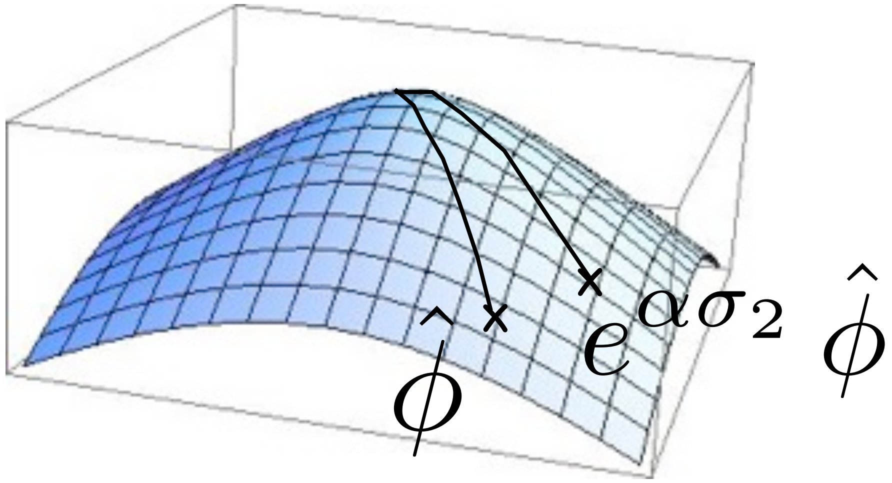
⇒ The symmetry transformations are well defined on the thimble.

⇒ This can be used to prove Ward Identities.



Perturbation Theory

One might expect PT on the thimble to be very complicated...
Instead, it is not difficult to compare the PT of the two formulations.
Here there are more terms.

$$\frac{d^p}{d\lambda^p}\left(\int_{\mathcal{J}_0(\lambda,\mu)} d\phi\; e^{-S[\phi;\lambda,\mu]}\mathcal{O}_{\lambda,\mu}[\phi]\right)_{|\lambda=0}$$

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↘

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ordinary PT

It is a **gaussian** integral (...) performed along the path of steepest descent. This coincides with the original integral as long as the latter is convergent (gaussian integrals have just one nontrivial class)

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 & \frac{d^p}{d\lambda^p}\left(\int_{\mathcal{J}_0(\lambda,\mu)} d\phi\; e^{-S[\phi;\lambda,\mu]}\mathcal{O}_{\lambda,\mu}[\phi]\right)_{|\lambda=0} \arrow[dl] \arrow[dr] & \\
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0 & & \text{ordinary PT}
\end{tikzcd}$$

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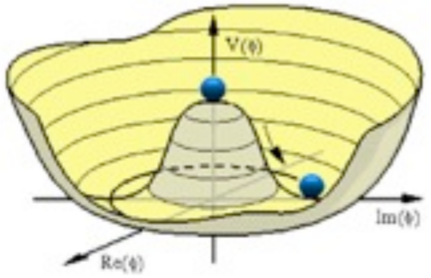
Spontaneous Symmetry Breaking with Mexican Hat Potential



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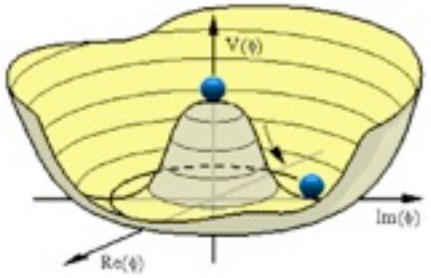

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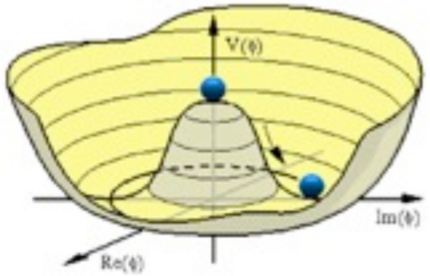

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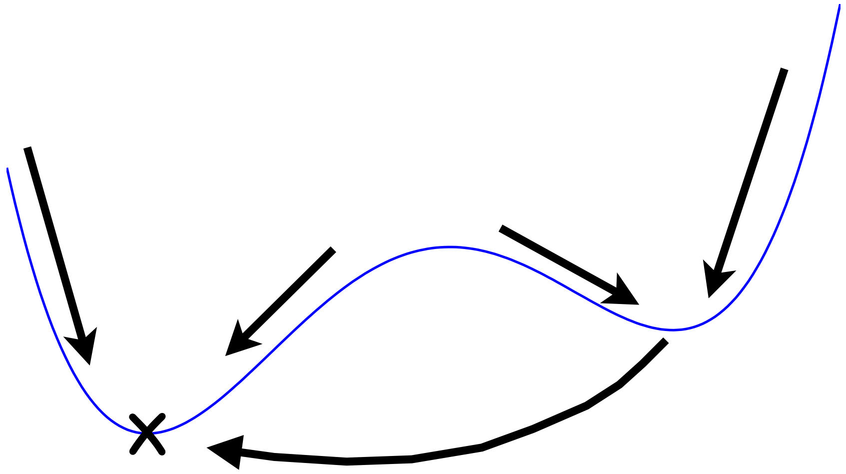

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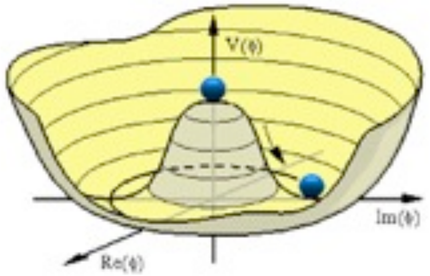

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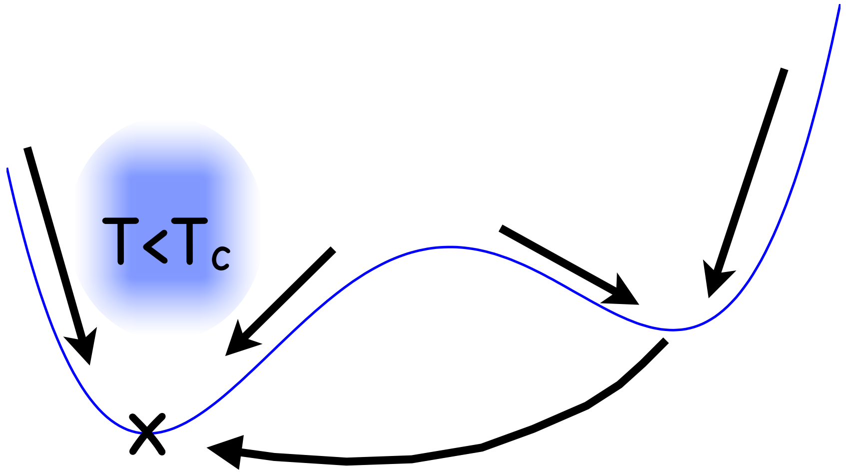

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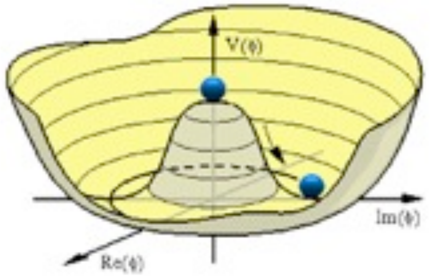

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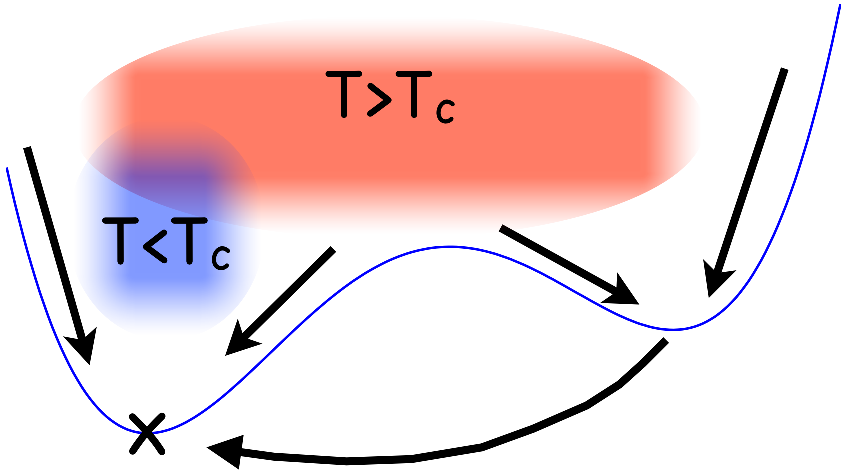

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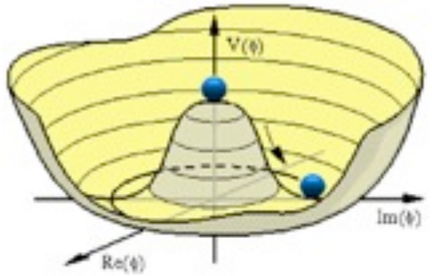

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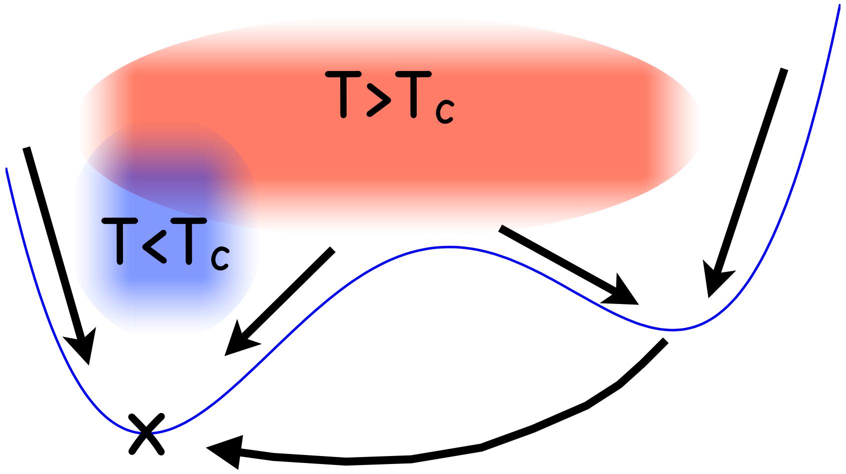

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(PT is again correct, since we also want to do PT around one of these global minima)

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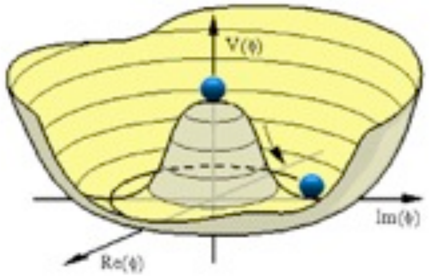

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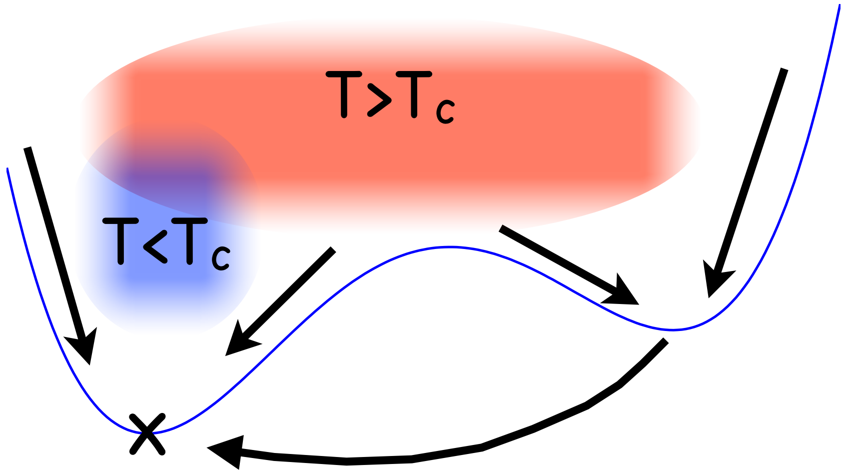


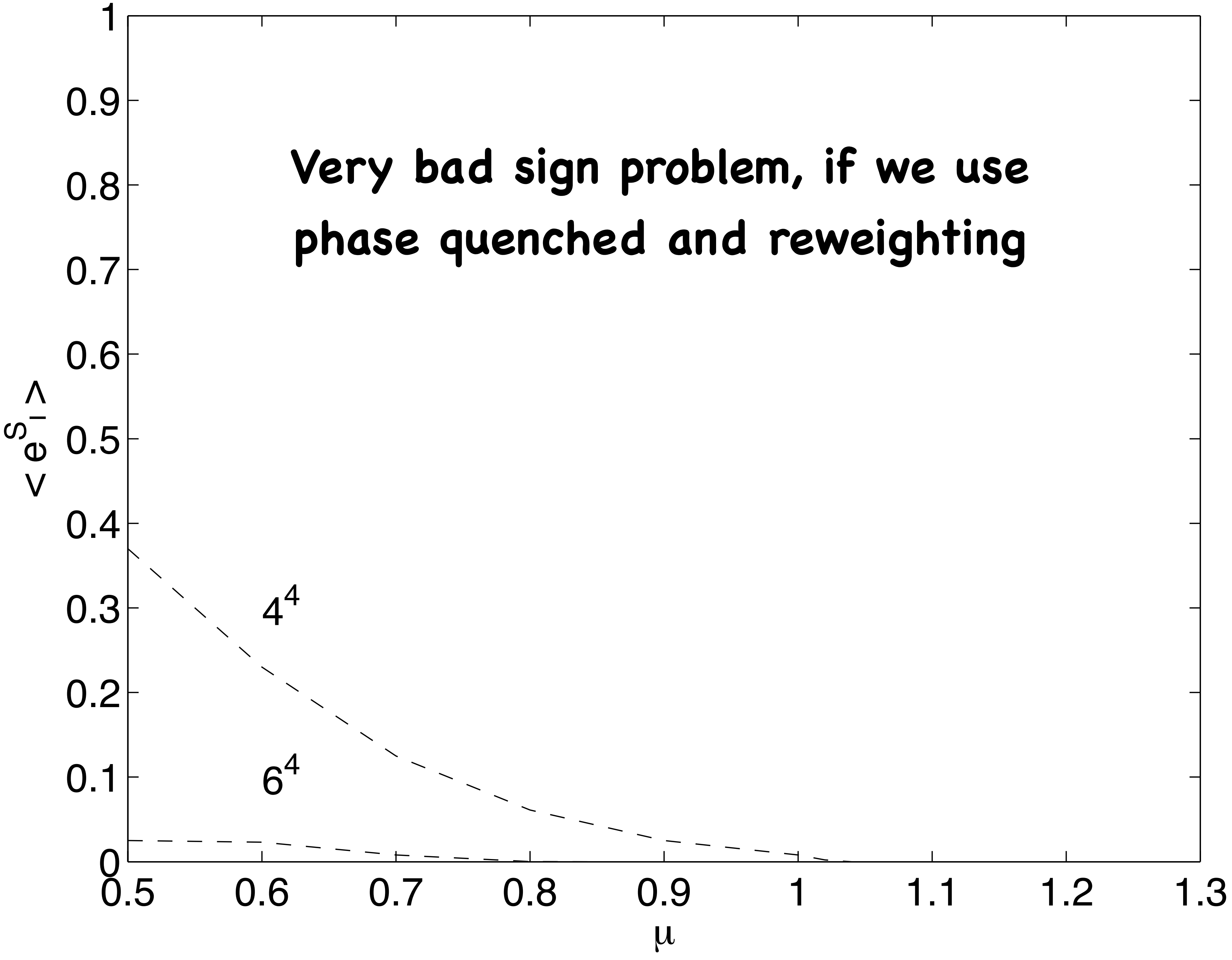
SSB is a dynamical question!

(PT is again correct, since we also want to do PT around one of these global minima)

(there is also another way to deal with symmetries. See gauge theories)

The sign problem in the Bose gas

(the complex scalar field with U(1) symmetry seen before)



m=λ=1

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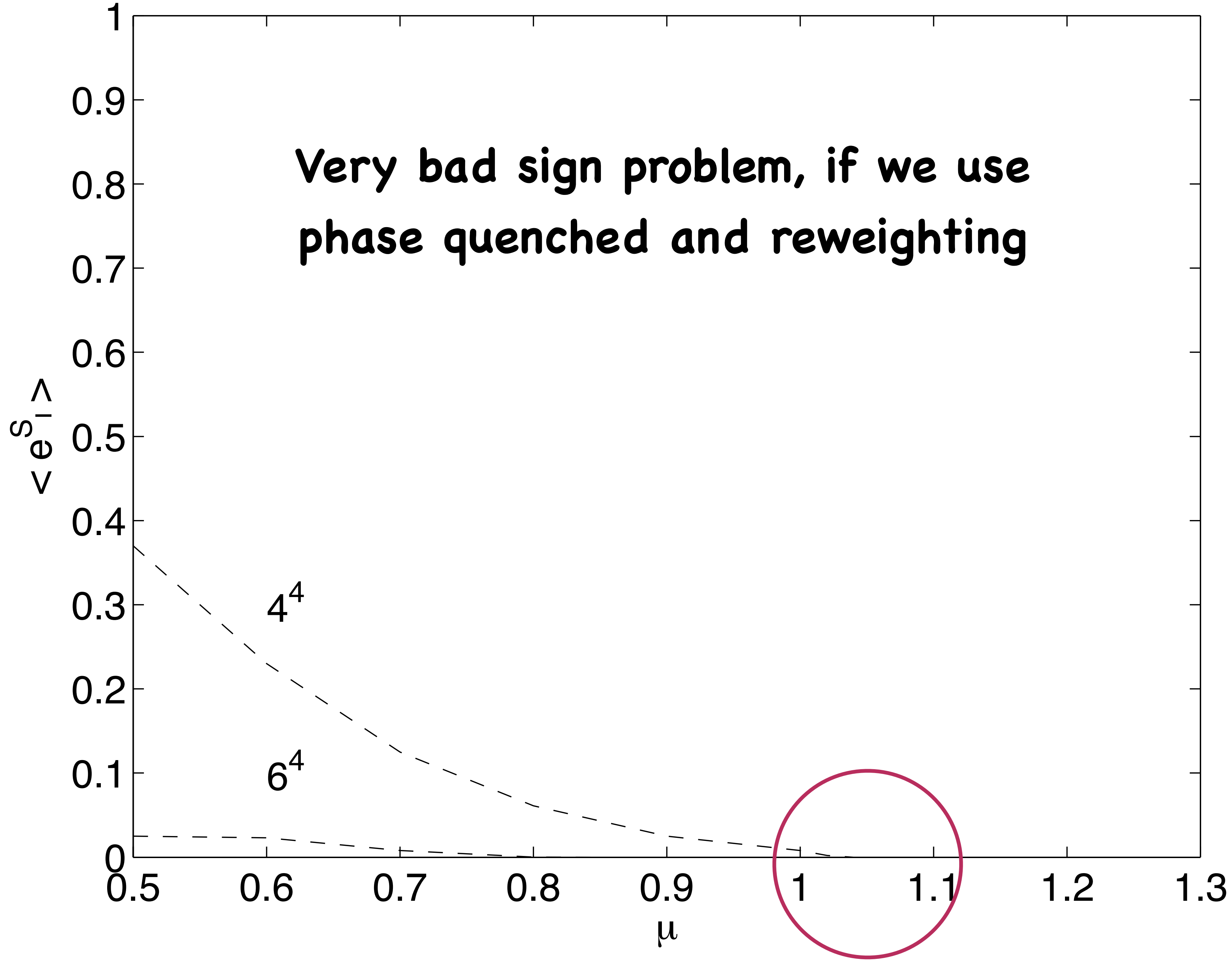

Very bad sign problem, if we use phase quenched and reweighting

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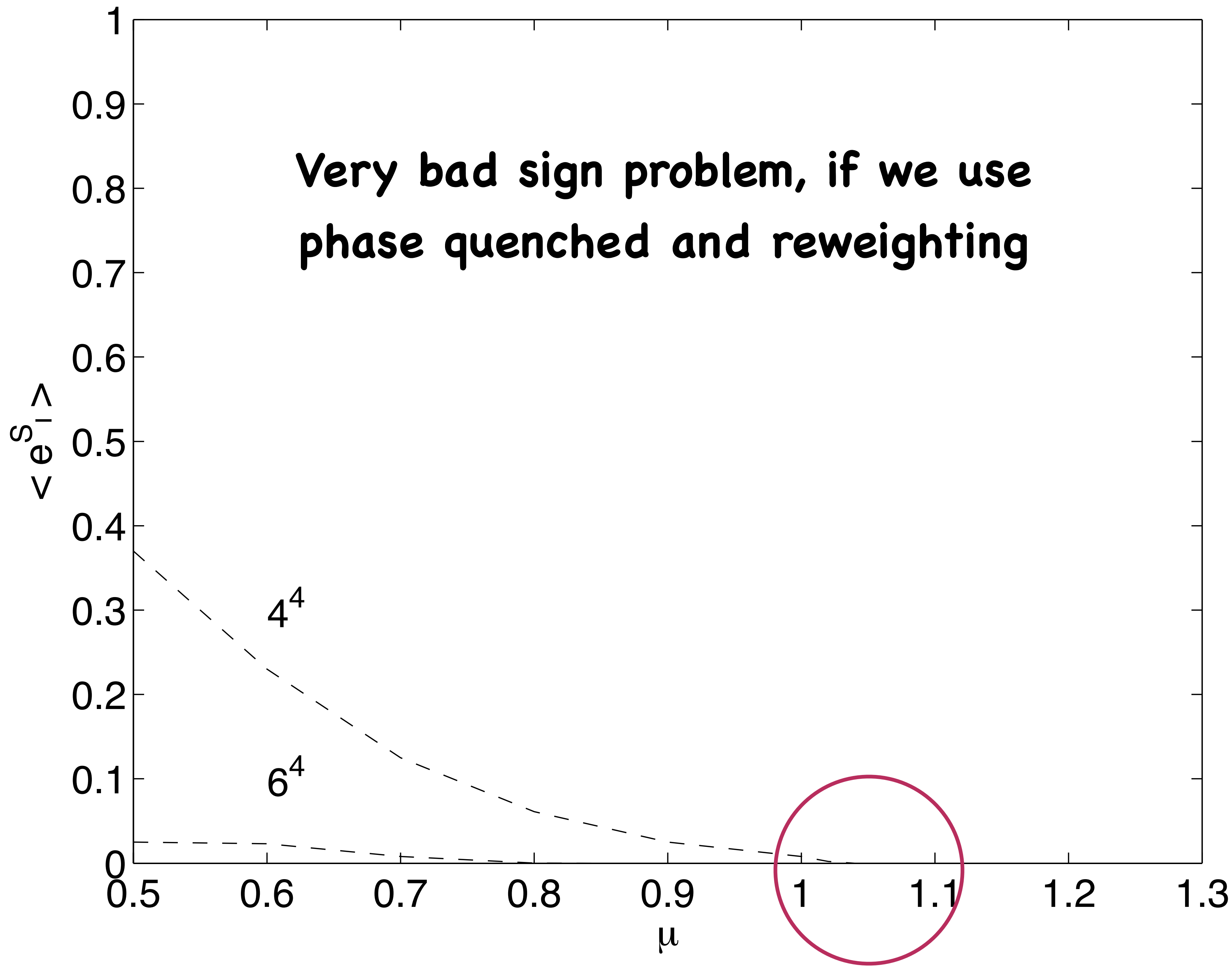

Very bad sign problem, if we use phase quenched and reweighting

$m=\lambda=1$

It has been solved through a reformulation with "flux/worldline" variables and Complex Langevin. → Great opportunity to check our approach.

How precisely should we approximate the thimble?

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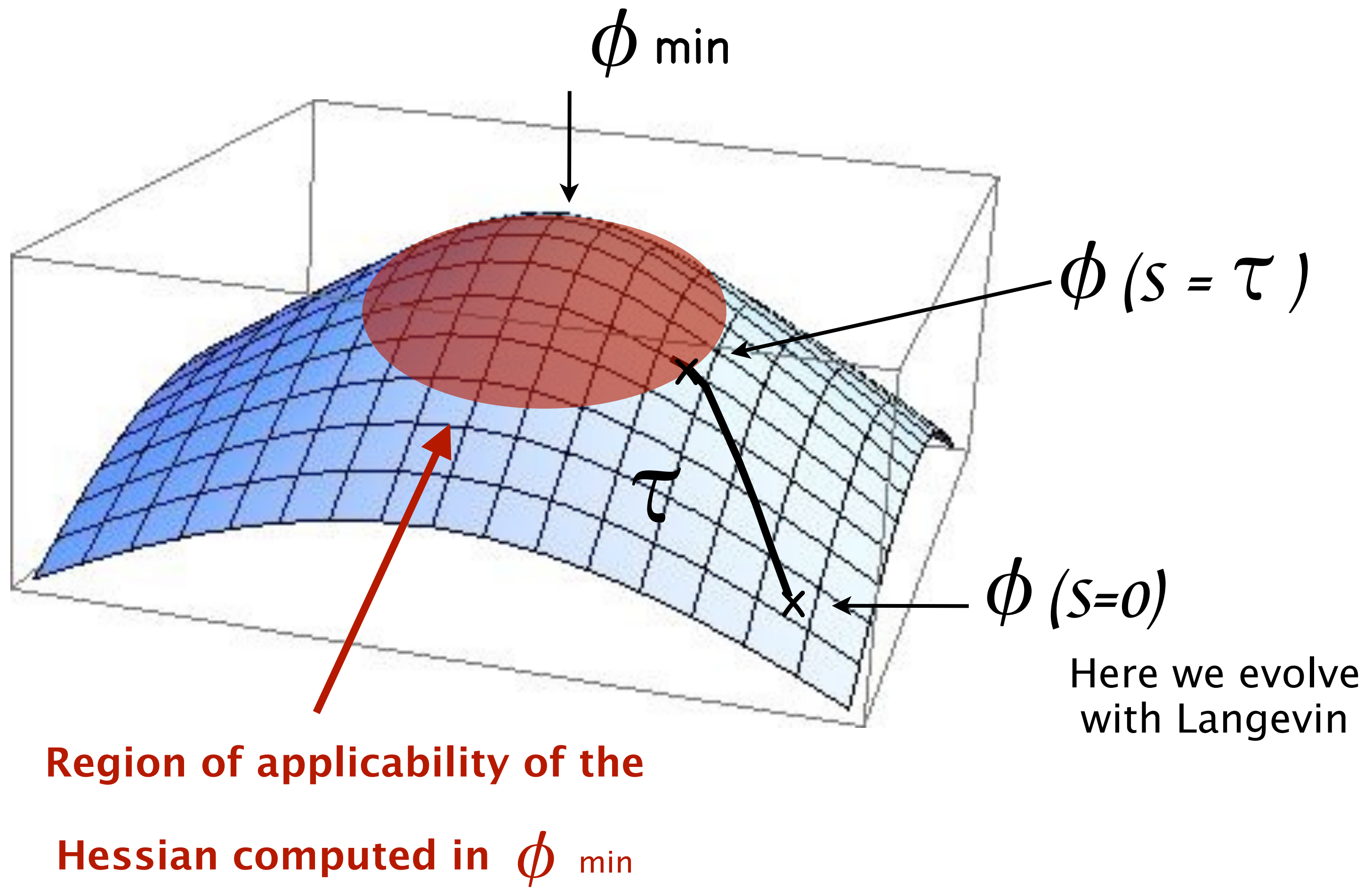
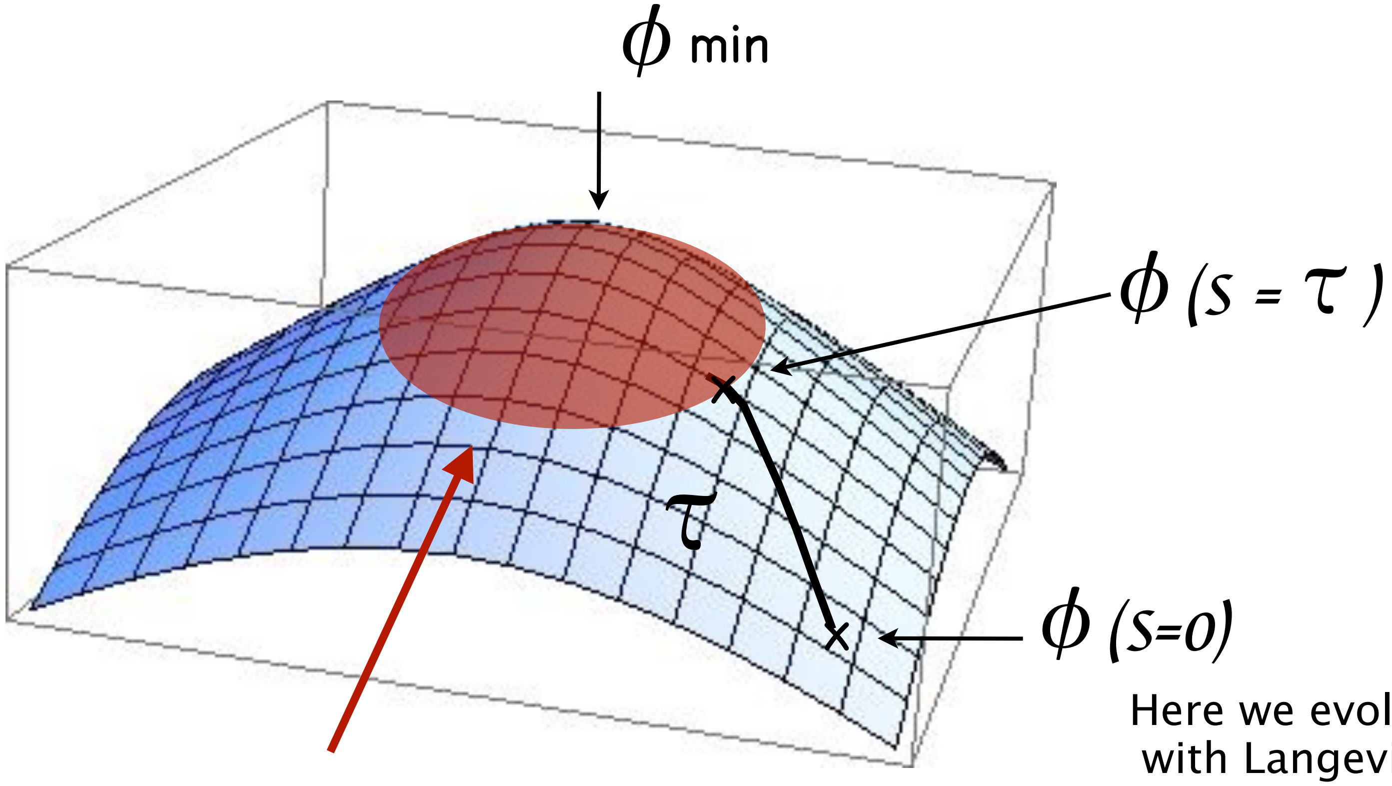


Equivalently:
how large is the (red) region where the flat thimble is enough?

How precisely should we approximate the thimble?



Here we evolve with Langevin

Region of applicability of the Hessian computed in ϕ min

Equivalently:
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Equivalently:
how long needs the 5th dimension be?

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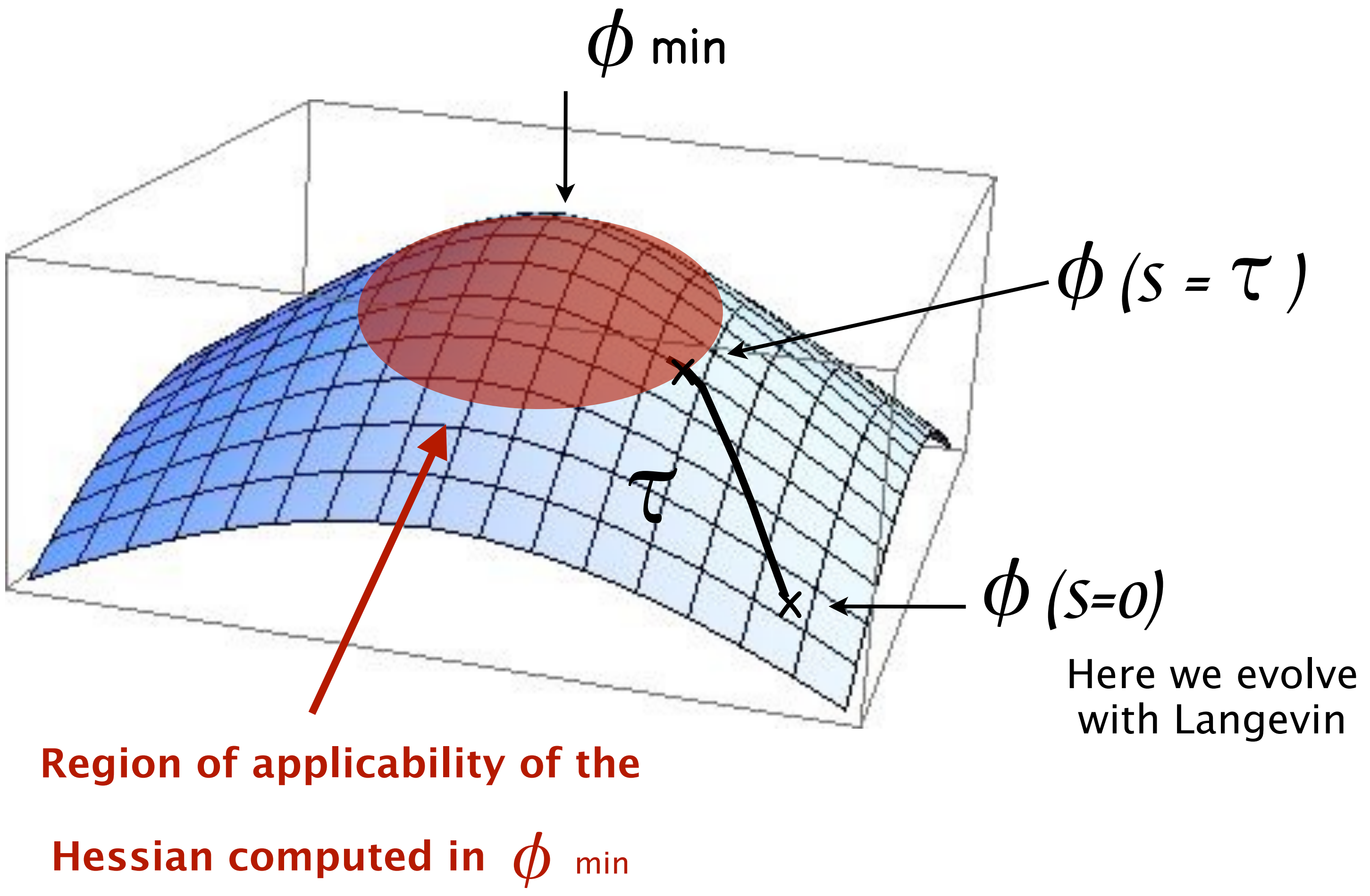


Here we evolve with Langevin

Region of applicability of the Hessian computed in ϕ min

Equivalently:
how large is the (red) region where the flat thimble is enough?

Equivalently:
how long needs the 5th dimension be?

Only as precise as to ensure that:

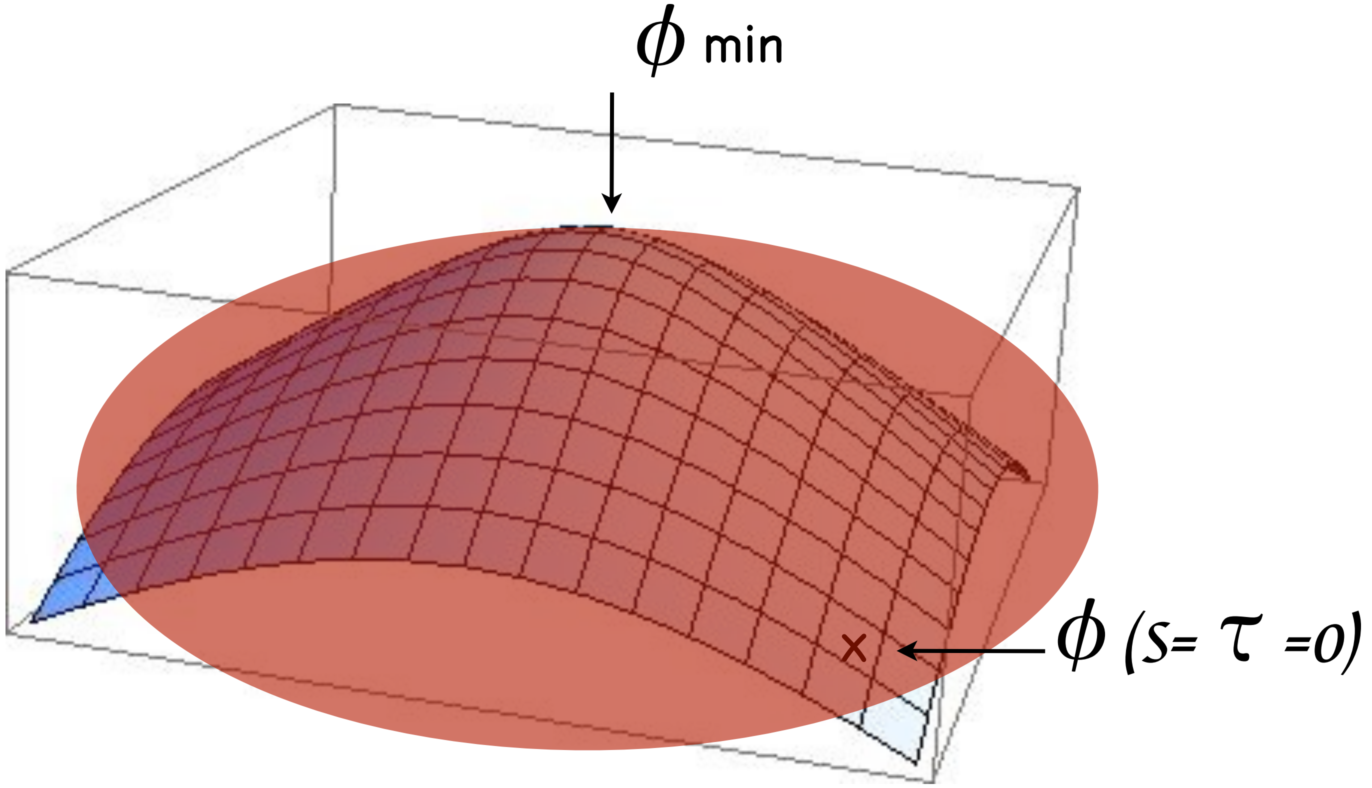
1. The homology class of the thimble should be preserved (when this is not the case, the system will diverge).
2. The fluctuations in S_I should be limited, in order not to produce a sign problem.

Crudest approximation of the thimble

i.e. the flat vector space associated to positive eigenvalues of the Hessian:

$$\partial^2 S_R[\phi]|_{\phi=\phi_{\text{global min}}}$$

In other words, project everywhere the configurations according to the Hessian computed at the saddle point



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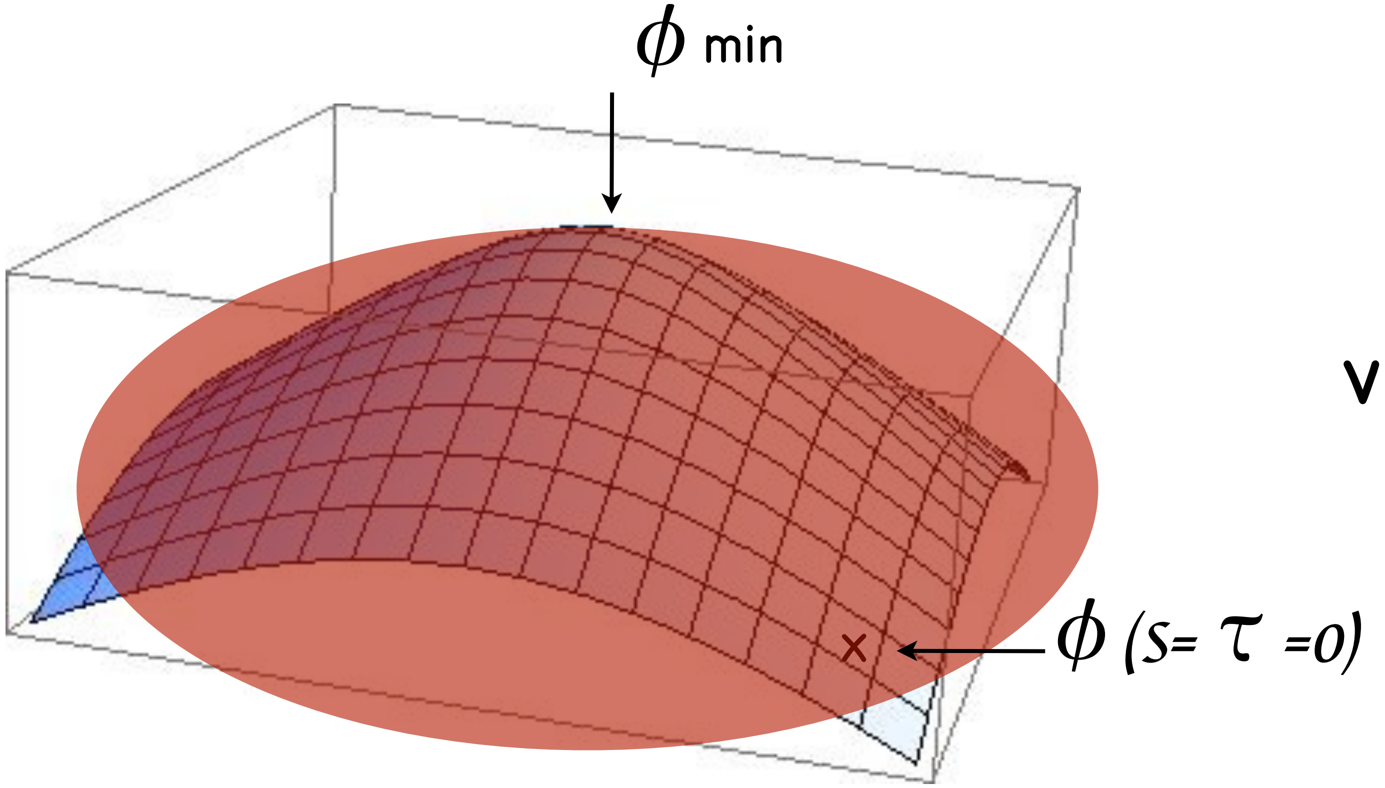
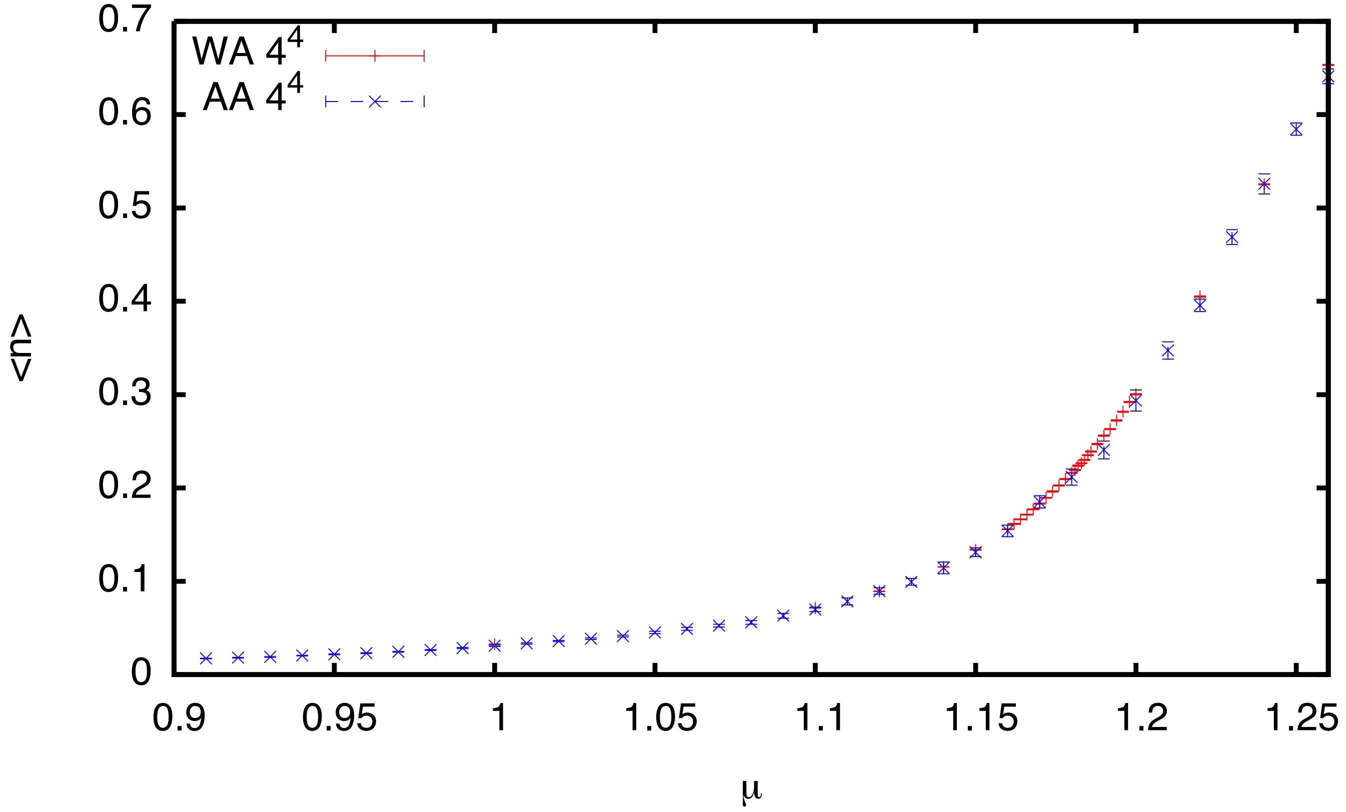
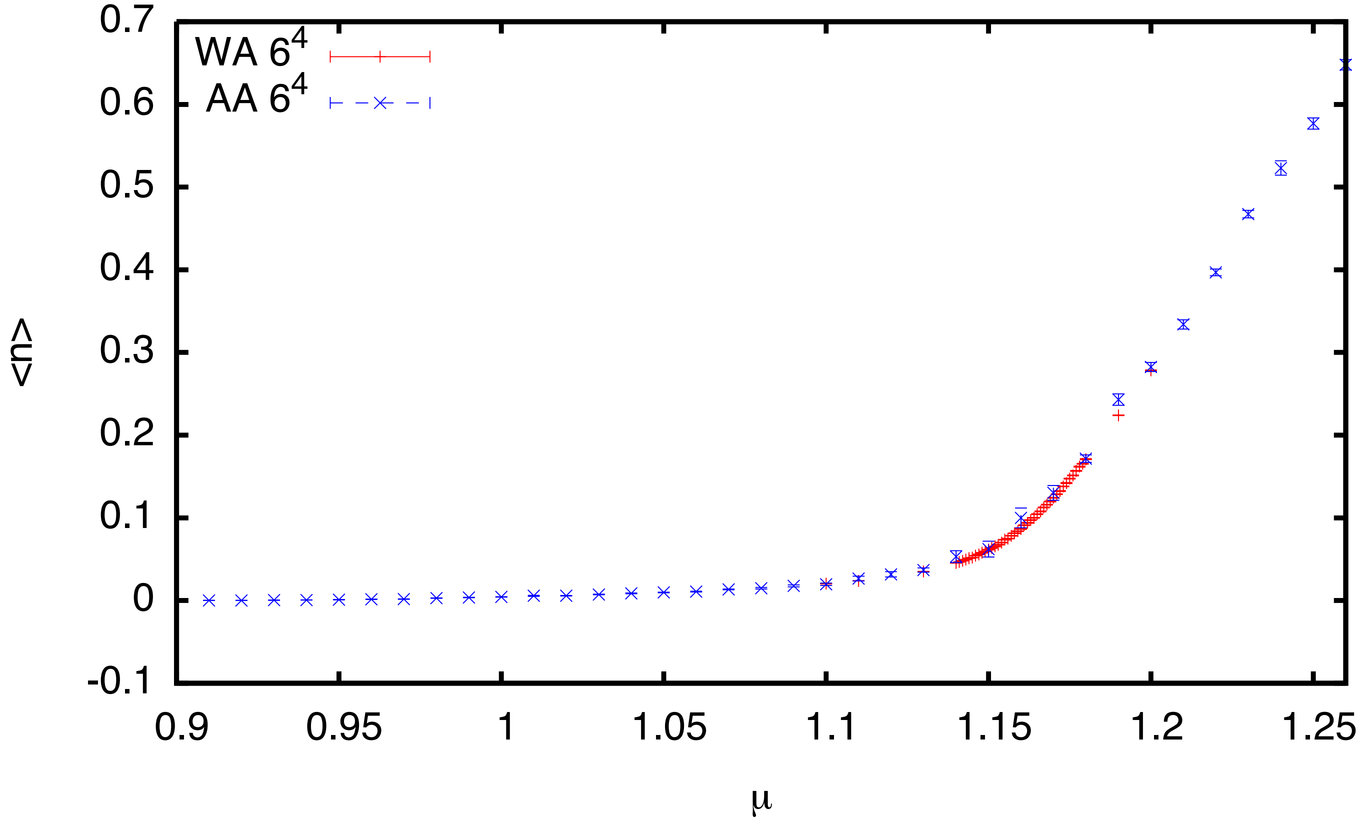


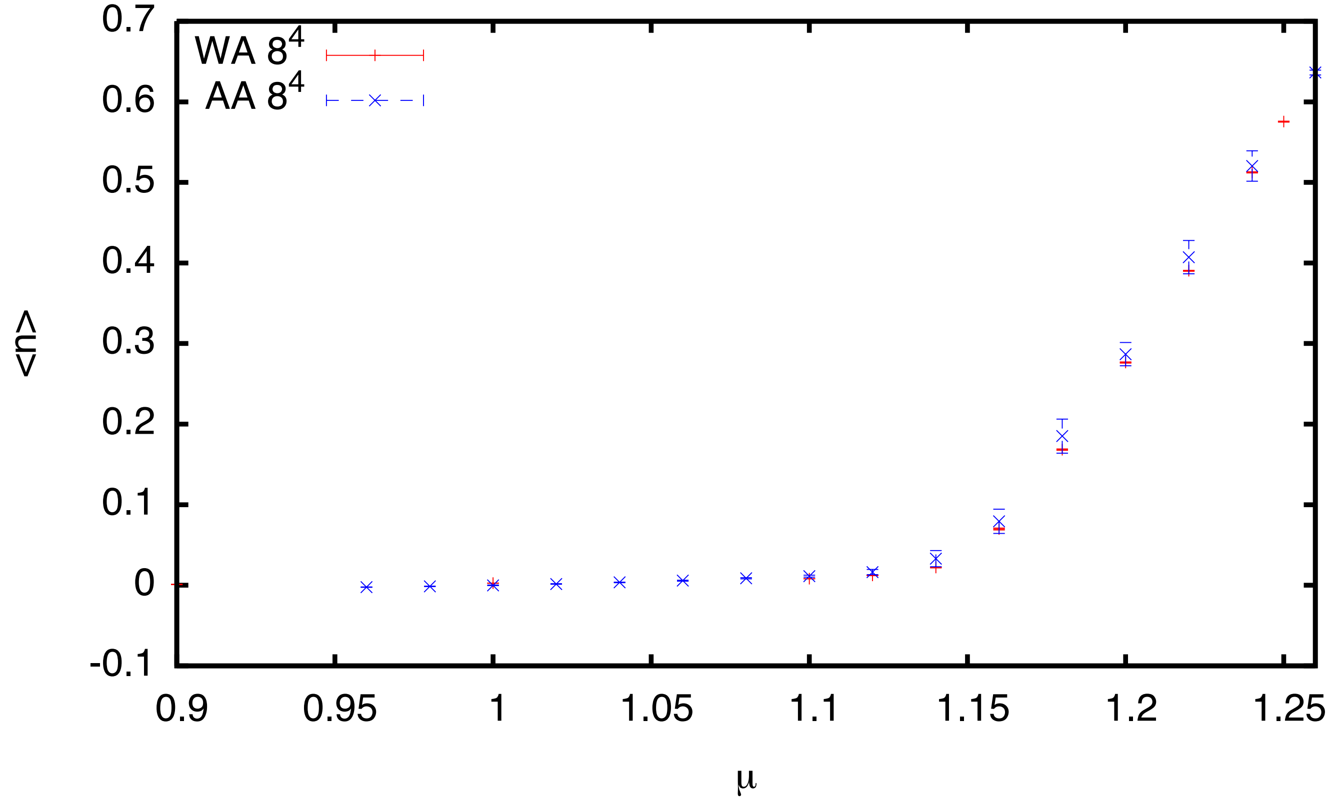
very crude but,...

Bose gas: results



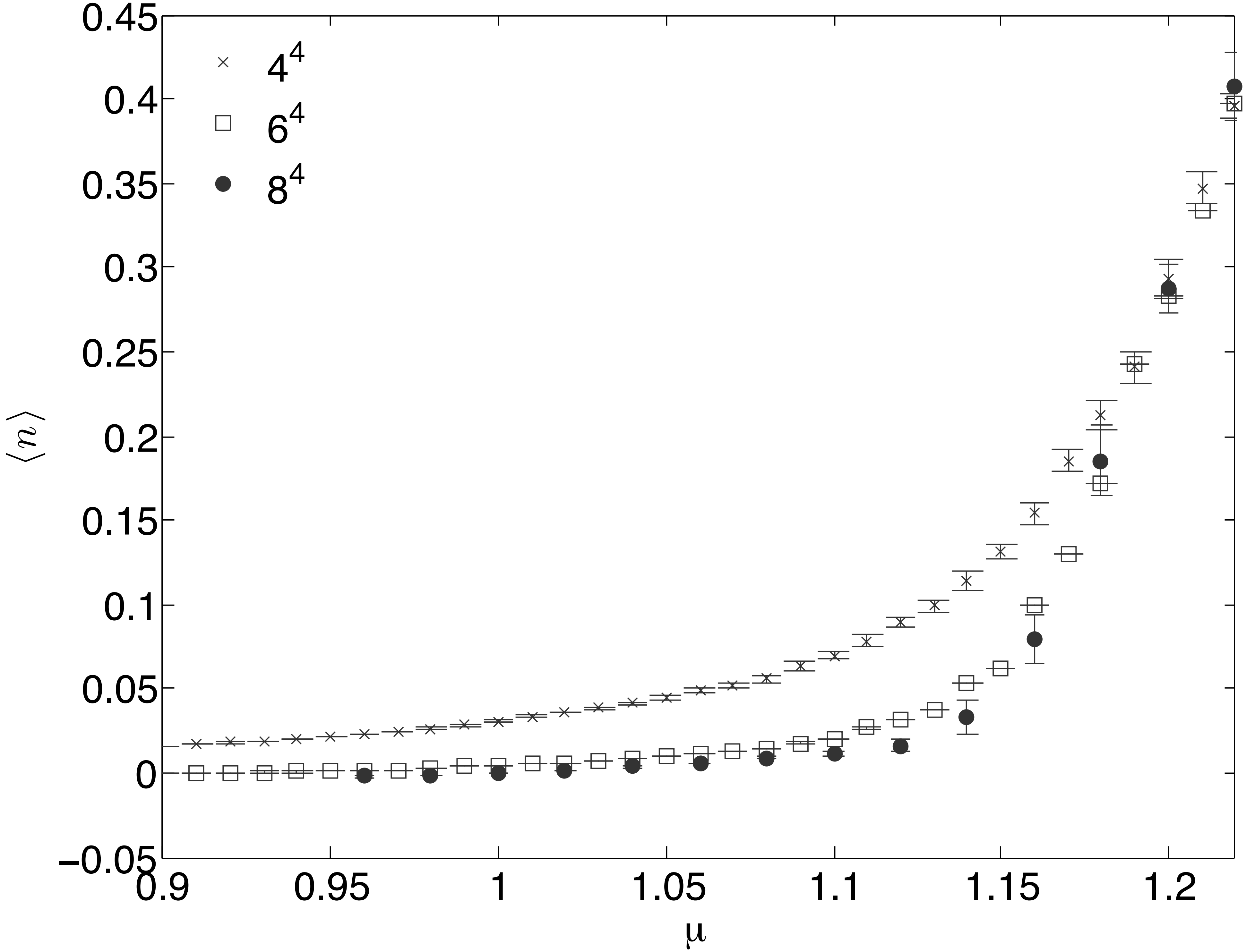
In fact, we find already **excellent agreement** with the known results! (Gattringer and Kloiber in red)





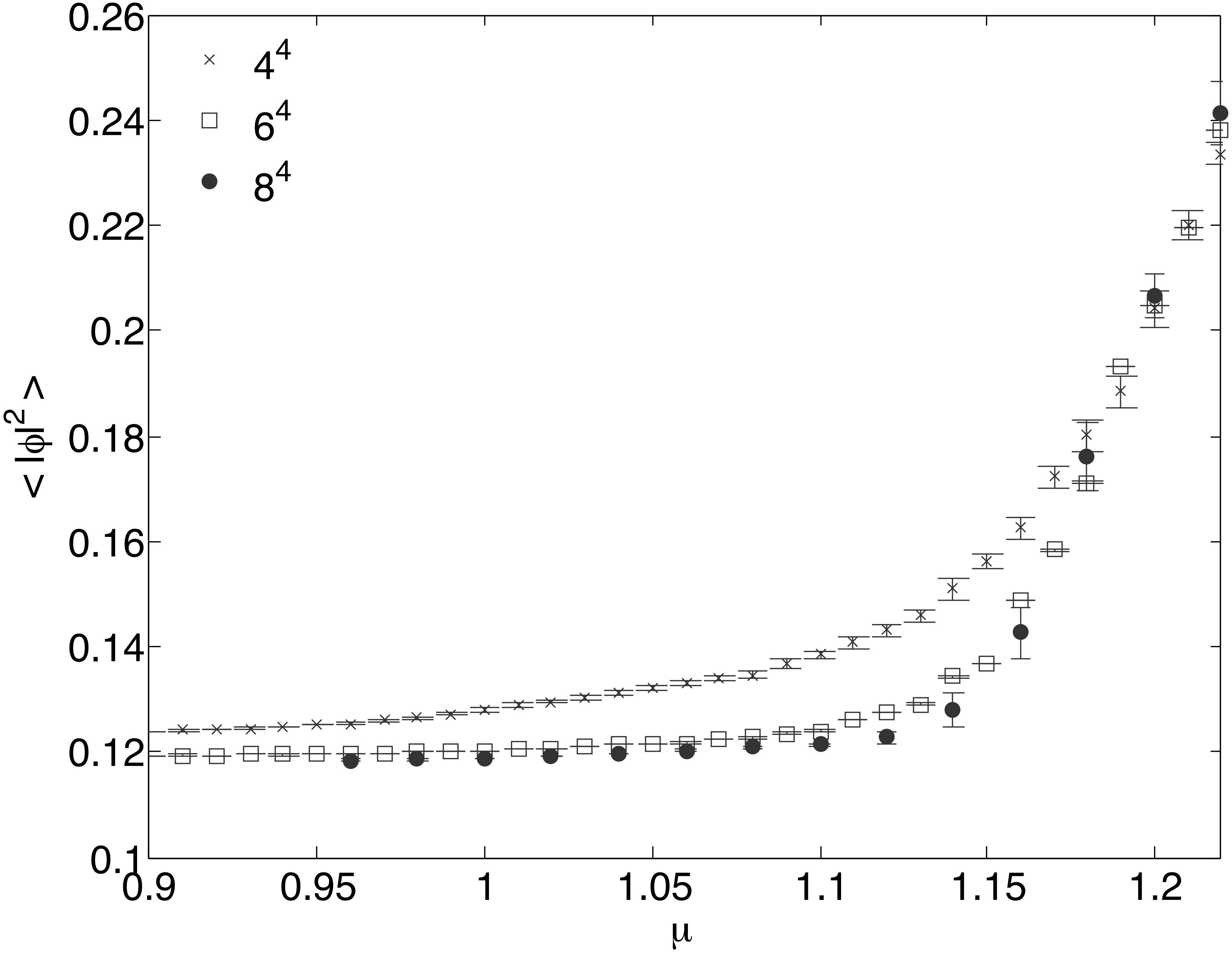
Bose gas: results

Putting the three volumes together, we see the **Silver Blaze** effect.



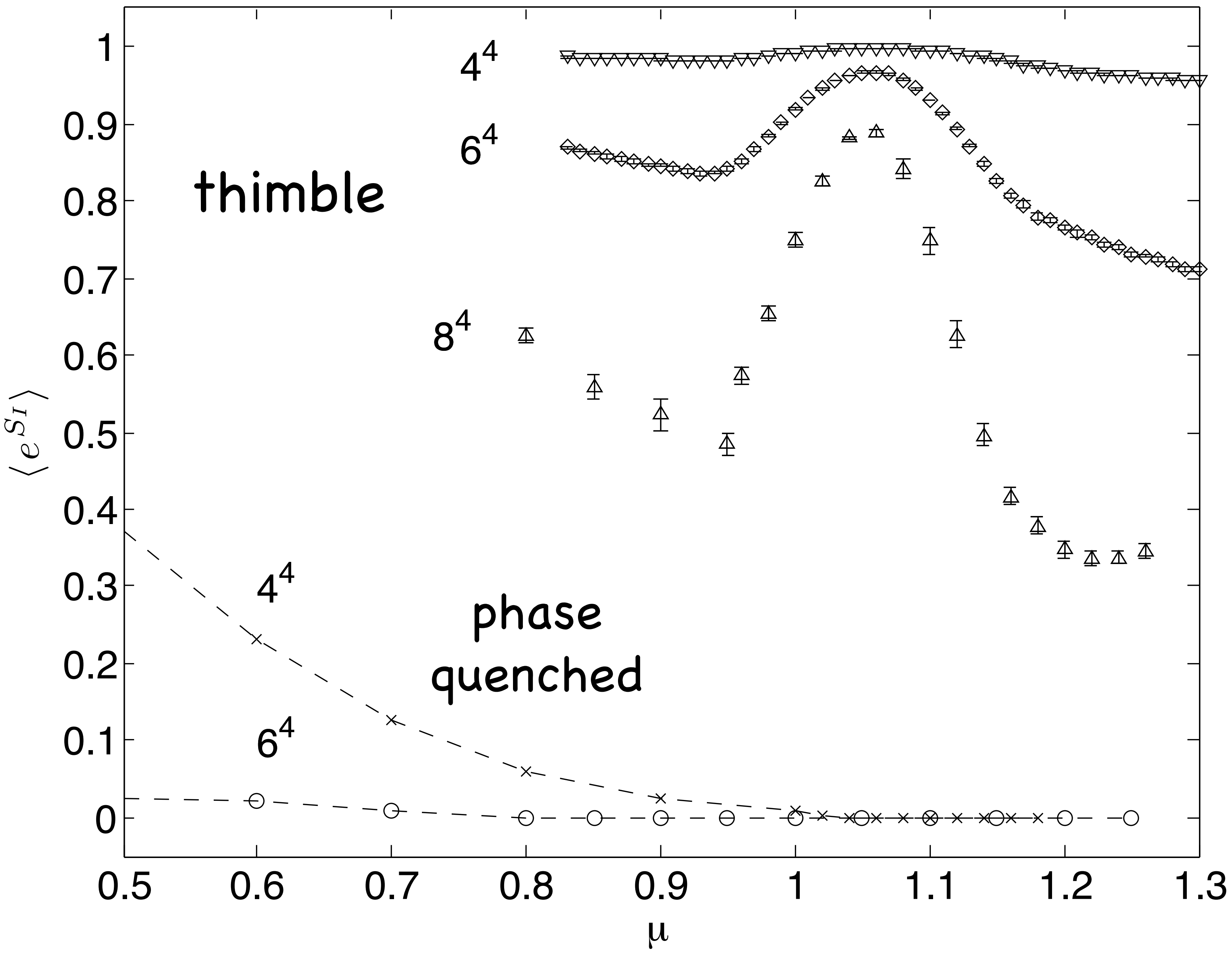
Bose gas: results

Same for the average modulus of the field



Bose gas: results

Since it is not exactly the thimble, S_I is not constant, but:



we see that the average phase is now far from ZERO and there is no sign problem in these lattices
(reweighting has essentially no visible effect, even in the hardest point)
no residual phase on the flat domain.

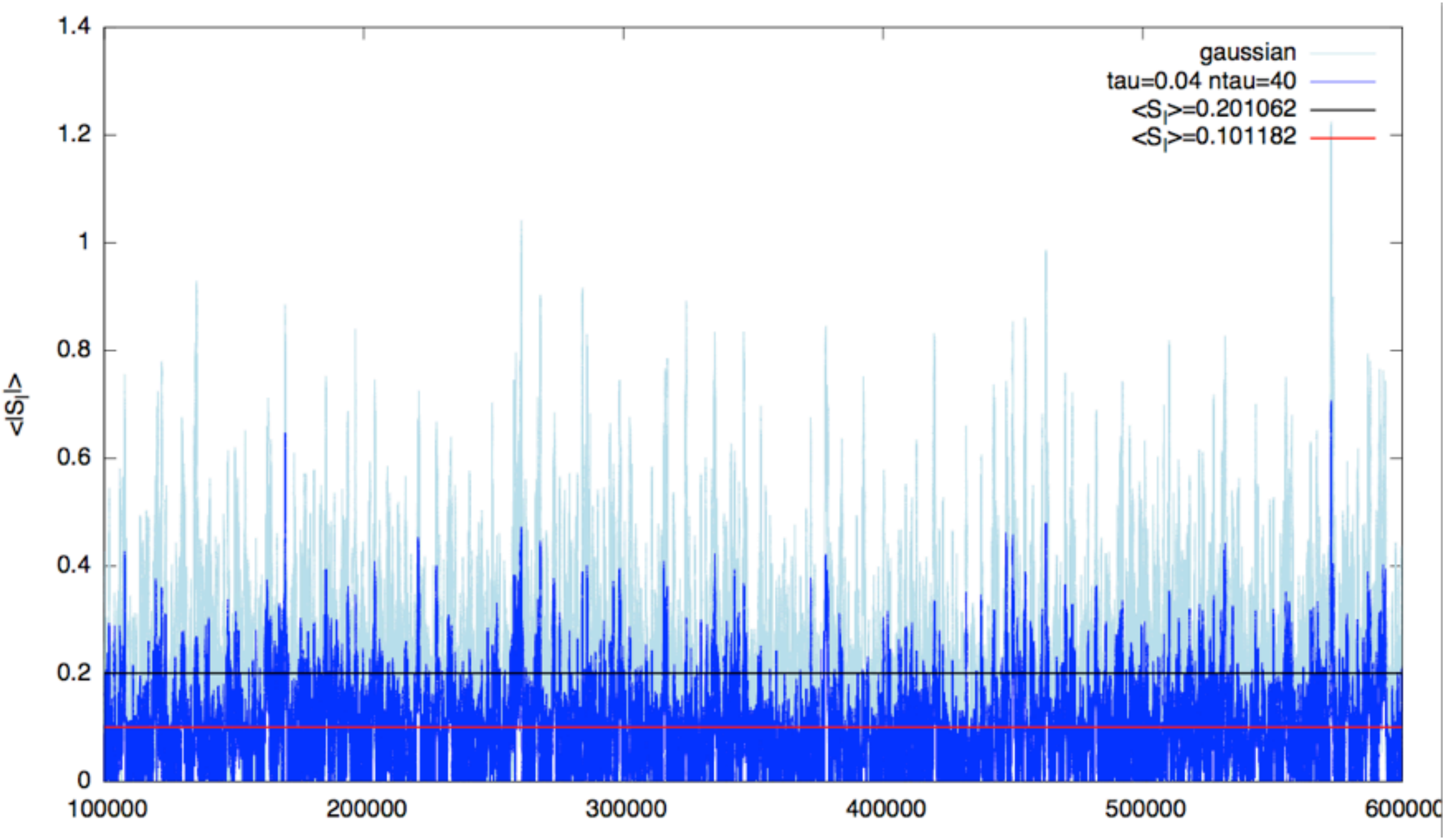
Approaching the thimble further

This is not enough:

there are a few (~1%) divergences, because the flat approximation is not converging asymptotically.

Discarding them introduces a cutoff that must be removed by approaching the thimble further.

Bose gas from flat to thimble



Indeed, we can approach the thimble better by following the SD equations:

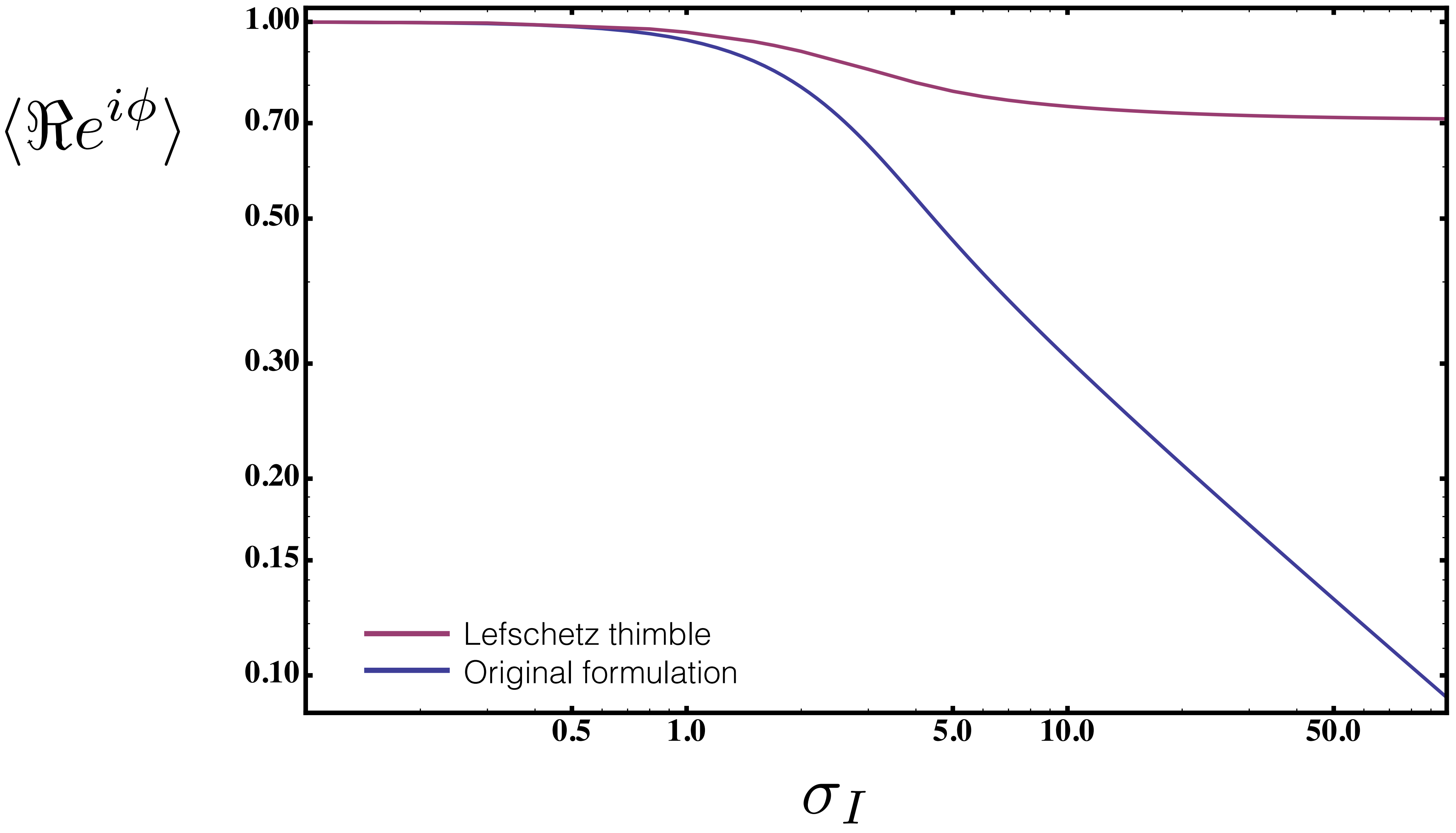
- the fluctuations are reduced;
- the results the same;
- we do not see divergences (but that's not statistically relevant).

IV. Numerical / analytical results on a 0-dim model

A 0-dim model

(see Aarts Phys.Rev. D88 (2013) 094501)

$$S[x] = \frac{1}{2}(\sigma_R + i\sigma_I)x^2 + \frac{1}{4}\lambda x^4$$



Thanks to
M.Cristoforetti

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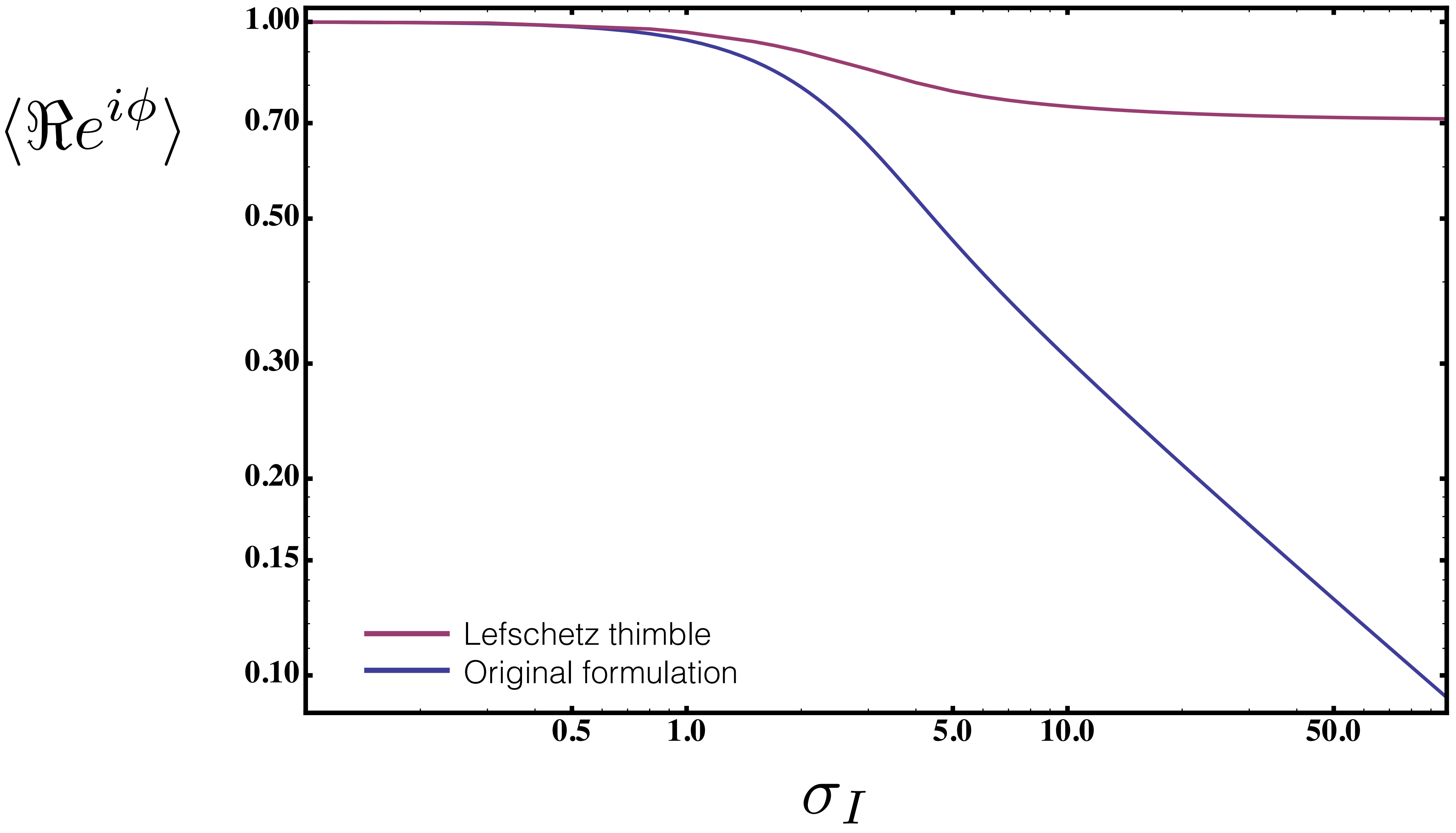

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The **residual phase** converges to a value ~0.7>>0 ⇒ finite correction, but no sign problem!

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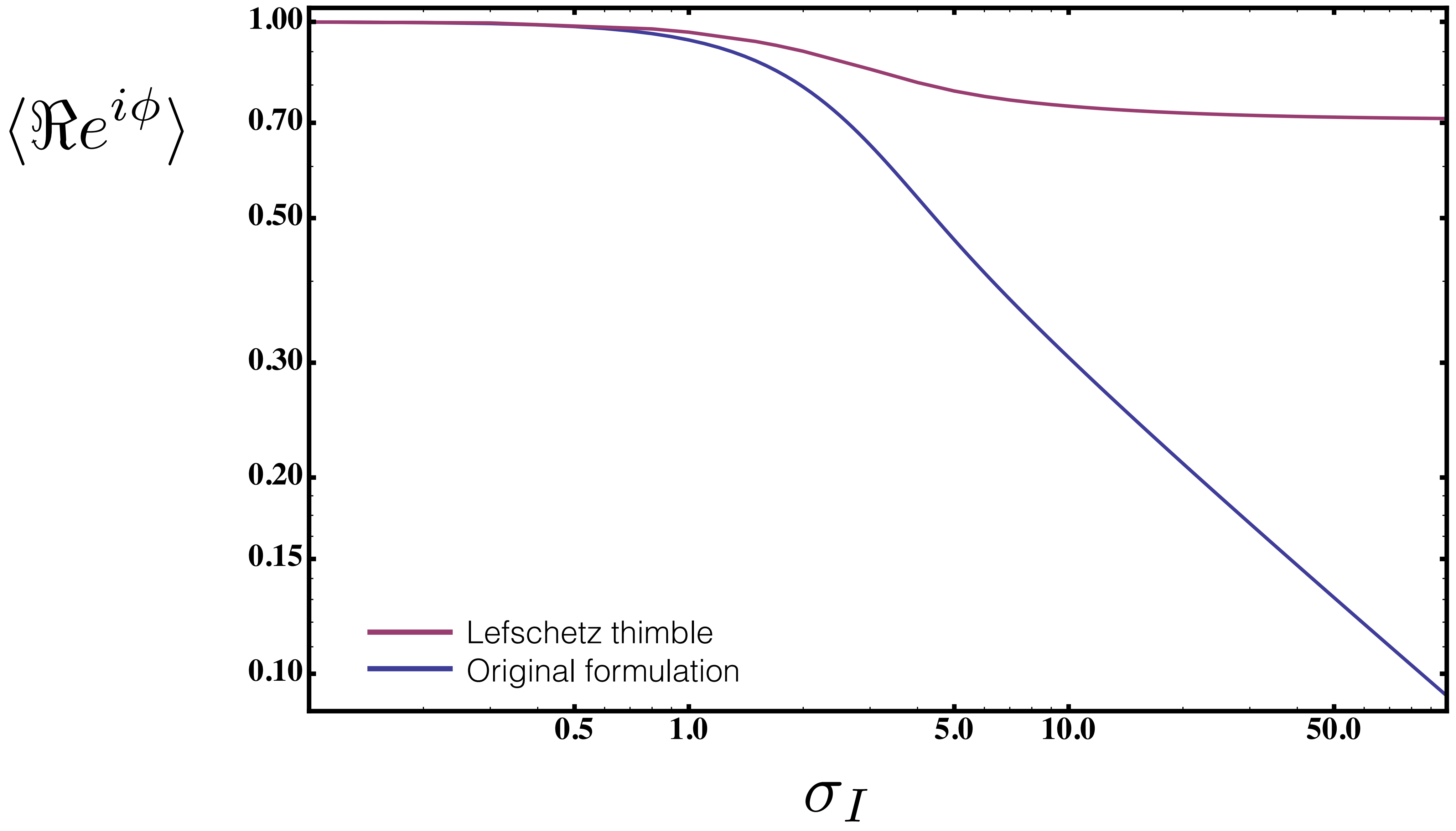

Thanks to
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The **residual phase** converges to a value ~0.7>>0 ⇒ finite correction, but no sign problem!
On larger systems it seems that the correction is even negligible (see Kikukawa's talk)

A 0-dim model

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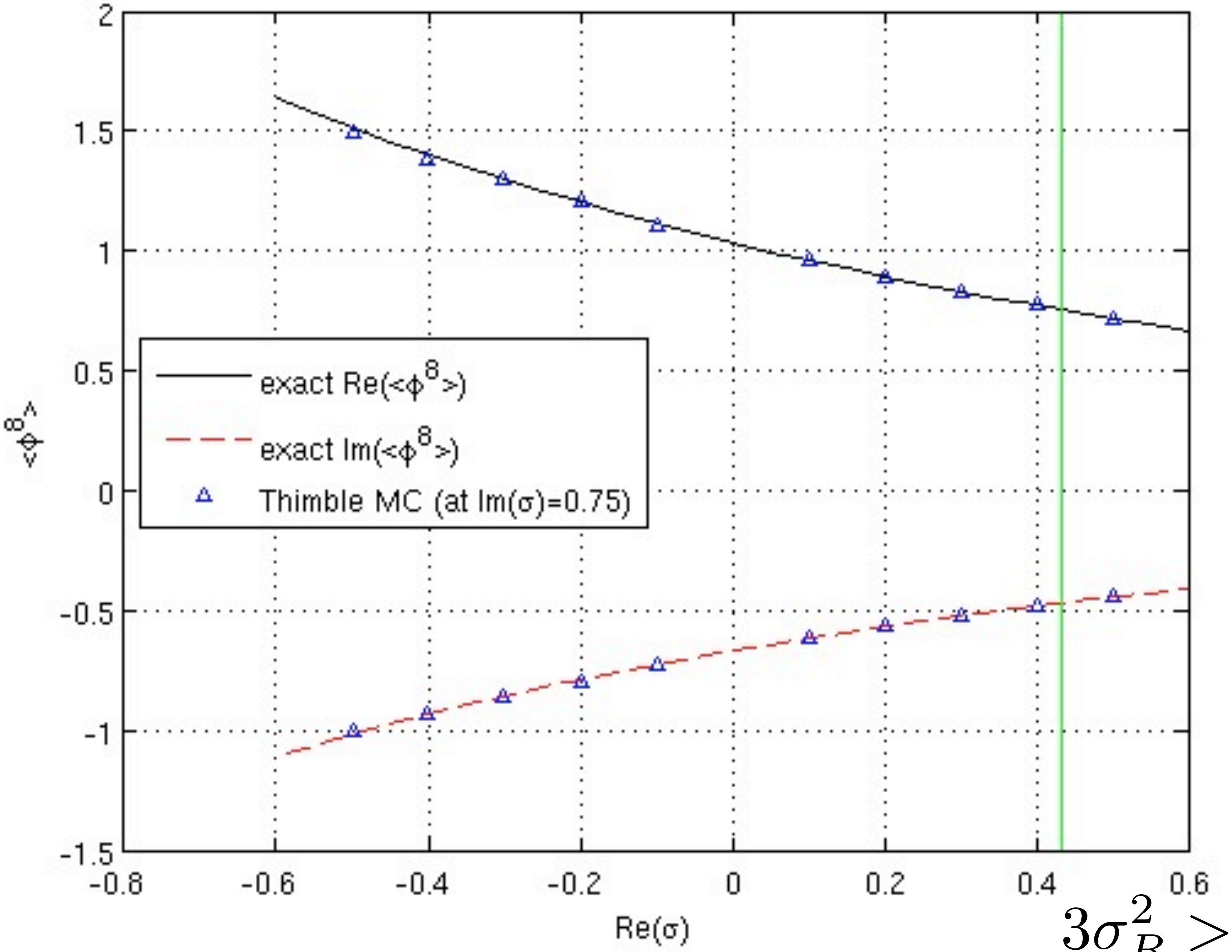
Thanks to
G. Eruzzi



$$3\sigma_R^2 > \sigma_I^2$$

A 0-dim model

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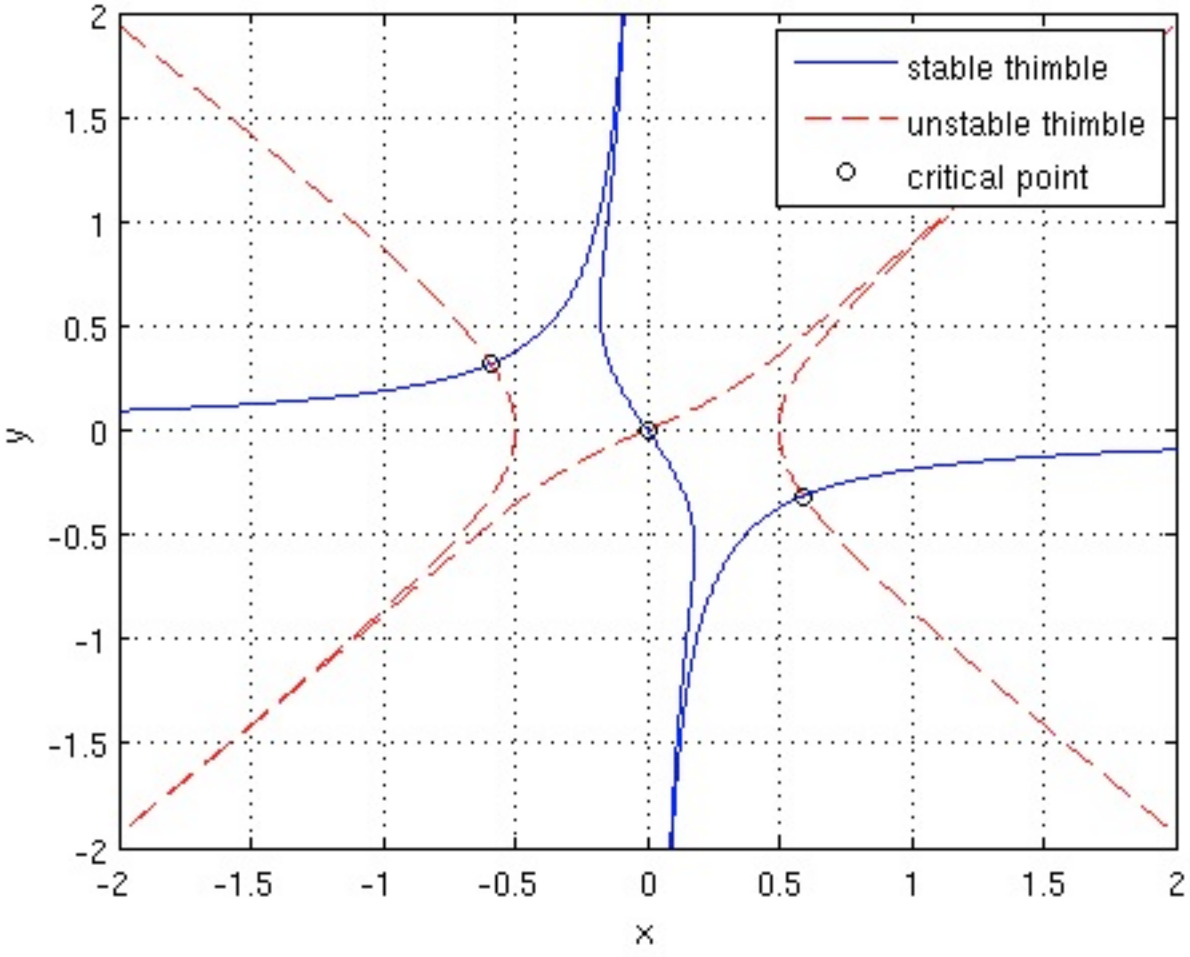
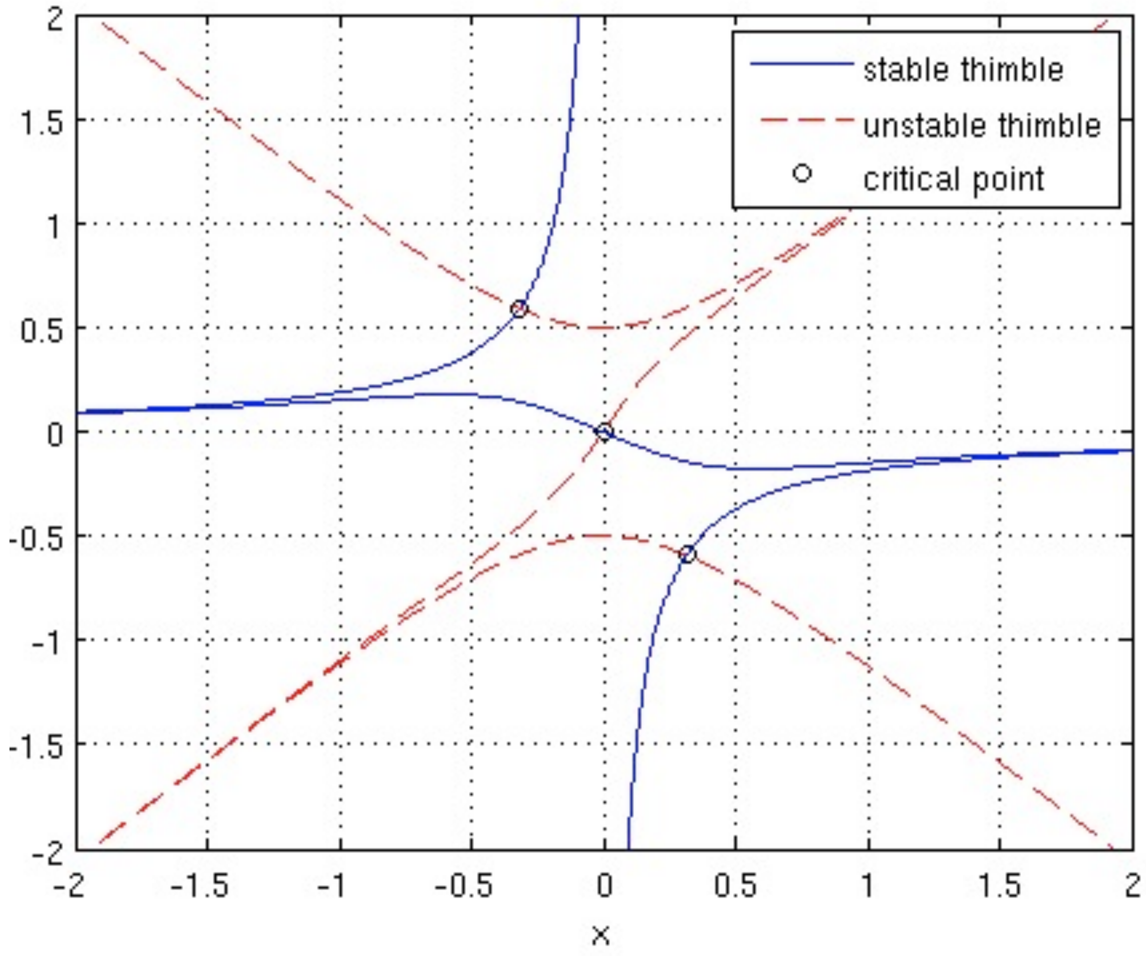


$\sigma_R < 0$



$\sigma_R > 0$

Does Complex Langevin visit the same thimbles?

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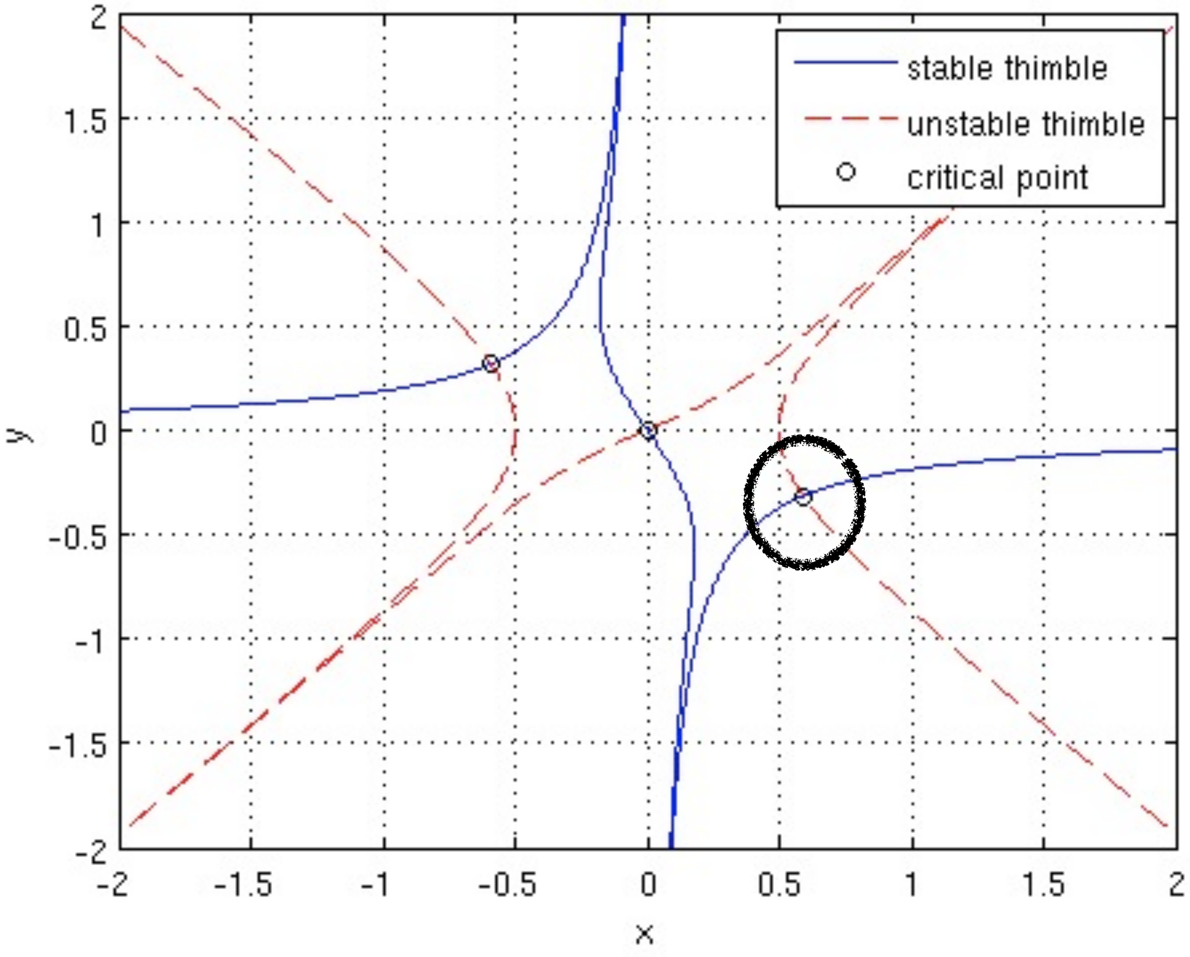

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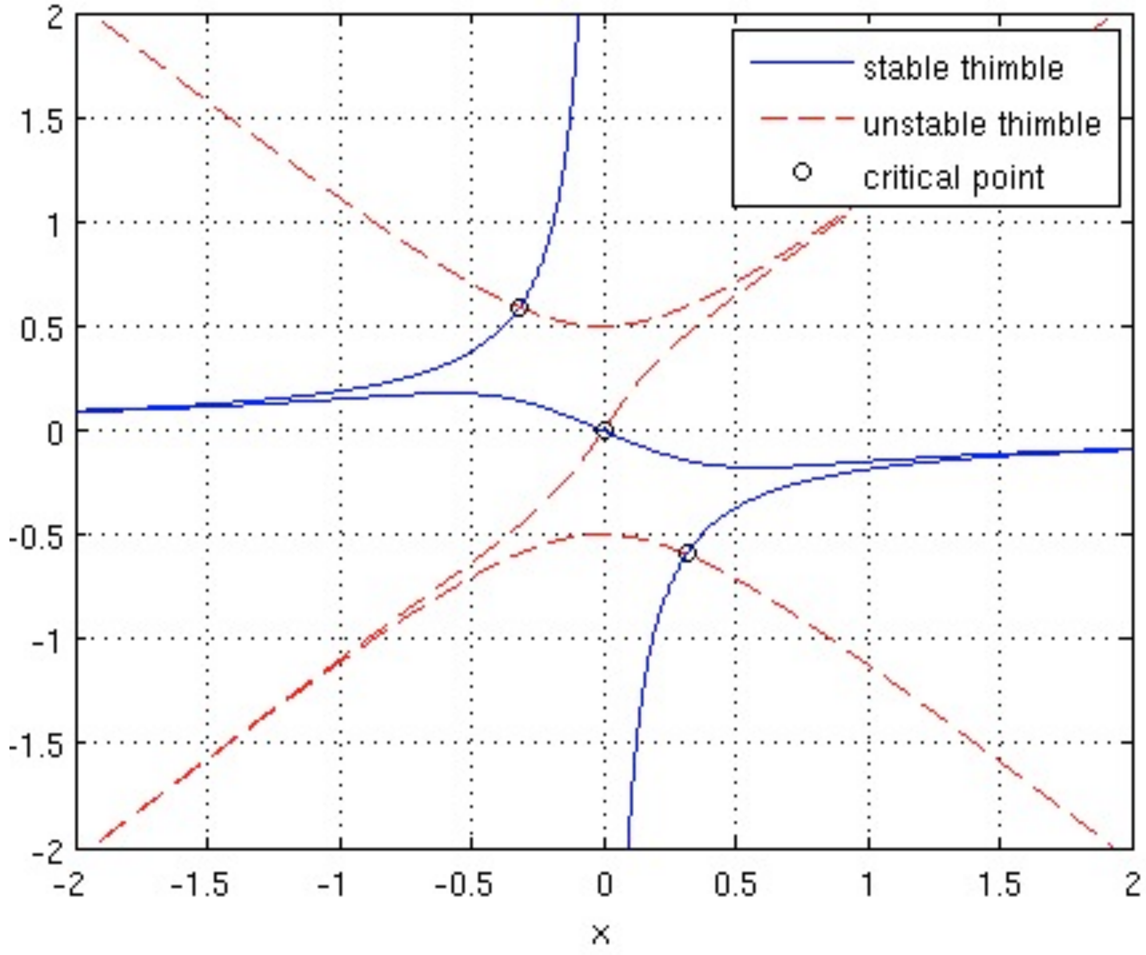

$\sigma_R > 0$

Does Complex Langevin visit the same thimbles?

Note that on large volumes one thimble is enough even with SSB

V. Hubbard Model

The Hubbard model

(See poster by Abhishek Mukherjee)

It is not a QFT (universality applies only in the critical regions)

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Different formulations are possible.
In some formulations the determinant is real (and sign ±1).
But, this is not a generic choice of parameters, so we are taking two approaches:

The Hubbard model

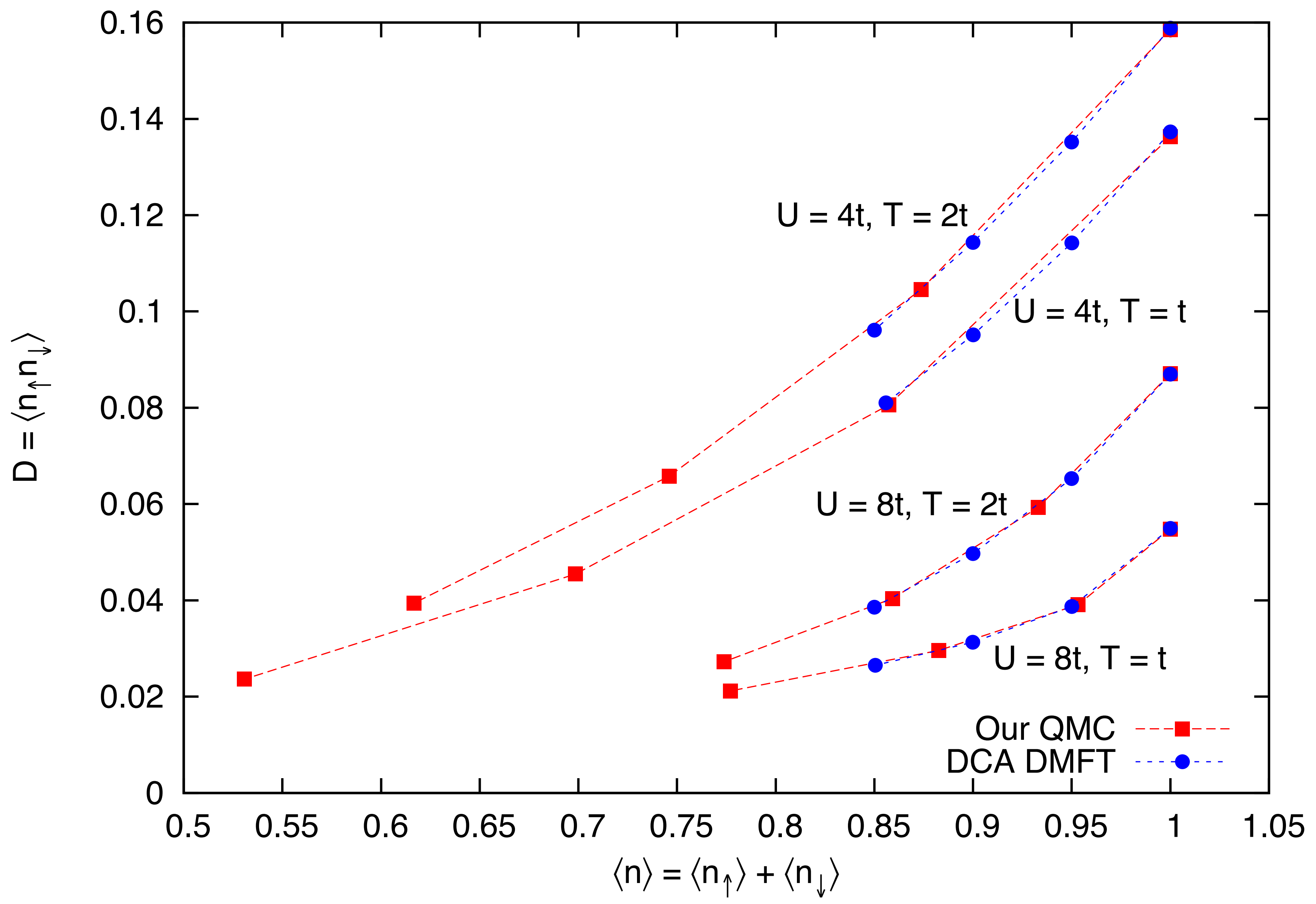
(See poster by Abhishek Mukherjee)

It is not a QFT (universality applies only in the critical regions)

Different formulations are possible.
In some formulations the determinant is real (and sign ±1).
But, this is not a generic choice of parameters, so we are taking two approaches:

- study a complex formulation on the thimble
- study the contribution from different real connected sectors

The Hubbard model



Thanks to
A.Mukherjee

Red: Cluster DMFT (LeBlanc and Gull, Phys. Rev. B 88, 155108 (2013))
Blue: QMC simulations on the single sector connected to the constant stationary configuration.
(…results from the thimble coming soon…)

VI. What about QCD ?!?

Complexification

$$A_\nu^a(x) \to A_\nu^{a,R}(x) + iA_\nu^{a,I}(x) \qquad a = 1 \dots N_c^2 - 1.$$

$$SU(3)^{4V} \to SL(3,\mathbb{C})^{4V}$$

Covariant Derivatives

$$\nabla_{x,\nu,a} F[U] := \frac{\partial}{\partial \alpha} F\left[e^{i\alpha T_a} U_\nu(x)\right]_{|\alpha=0}$$

and similar definitions for: $\nabla^R_{x,\nu,a},\ \nabla^I_{x,\nu,a},\ \overline{\nabla}_{x,\nu,a}.$

Such that: $\nabla_{x,\nu,a} = \nabla^R_{x,\nu,a} - i\nabla^I_{x,\nu,a},$ And Cauchy-Riemann hold.

$$\overline{\nabla}_{x,\nu,a} = \nabla^R_{x,\nu,a} + i\nabla^I_{x,\nu,a}$$

Note that the covariant derivatives do not commute:

$$\left[\nabla_{x,\nu,a}, \nabla_{y,\sigma,b}\right] = \delta_{x,y}\delta_{\nu,\sigma} f_{abc} \nabla_{x,\nu,c},$$ where: $[T_a, T_b] = i f_{abc} T_c$

But the Hessian is still well defined and symmetric in the stationary points!

Equations of Steepest Descent

with covariant derivatives, they take the form:

$$\frac{d}{d\tau}U_\nu(x;\tau) = (-iT_a\overline{\nabla}_{x,\nu,a}\overline{S[U]})U_\nu(x;\tau)$$

Note that this implies the following essential relations:

$$\frac{d}{d\tau}S_{R/I} = \frac{1}{2}\frac{d}{d\tau}(S \pm \overline{S}) = -\frac{1}{2}\nabla_j S \cdot \overline{\nabla}_j \overline{S} \mp \frac{1}{2}\overline{\nabla}_j \overline{S} \cdot \nabla_j S = \begin{cases} \quad - \parallel \nabla S \parallel^2 \\ \qquad 0 \end{cases}$$

Defining the thimbles for gauge theories

How does the gauge invariance affects the construction of the thimble $\mathcal{J}_0$?

Discussed by **Atiyah-Bott (1982)** and reviewd by **Witten (2010)**.

☛ Substitute the concept of non-degenerate critical point with that of non-degenerate critical manifold (Bott 1956)

Gauge Symmetry of the thimble

Consider the SD equation:

$$\frac{d}{d\tau}U_\nu(x;\tau) = (-iT_a\overline{\nabla}_{x,\nu,a}\overline{S[U]})U_\nu(x;\tau)$$

Under an $SL(3,\mathbb{C})$ gauge transformations it changes as:

$$(T_a\overline{\nabla}_{x,\nu,a}\overline{S[U]}) \to \left(\Lambda(x)^{-1}\right)^\dagger (T_a\overline{\nabla}_{x,\nu,a}\overline{S[U]})\Lambda(x)^\dagger$$

$$U_\nu(x) \to \Lambda(x)U_\nu(x)\Lambda(x+\hat{\nu})^{-1}$$

Note that the full SD equation is covariant only under the $SU(3)$ subgroup of $SL(3,\mathbb{C})$.

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$$\Lambda(x)^\dagger = \Lambda(x)^{-1}$$

The thimble is symmetric under $SU(3)$ transformations.

But the gauge links are not in $SU(3)$ ... Why should they be?

Perturbation Theory

We need to compute:

$$\frac{d^p}{dg^p}\left(\int_{\mathcal{J}_0(g;\mu)} dA\; e^{-S_2[A]+gS_{\rm int}[A]}\;\det(Q[A=0])\;F[A;g,\mu]\;Q[A=0;\mu]^{-1}\ldots Q[A=0;\mu]^{-1}\right)_{|g=0}$$

In this expression, the fermion field is integrated out.

This leaves the determinant and the inverse fermion matrices (free propagators).

The integrand has the form of a gaussian times polynomials

Proof of equivalence is essentially identical to the scalar case.

Conclusions

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- The ϕ^4 QFT has been a great testbed and we are currently working on new problems.
- See Abhi's poster!

1st Aurora prototype

The two installations of the Aurora architecture that followed it became the two most power-efficient computers in the world in June 2013

The Green500 List

Listed below are the June 2013 The Green500's energy-efficient supercomputers ranked from 1 to 10.

Green500 Rank	MFLOPS/W	Site*	Computer*	Total Power (kW)
1	3,208.83	CINECA	Eurora - Eurotech Aurora HPC 10-20, Xeon E5-2687W 8C 3.100GHz, Infiniband QDR, NVIDIA K20	30.70
2	3,179.88	Selex ES Chieti	Aurora Tigon - Eurotech Aurora HPC 10-20, Xeon E5-2687W 8C 3.100GHz, Infiniband QDR, NVIDIA K20	31.02
3	2,449.57	National Institute for Computational Sciences/University of Tennessee	Beacon - Appro GreenBlade GB824M, Xeon E5-2670 8C 2.600GHz, Infiniband FDR, Intel Xeon Phi 5110P	45.11
4	2,351.10	King Abdulaziz City for Science and Technology	SANAM - Adtech, ASUS ESC4000/FDR G2, Xeon E5-2650 8C 2.000GHz, Infiniband FDR, AMD FirePro S10000	179.15
5	2,299.15	IBM Thomas J. Watson Research Center	BlueGene/Q, Power BQC 16C 1.60 GHz, Custom	82.19
6	2,299.15	DOE/SC/Argonne National Laboratory	Cetus - BlueGene/Q, Power BQC 16C 1.600GHz, Custom Interconnect	82.19
7	2,299.15	Ecole Polytechnique Federale de Lausanne	CADMOS BG/Q - BlueGene/Q, Power BQC 16C 1.600GHz, Custom Interconnect	82.19
8	2,299.15	Interdisciplinary Centre for Mathematical and Computational Modelling, University of Warsaw	BlueGene/Q, Power BQC 16C 1.600GHz, Custom Interconnect	82.19
9	2,299.15	DOE/SC/Argonne National Laboratory	Vesta - BlueGene/Q, Power BQC 16C 1.60GHz, Custom	82.19
10	2,299.15	University of Rochester	BlueGene/Q, Power BQC 16C 1.60GHz, Custom	82.19