The Lefschetz thimble and the sign problem

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(LISC & ECT*, Trento)

See:
M.Cristoforetti, F.Di Renzo, L.S. 1205.3996
M.Cristoforetti, F.Di Renzo, L.S. 1210.8026
M.Cristoforetti, A. Mukherjee, F.Di Renzo, L.S. 1303.7204
M.Cristoforetti, A. Mukherjee, L.S. 1308.0233

31st Lattice Conference — Mainz, 2 August 2013

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Saddle-point integration

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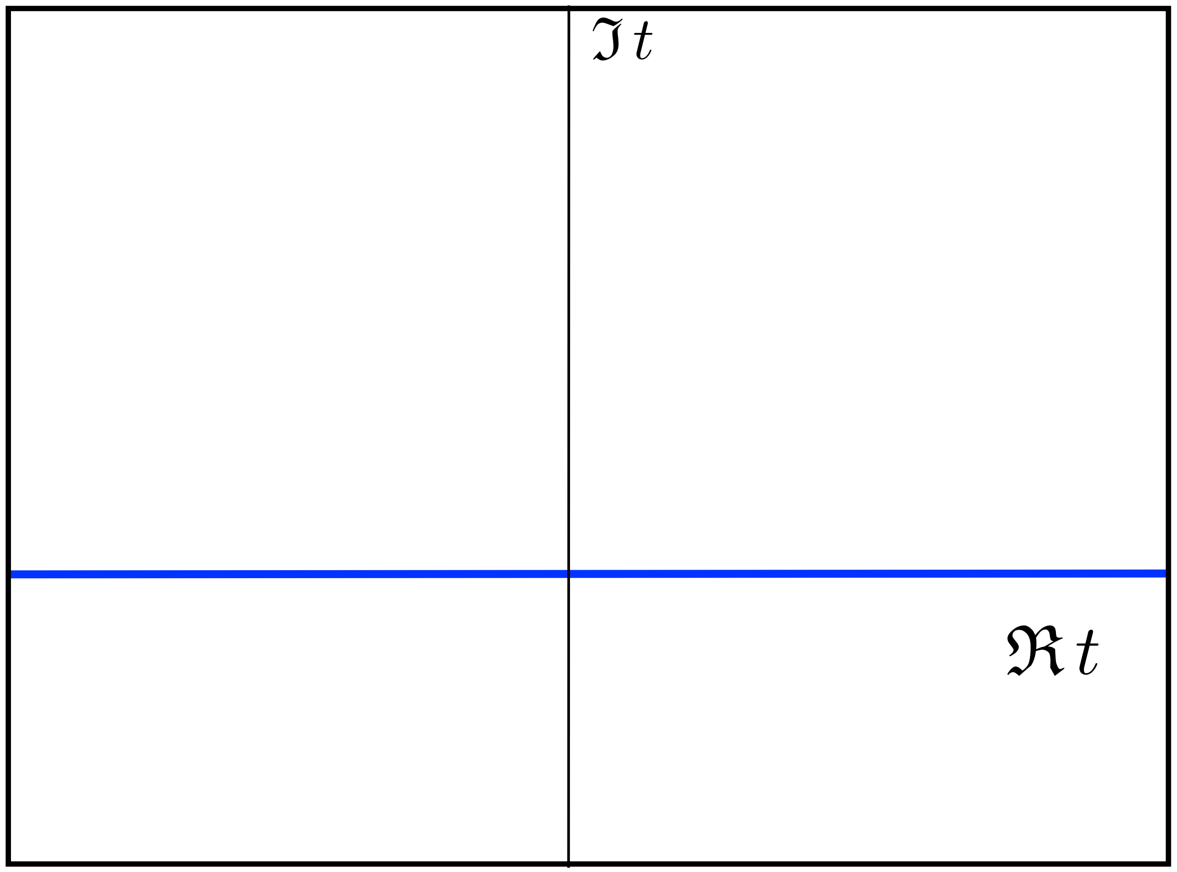

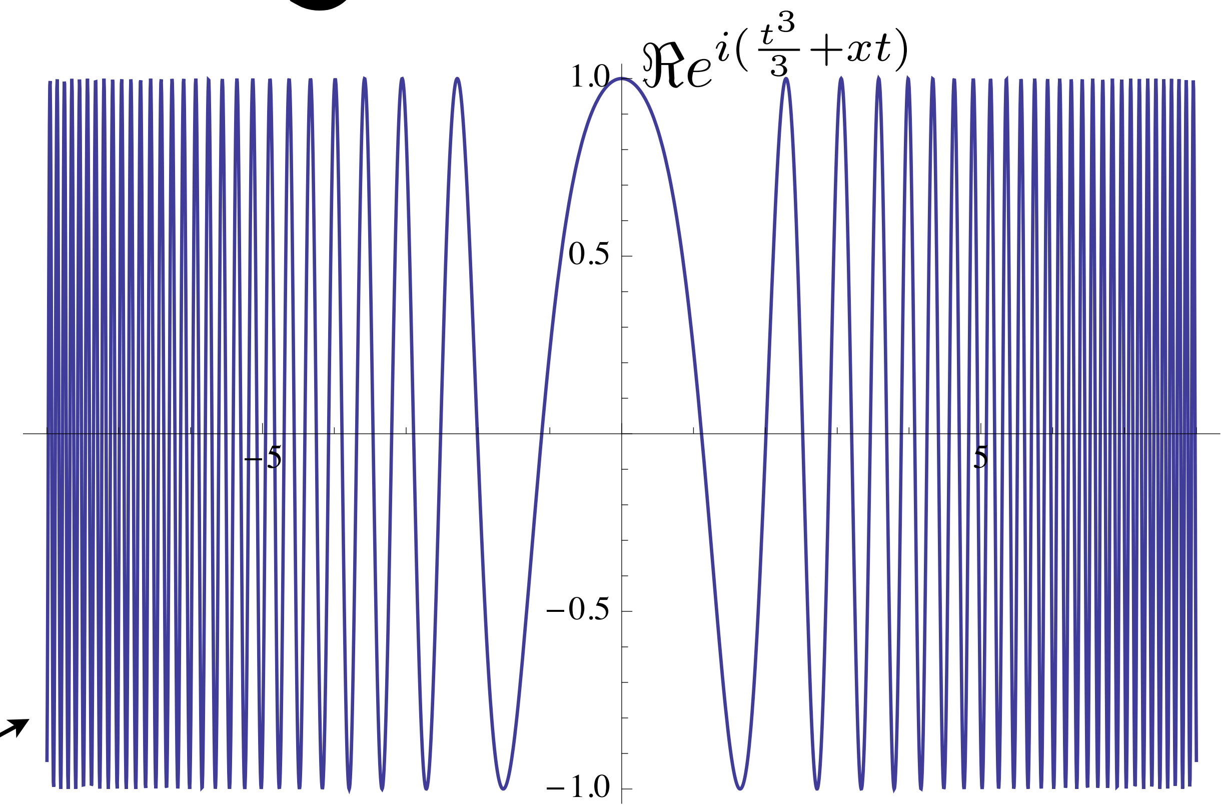

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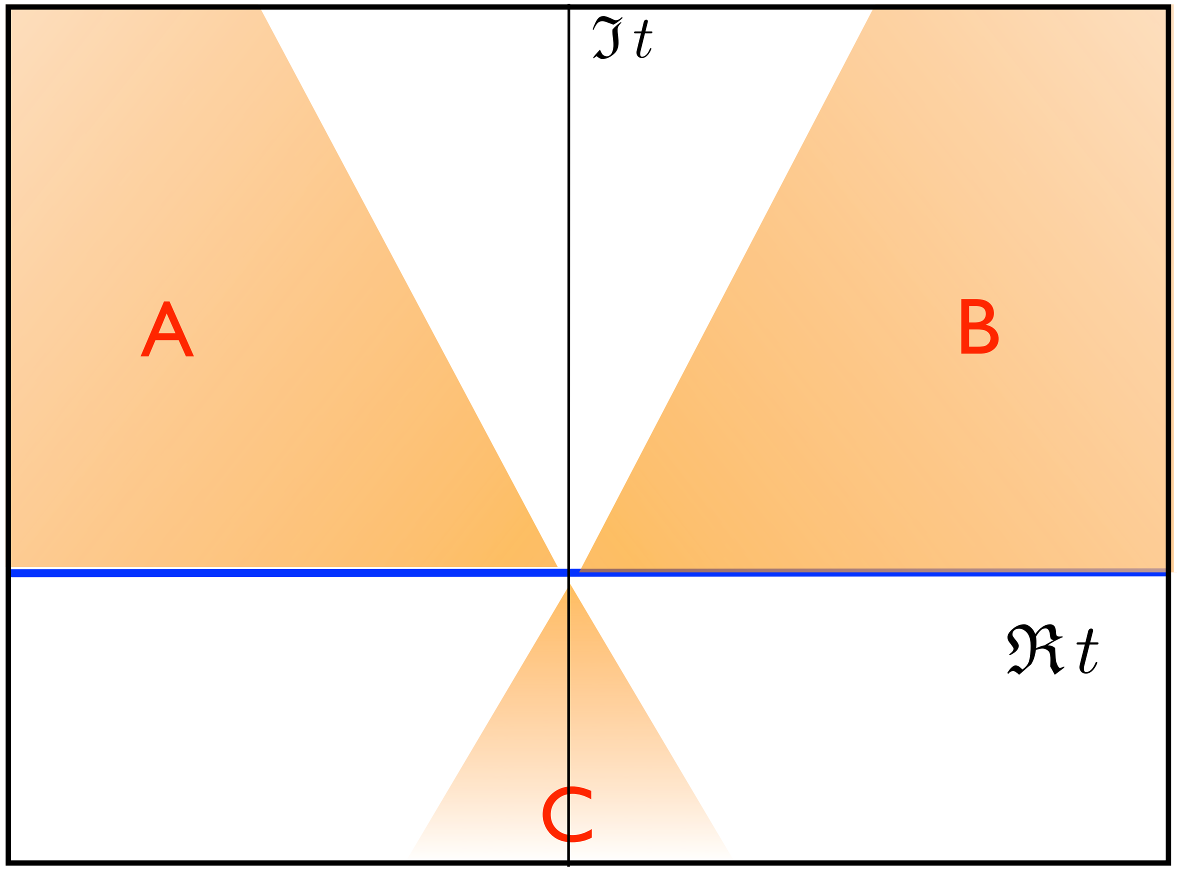

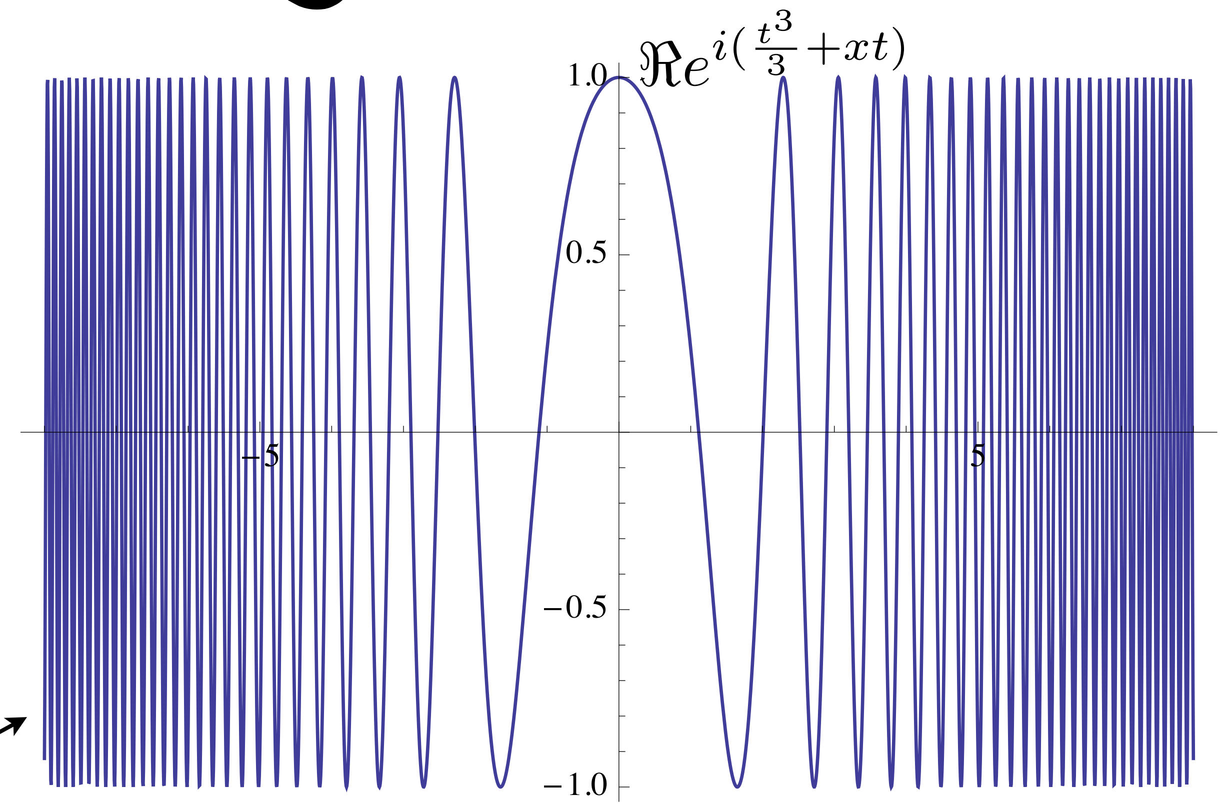

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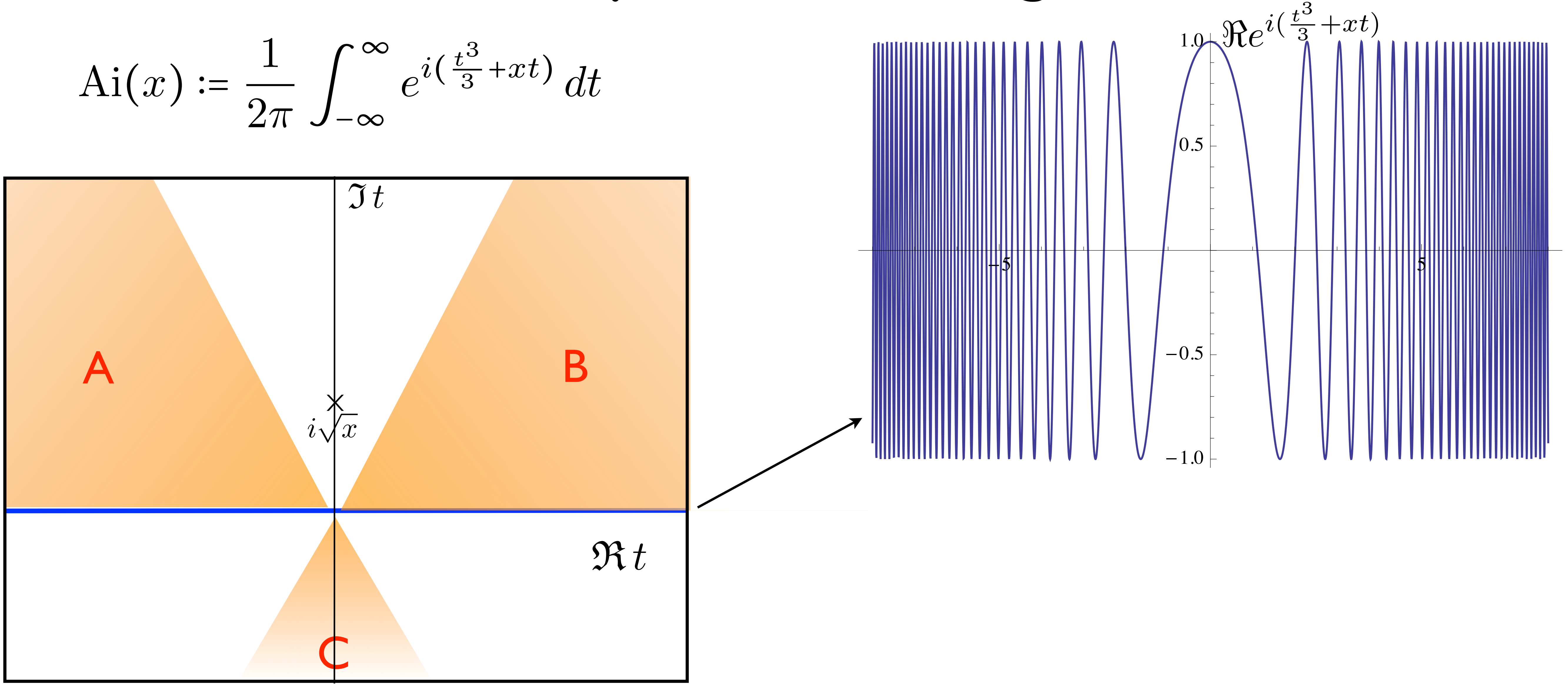

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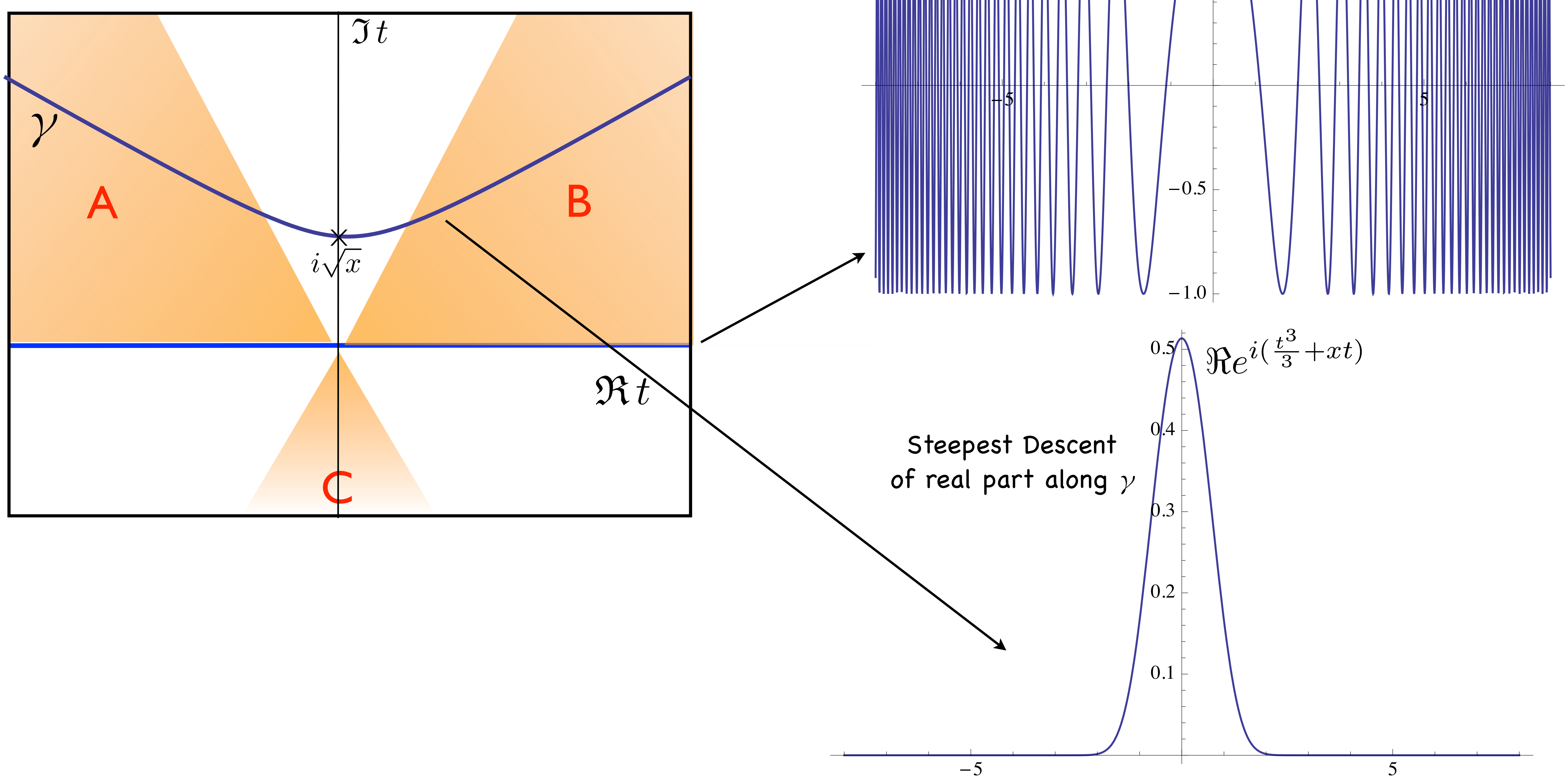

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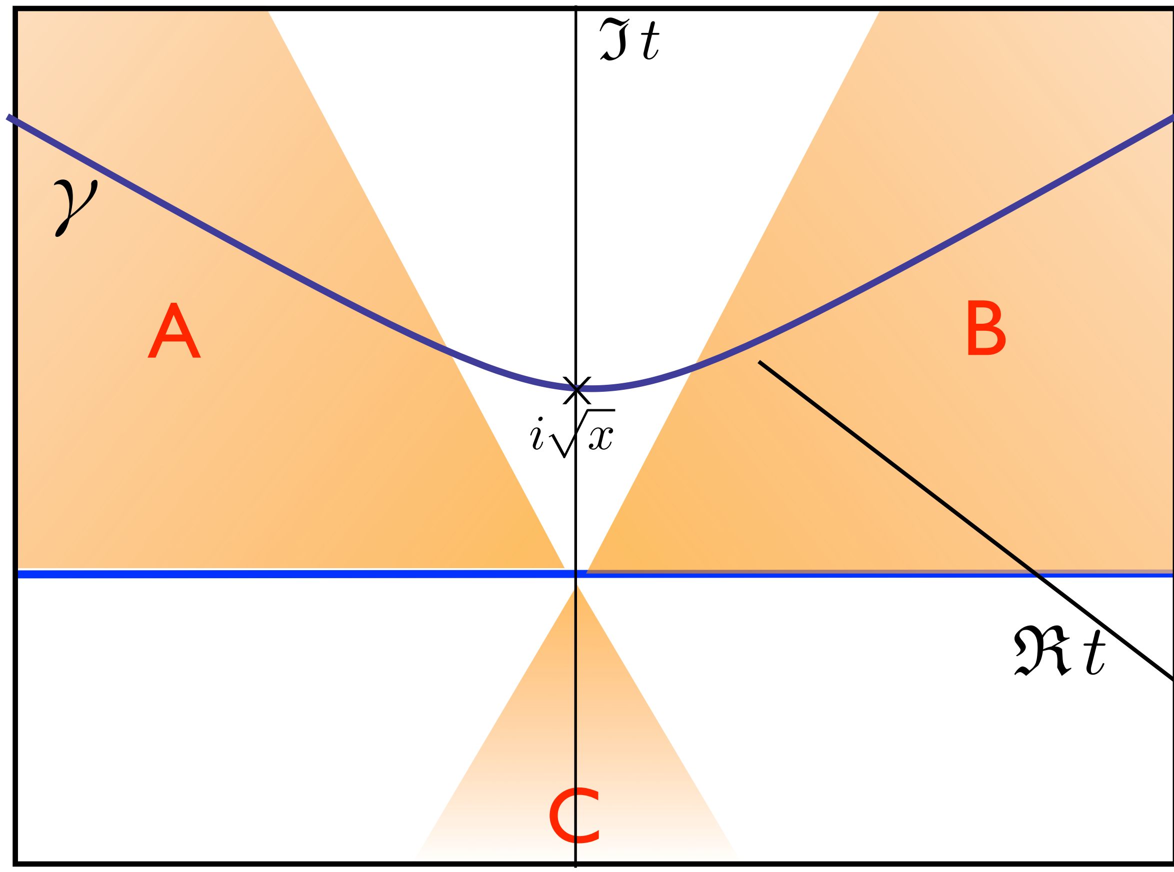

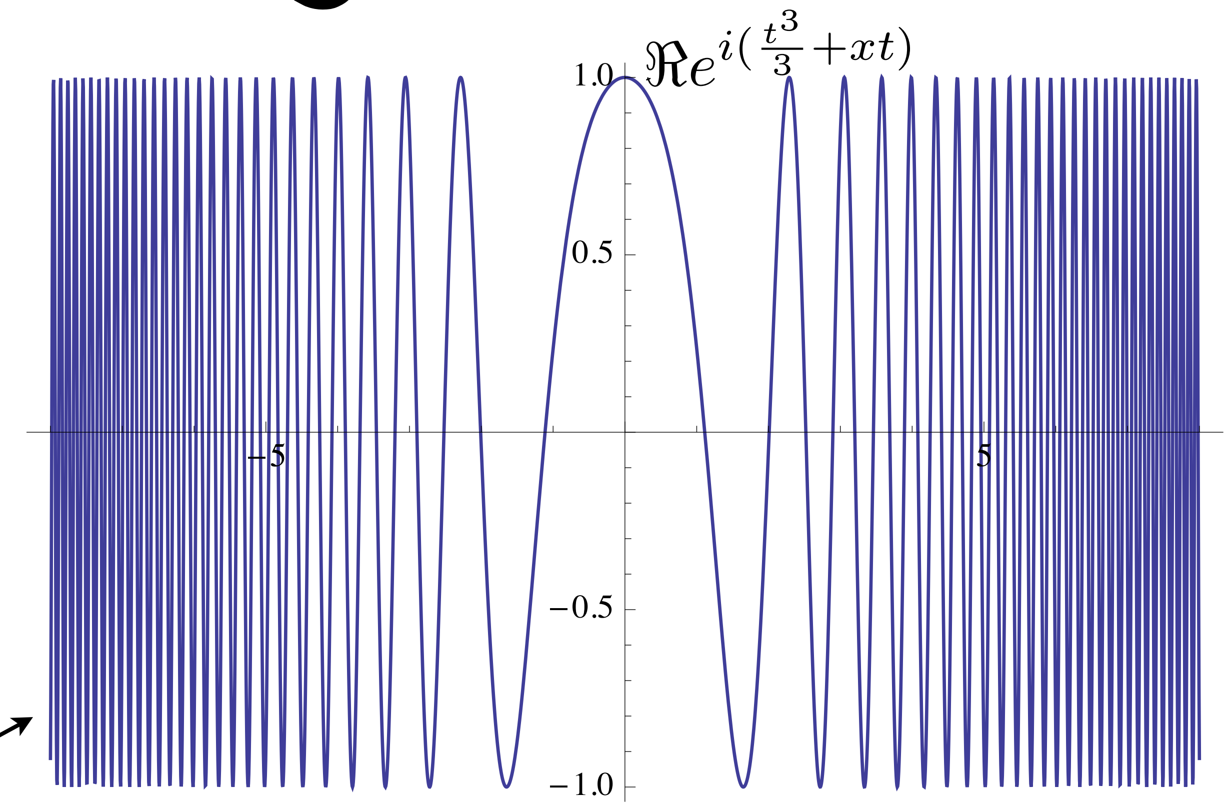

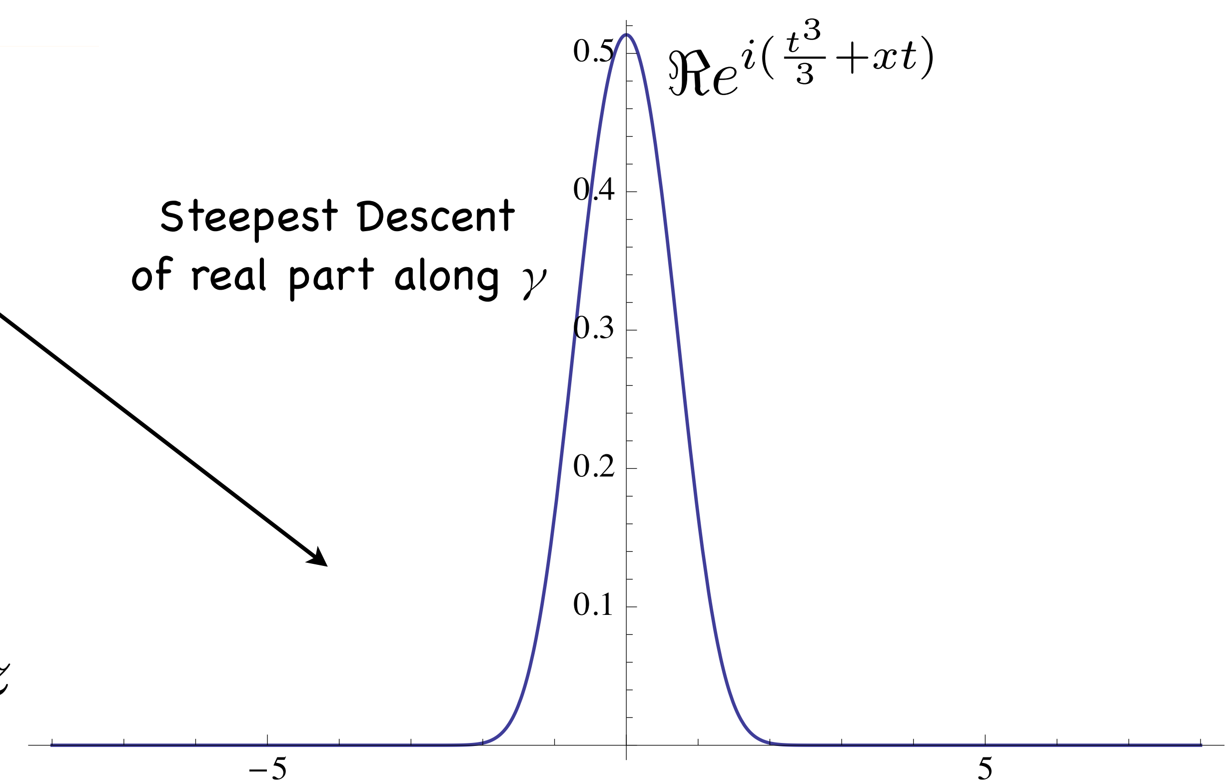

Stationary phase along γ

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

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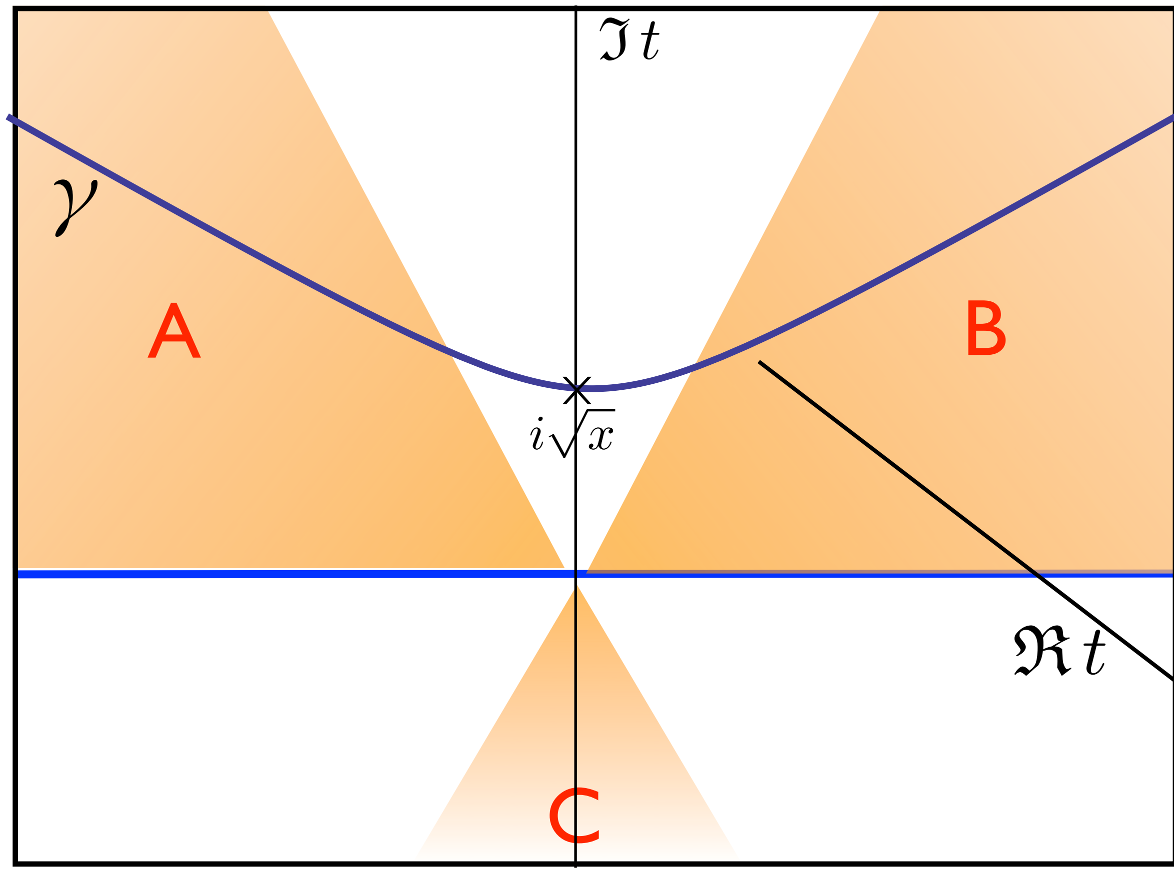

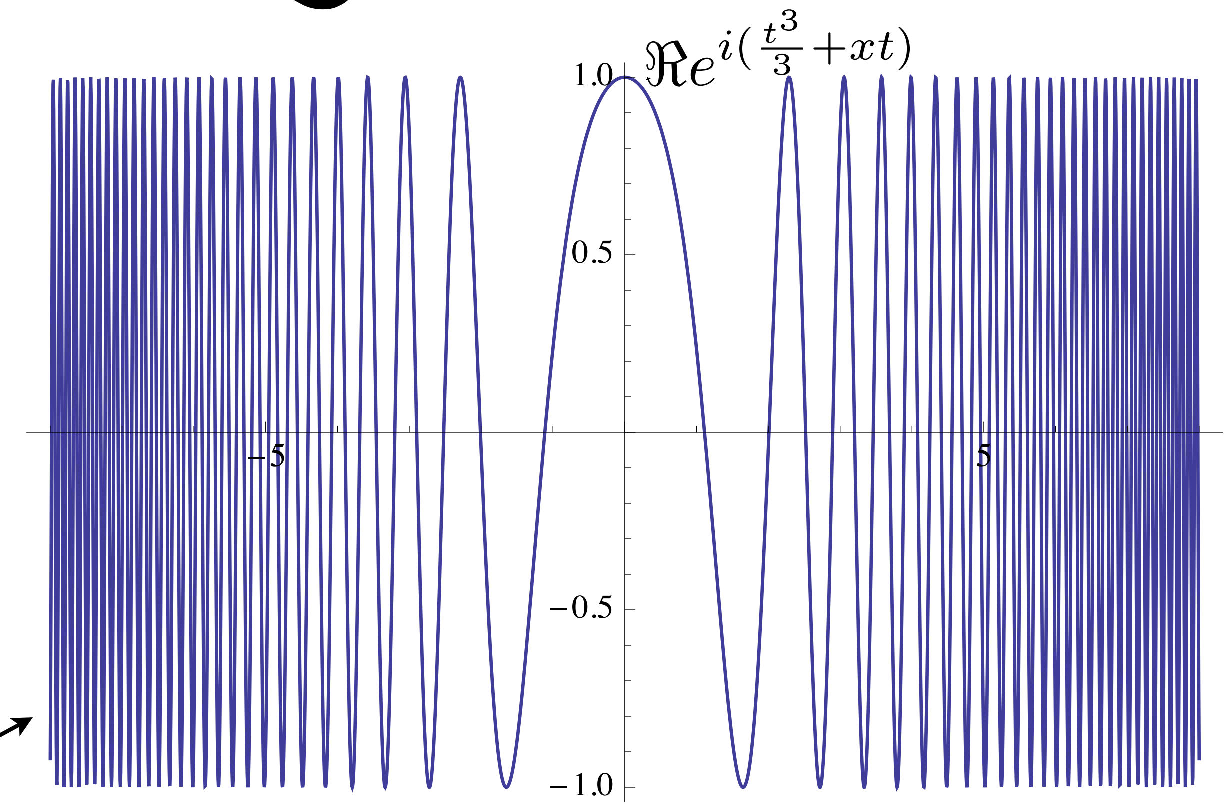

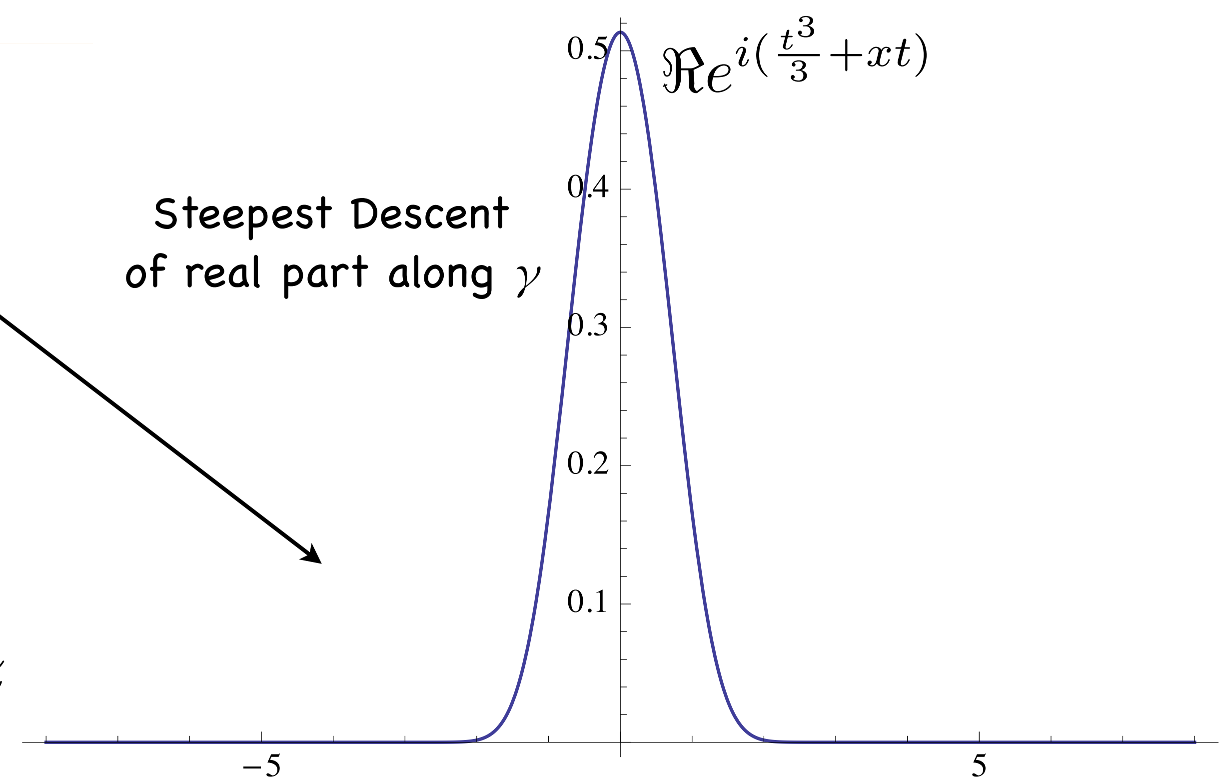

Steepest Descent
of real part along γ

Stationary phase along γ

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

NOTE γ' is not constant, but changes smoothly!

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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.

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  - What about a Monte Carlo integral along the curves of steepest descent (SD)?

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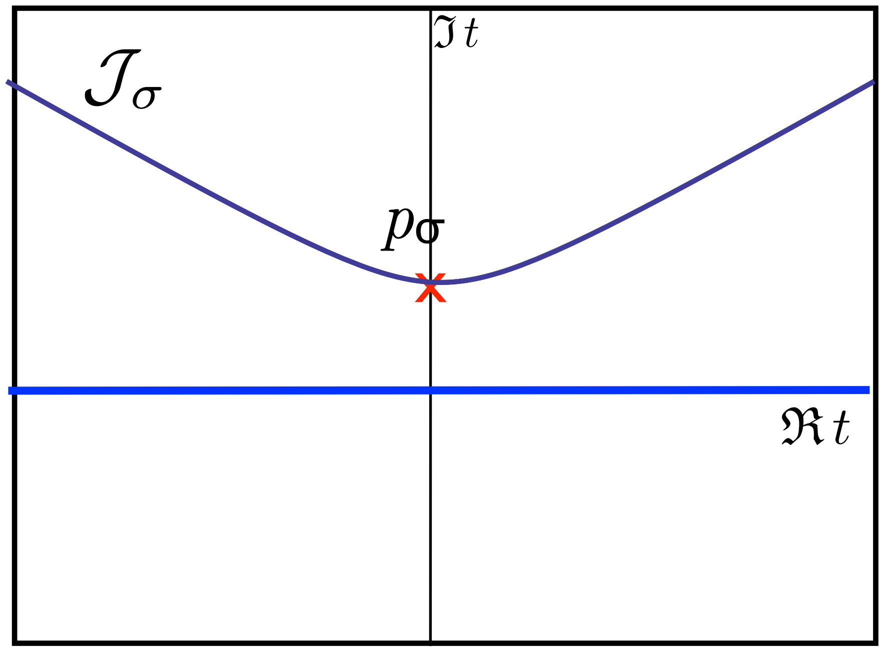

The generalization of the paths of SD are called Lefschetz thimbles $\mathcal{J}_\sigma$,

For each stationary point p_σ of the complexified $f(z)$, $\mathcal{J}_\sigma$ is the union of the paths

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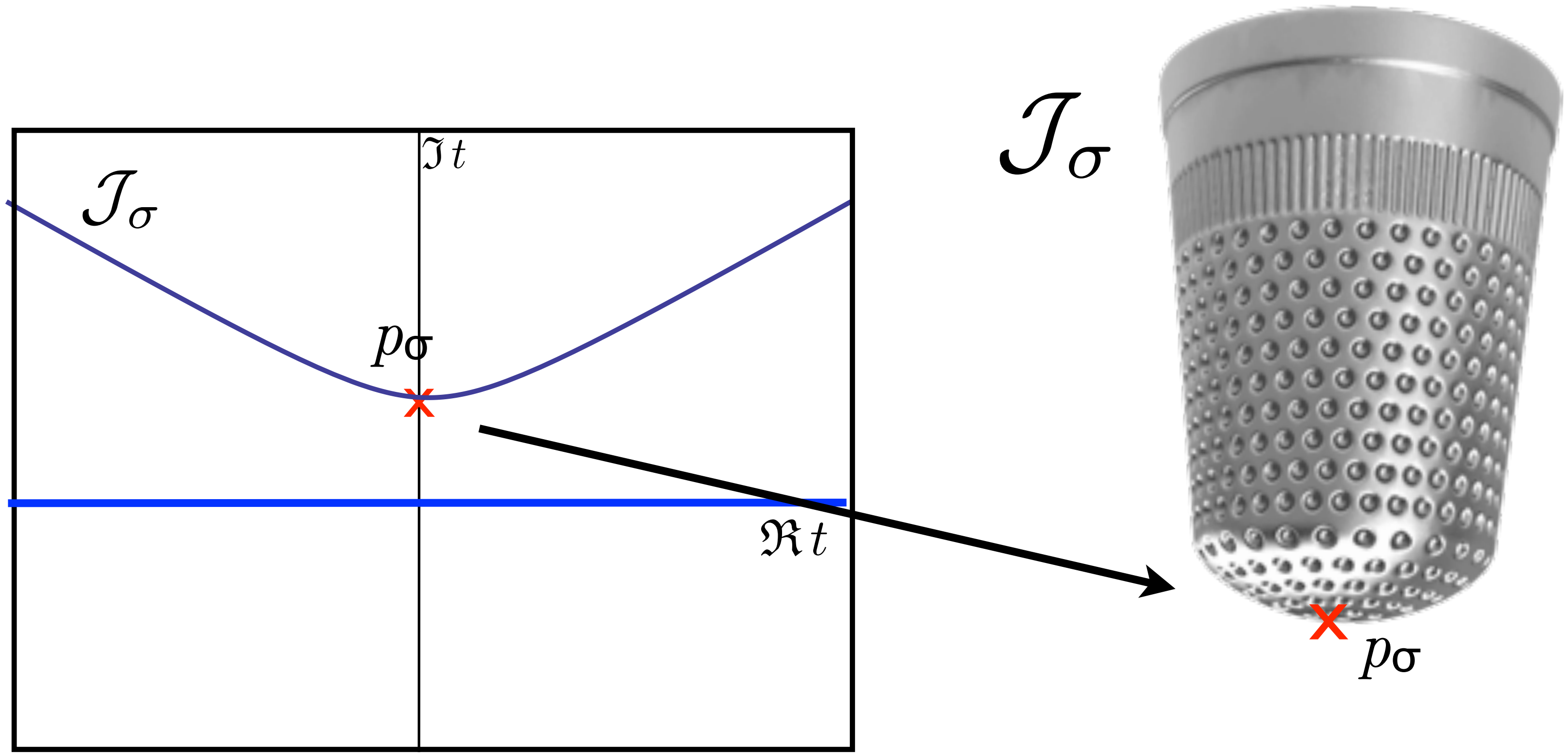

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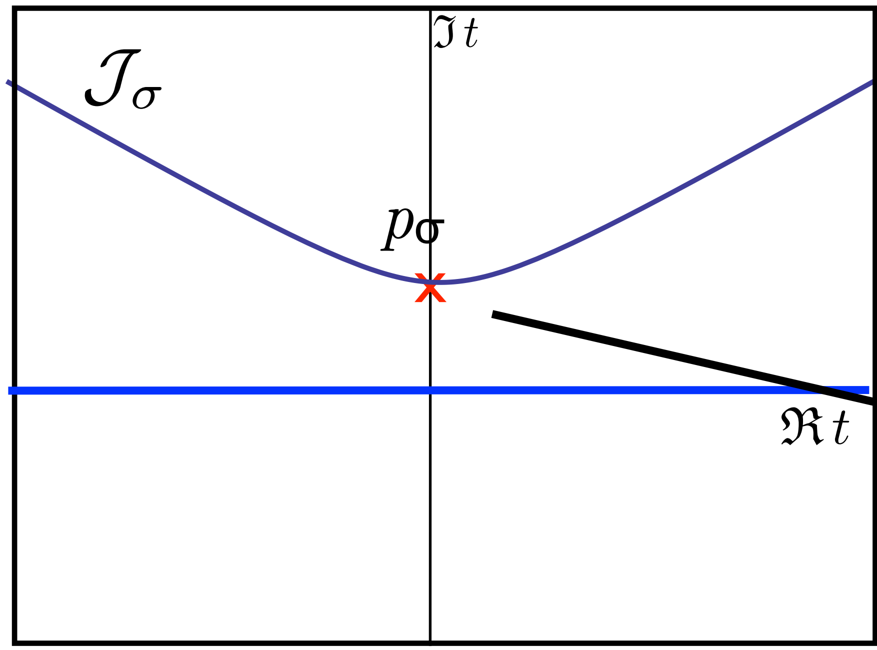

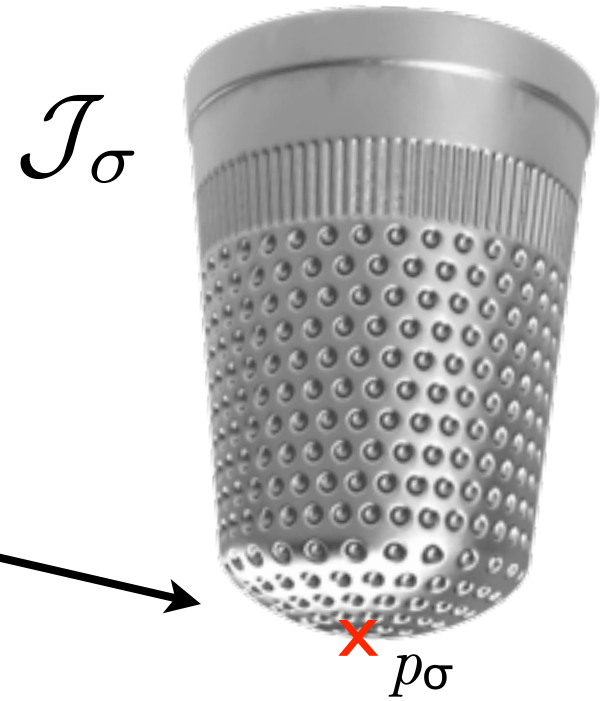

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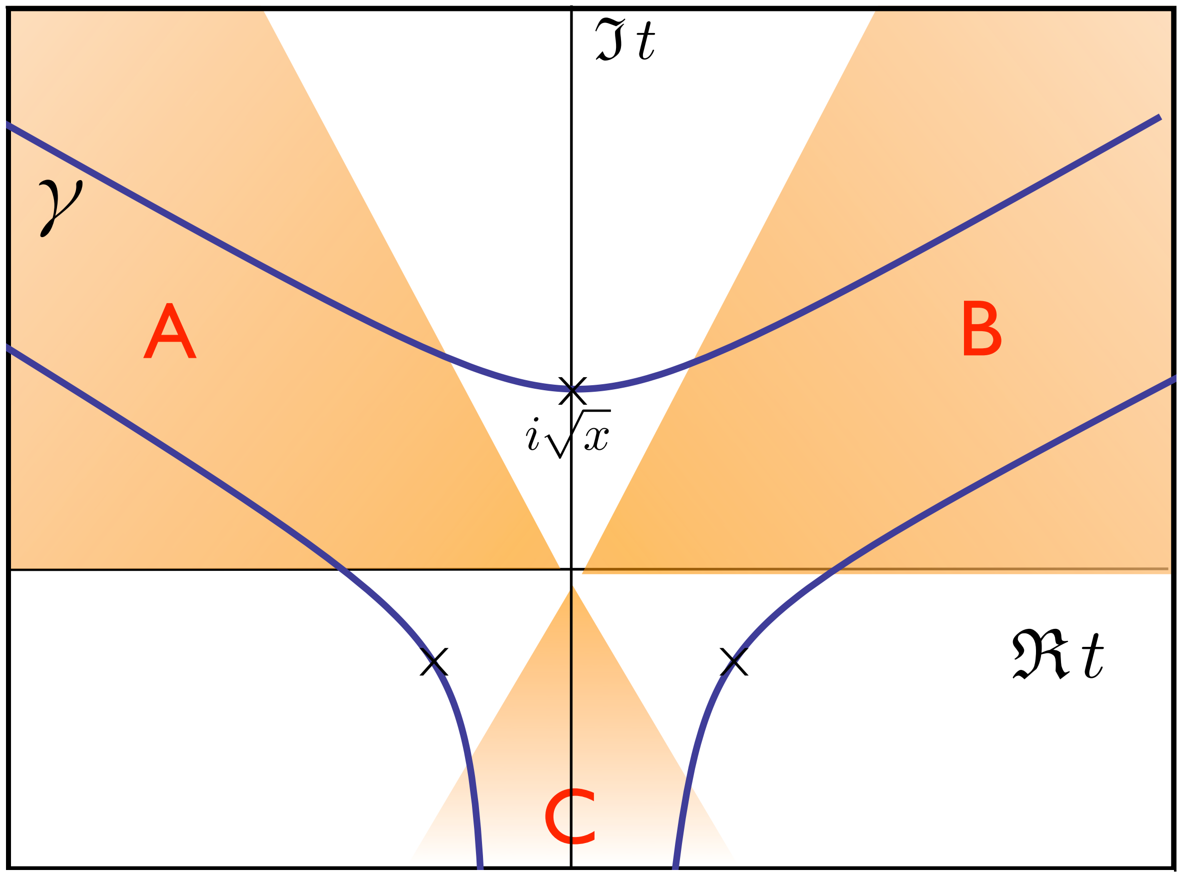
Under suitable conditions on $f(x)$ and $g(x)$, **Morse theory** (Pham '83, Witten '10) tells us that for each cycle C, where the integral converges:

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

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.



$$\mathrm{Ai}(x) := \frac{1}{2\pi}\int_{\mathcal{C}} e^{i\left(\frac{t^3}{3}+xt\right)}\,dt$$

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 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:

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

Is it necessary? No!

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- Consider the global minimum of S_R (e.g. ϕ =0), (which is a stationary point also of the complexified action, in the theories that we consider). We will see that the thimble $\mathcal{J}_0$ associated to that point alone, defines a local QFT with the same degrees of freedom, the same symmetries and symmetry representations and also the same perturbative expansion as the original formulation.

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→ regularize the QFT on that single $\mathcal{J}_0$ attached to the global min.

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

thimble attached to the global minimum of S_R

To be specific, let me discuss a simple model,
which already contains most of the interesting aspects

A complex scalar field with U(1) symmetry

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

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

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- the Symmetries
- Perturbation Theory

What about symmetries? The only interesting one is the

U(1) Symmetry

One can prove that the thimble is invariant under U(1) if $\phi_{\text{glob-min}}$ is so.

Skipping details, the reason is the covariance of the SD equation:

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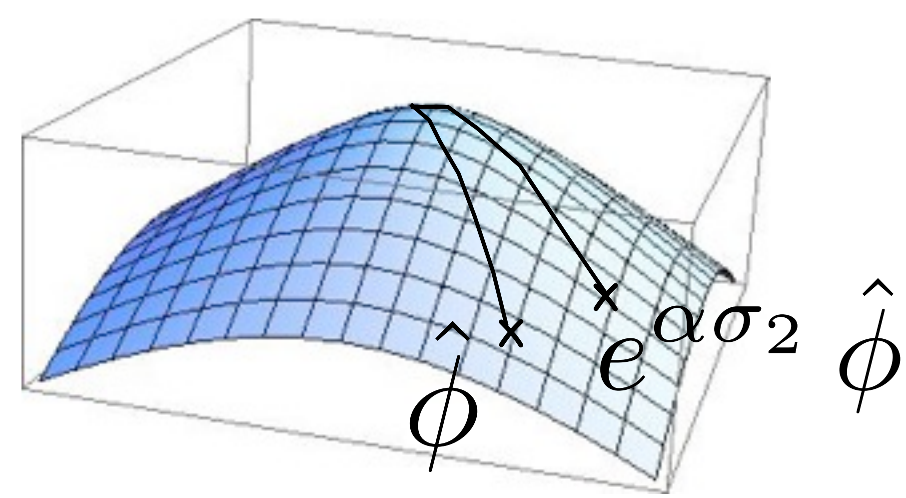
$\Rightarrow$ This can be used to prove Ward Identities.



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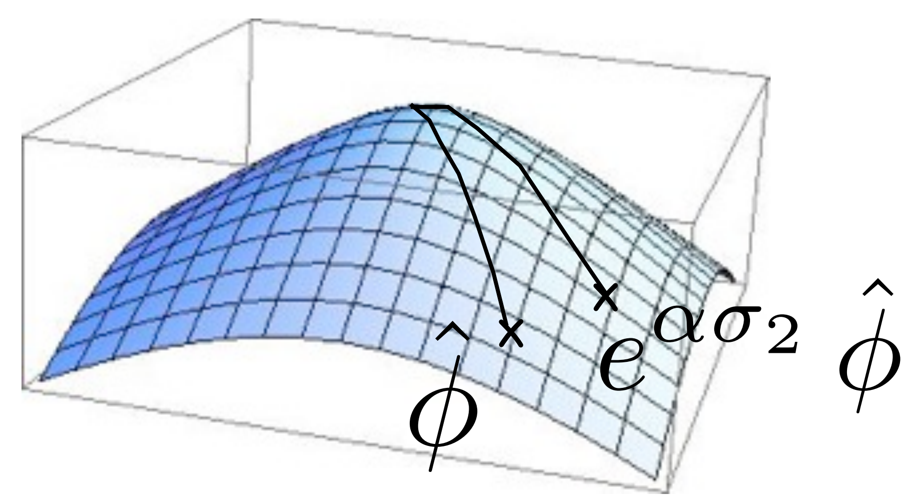

Perturbation Theory

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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The integral is constant under small variations of the path around the path of steepest descent.

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Message #1

Designing regularizations that are better suited to deal with the sign problem is possible and should be pursued.

A Monte Carlo algorithm for a Lefschetz thimble?

Monte Carlo on a thimble

I want to compute: $$\frac{1}{Z_0}\int_{\mathcal{J}_0}\prod_x d\phi_x\, e^{-S[\phi]}\mathcal{O}[\phi]$$

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Bounded, real action: use MC.

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... But it is feasible in 5D !!

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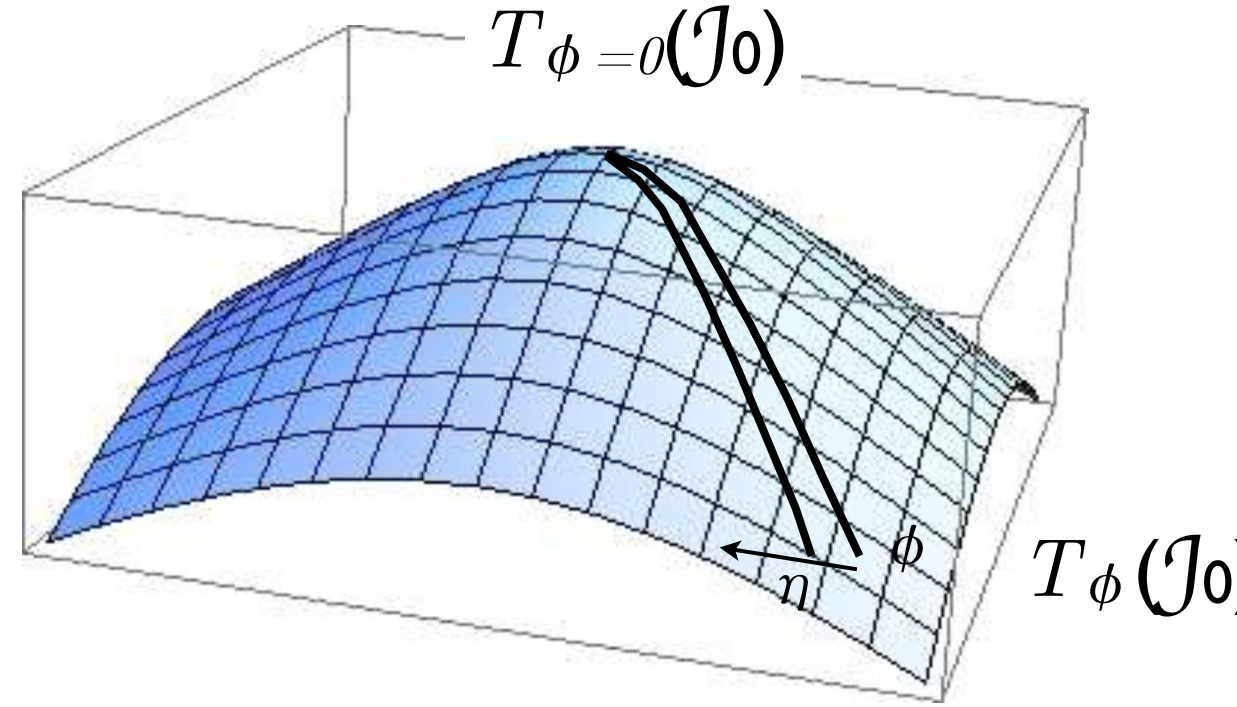

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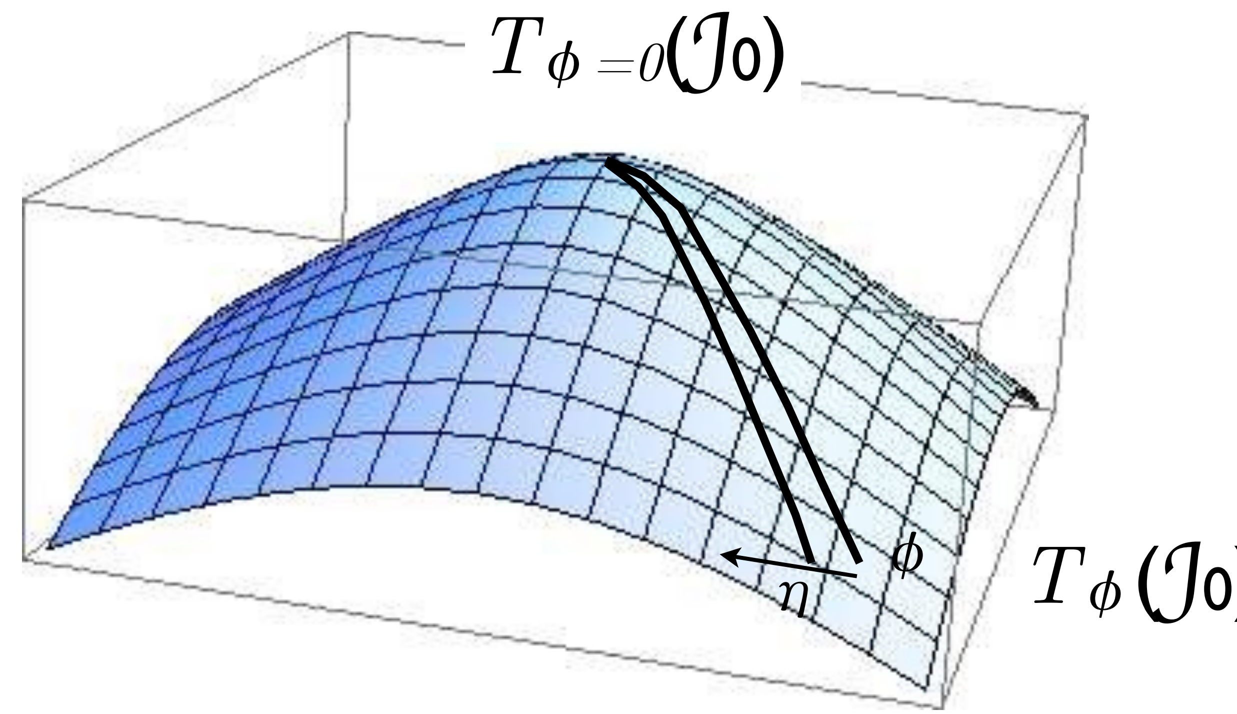

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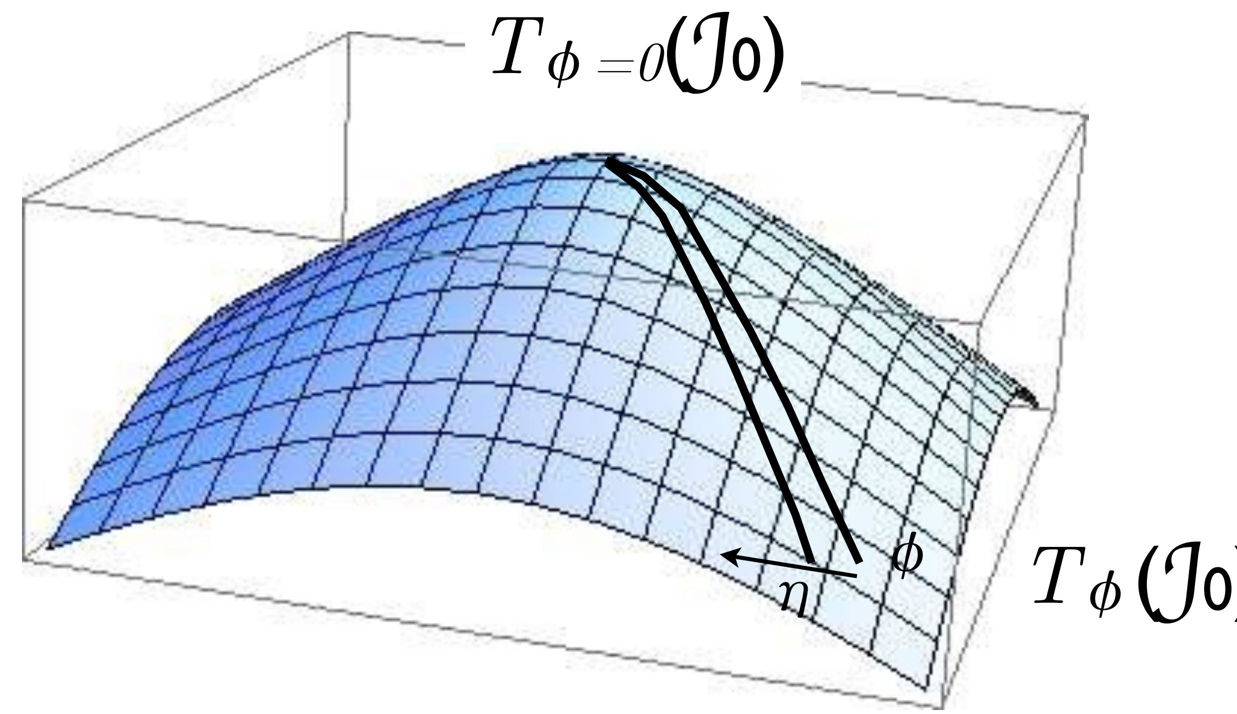

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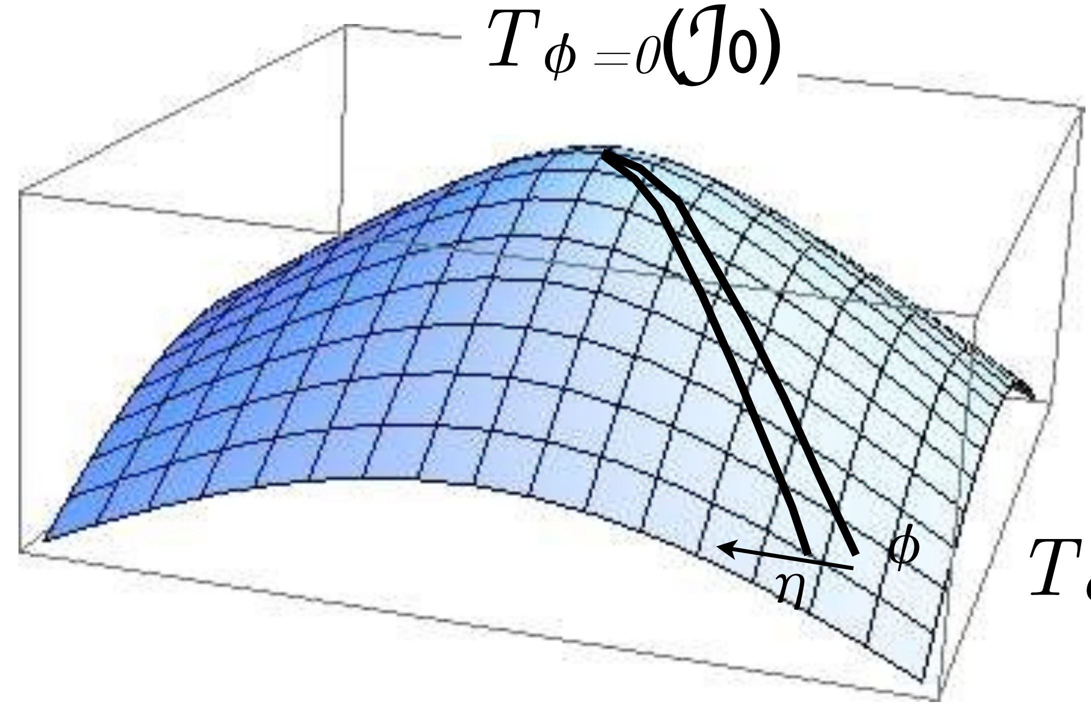

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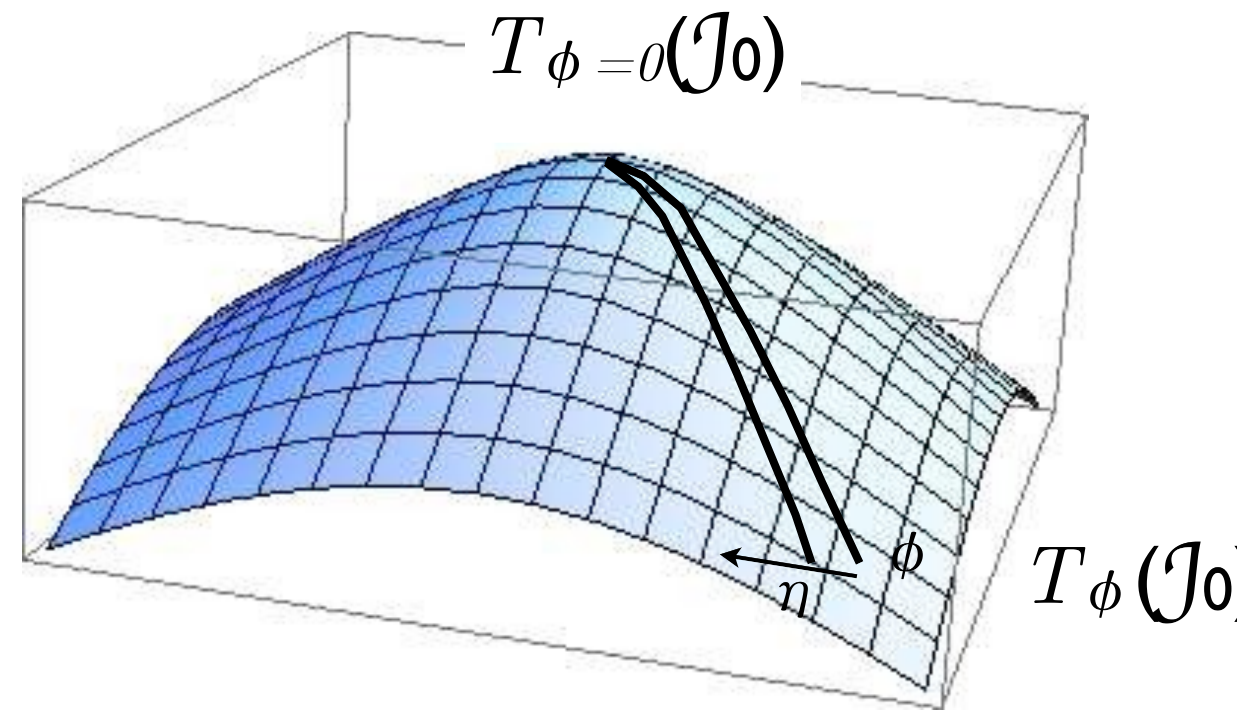

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GREAT!!

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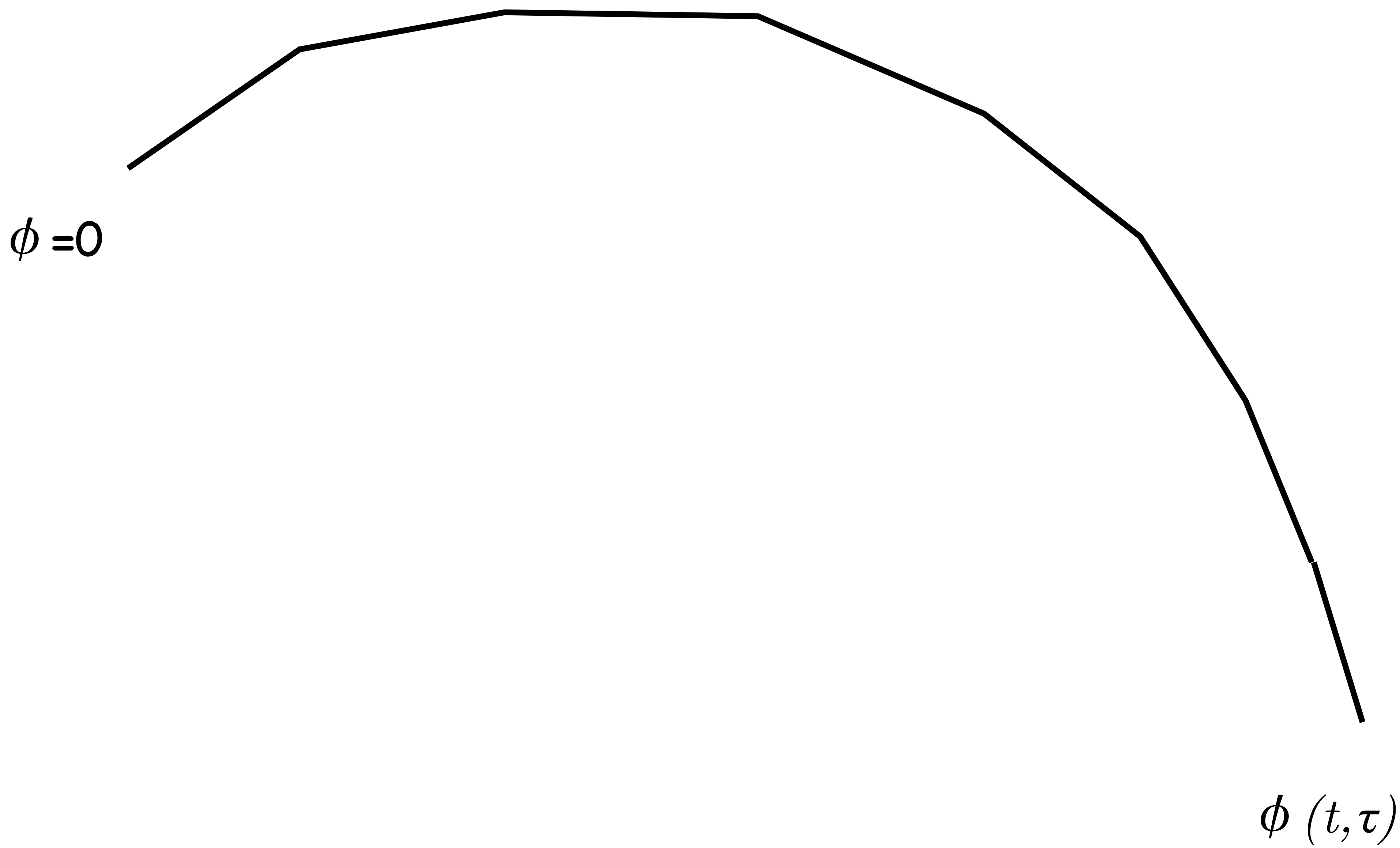

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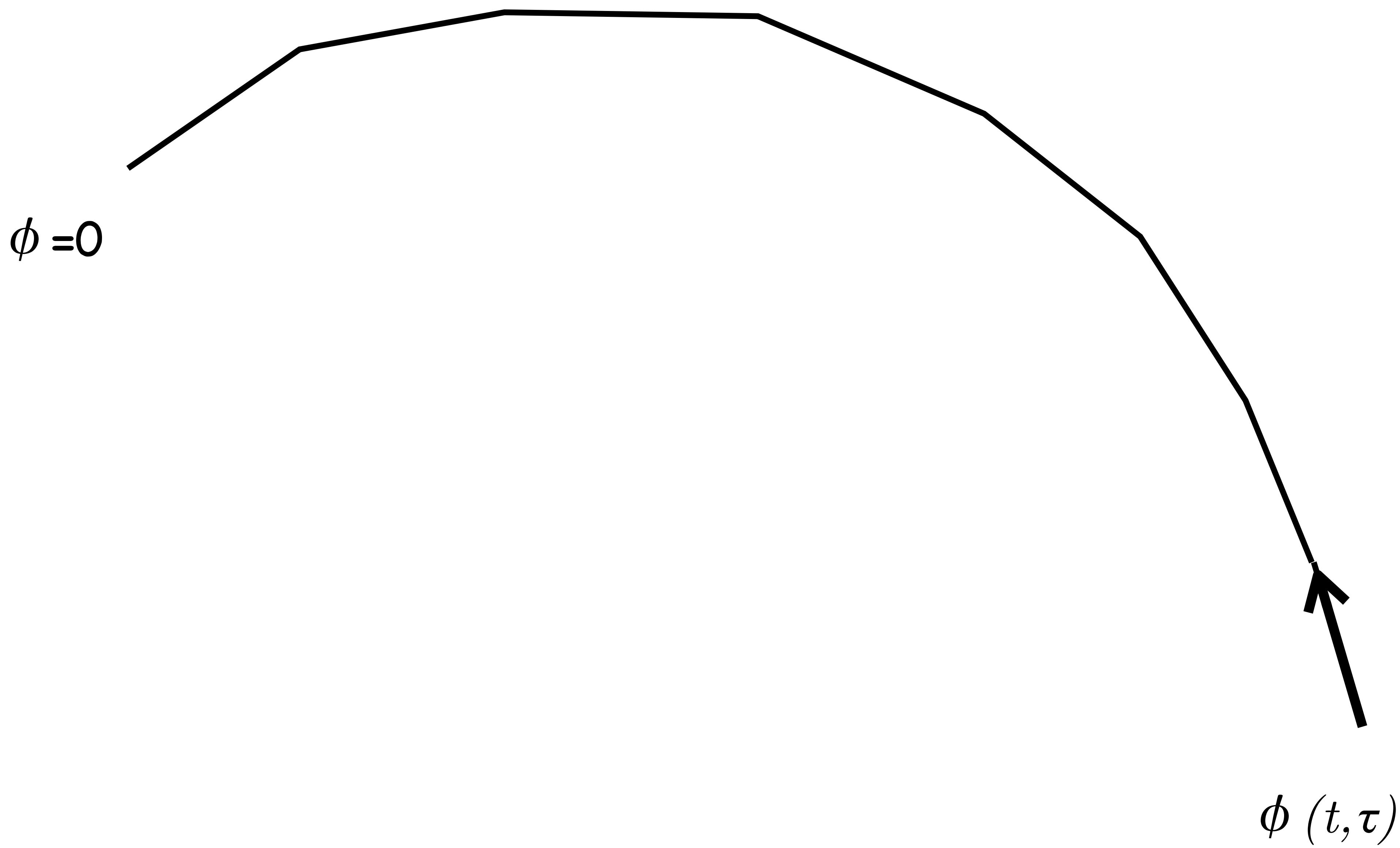

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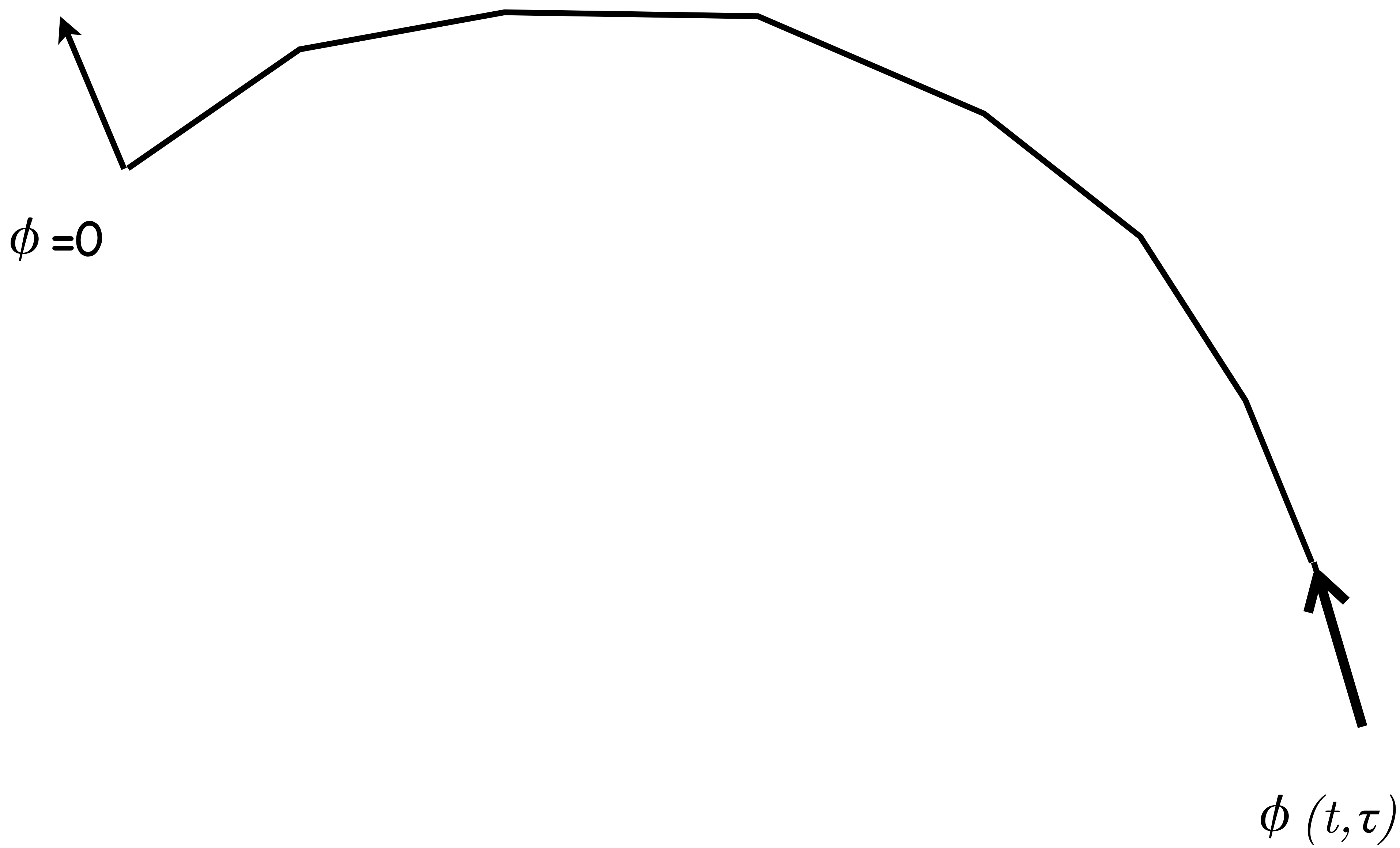

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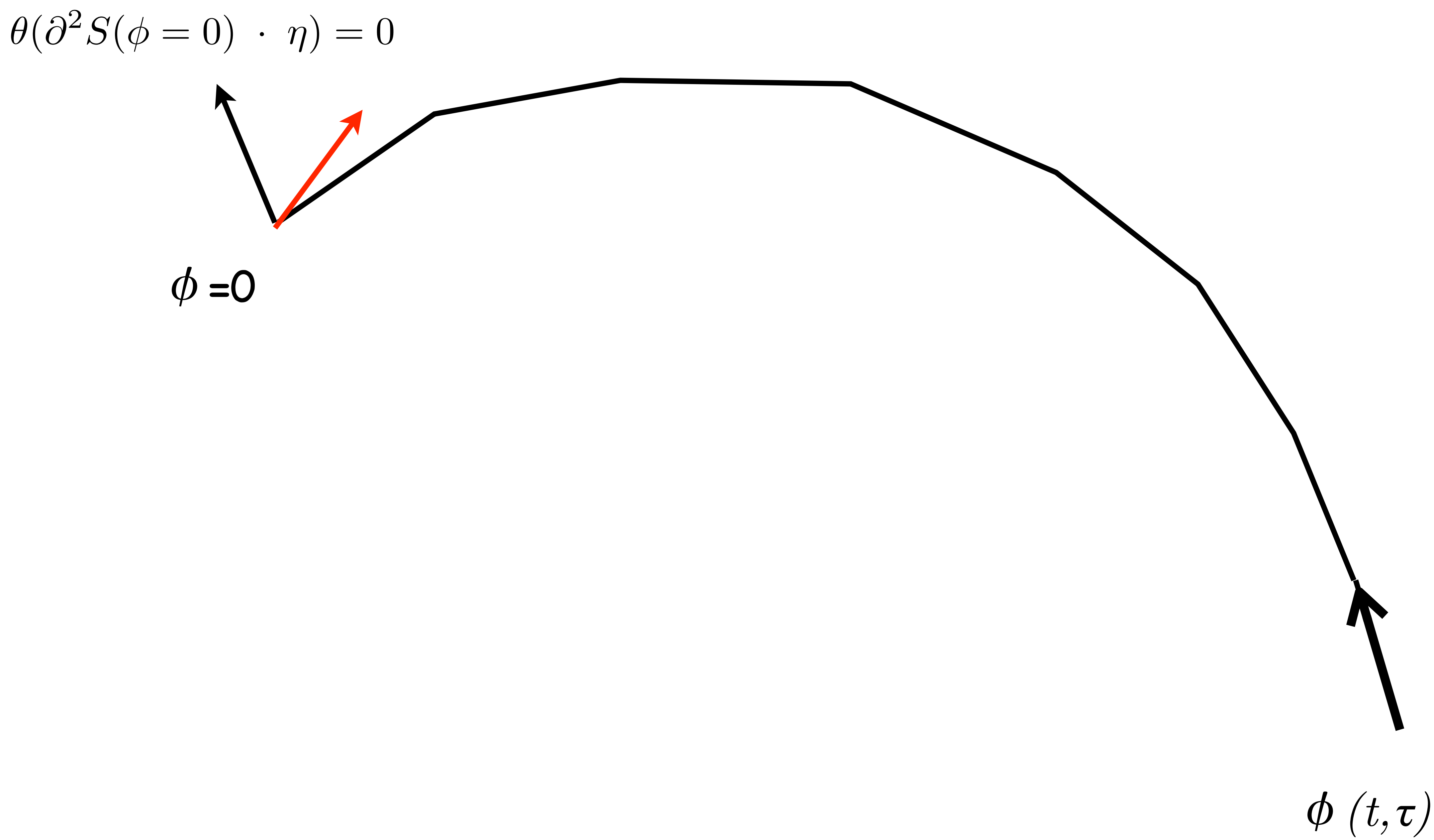

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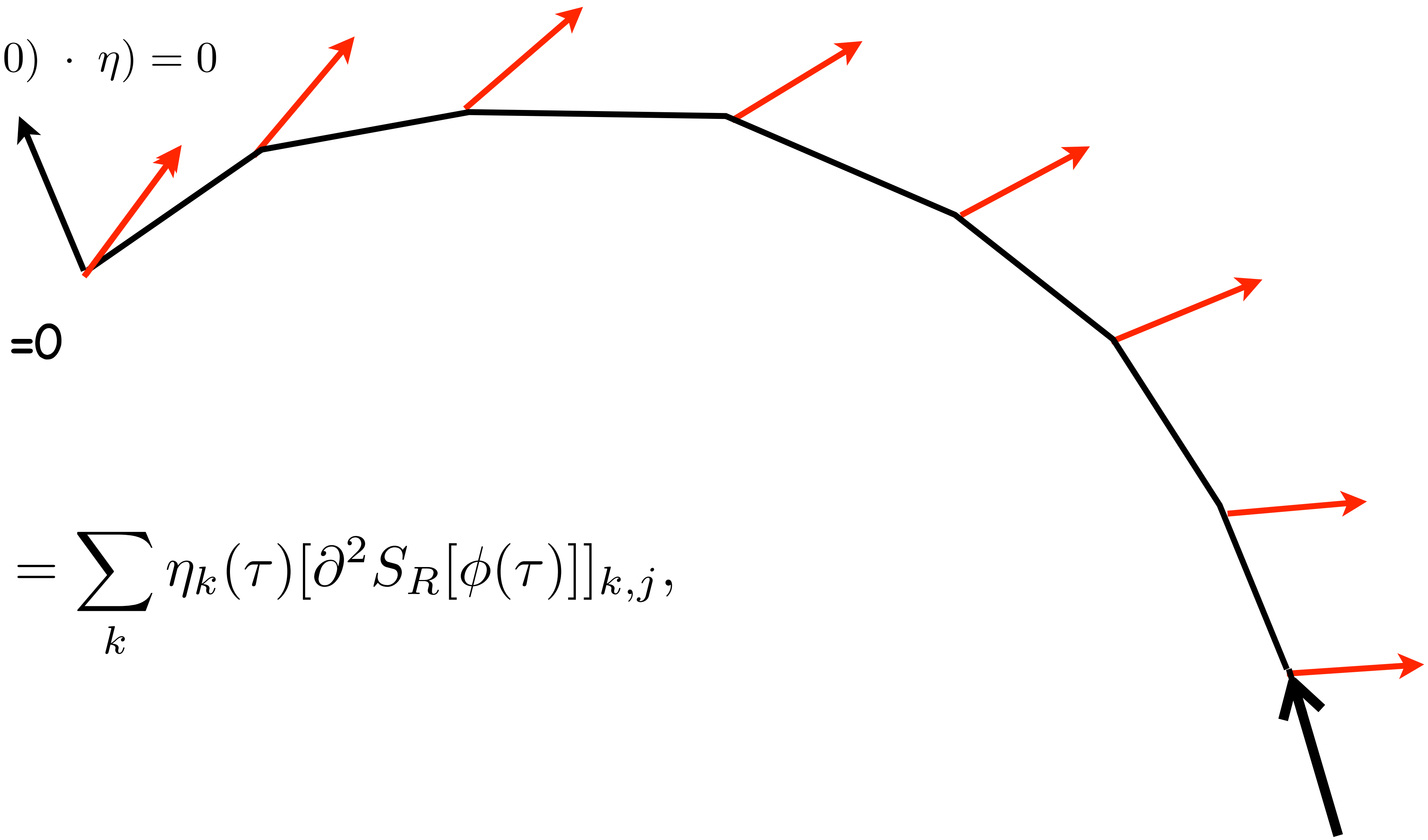

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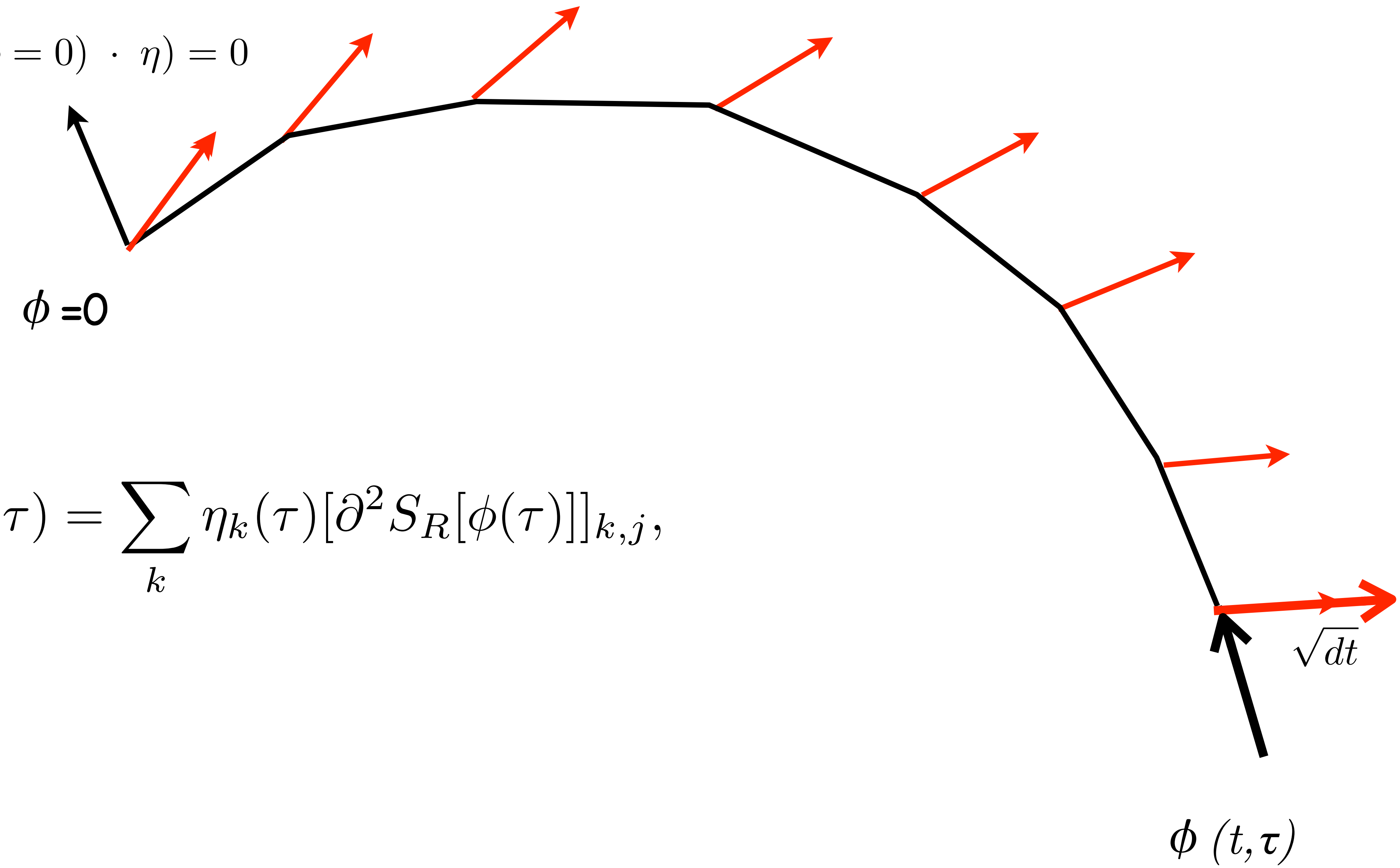

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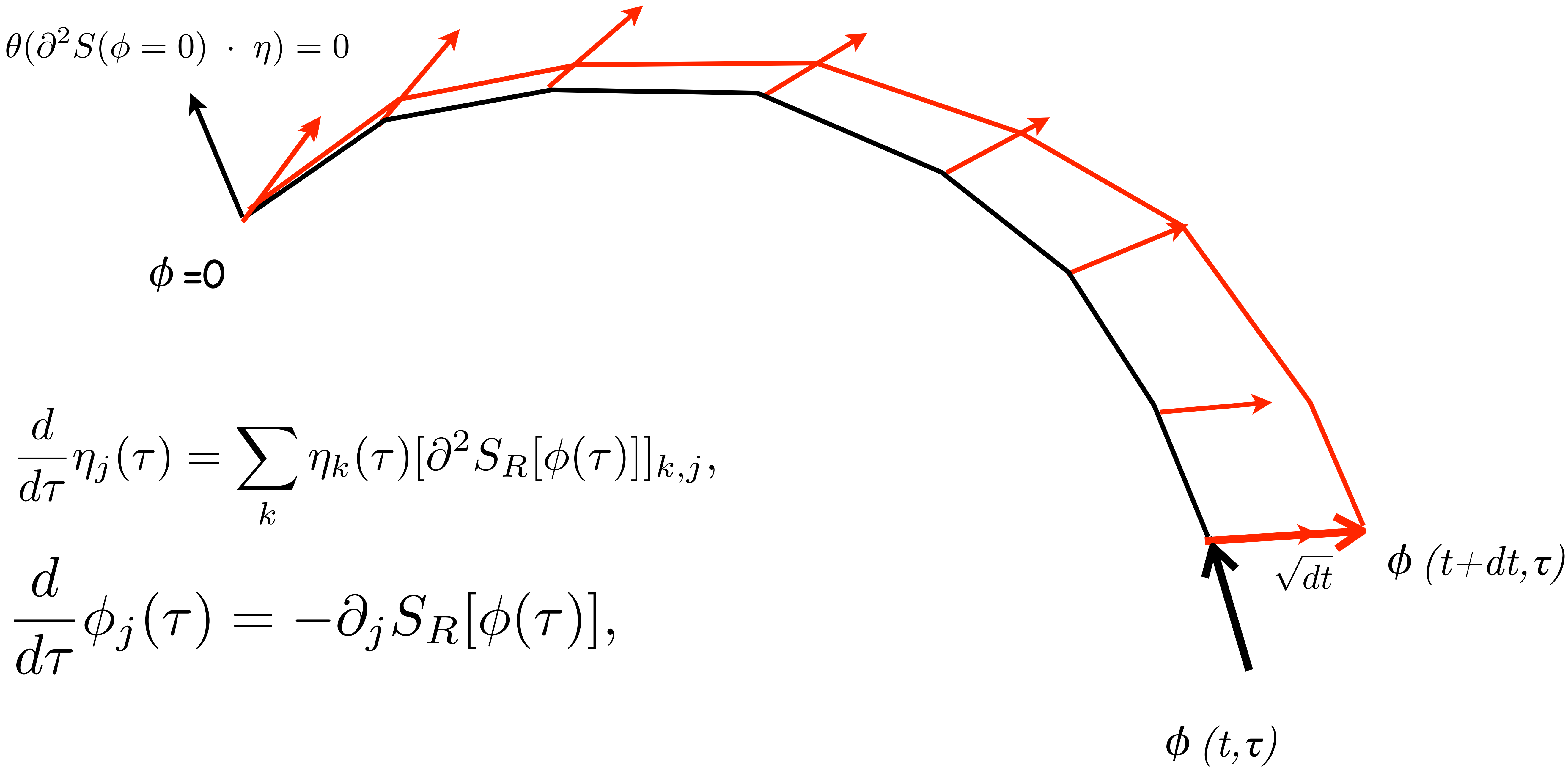

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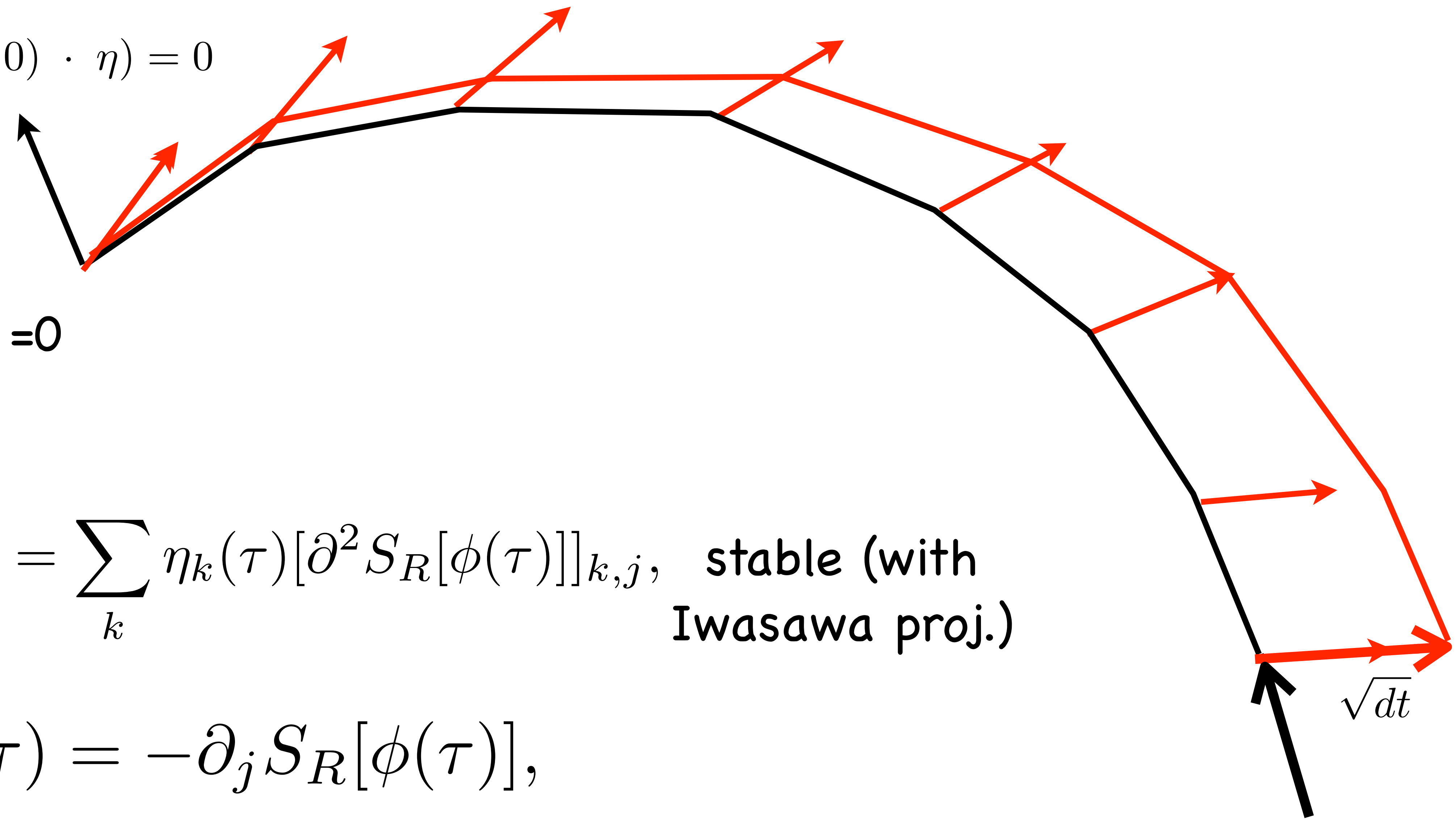

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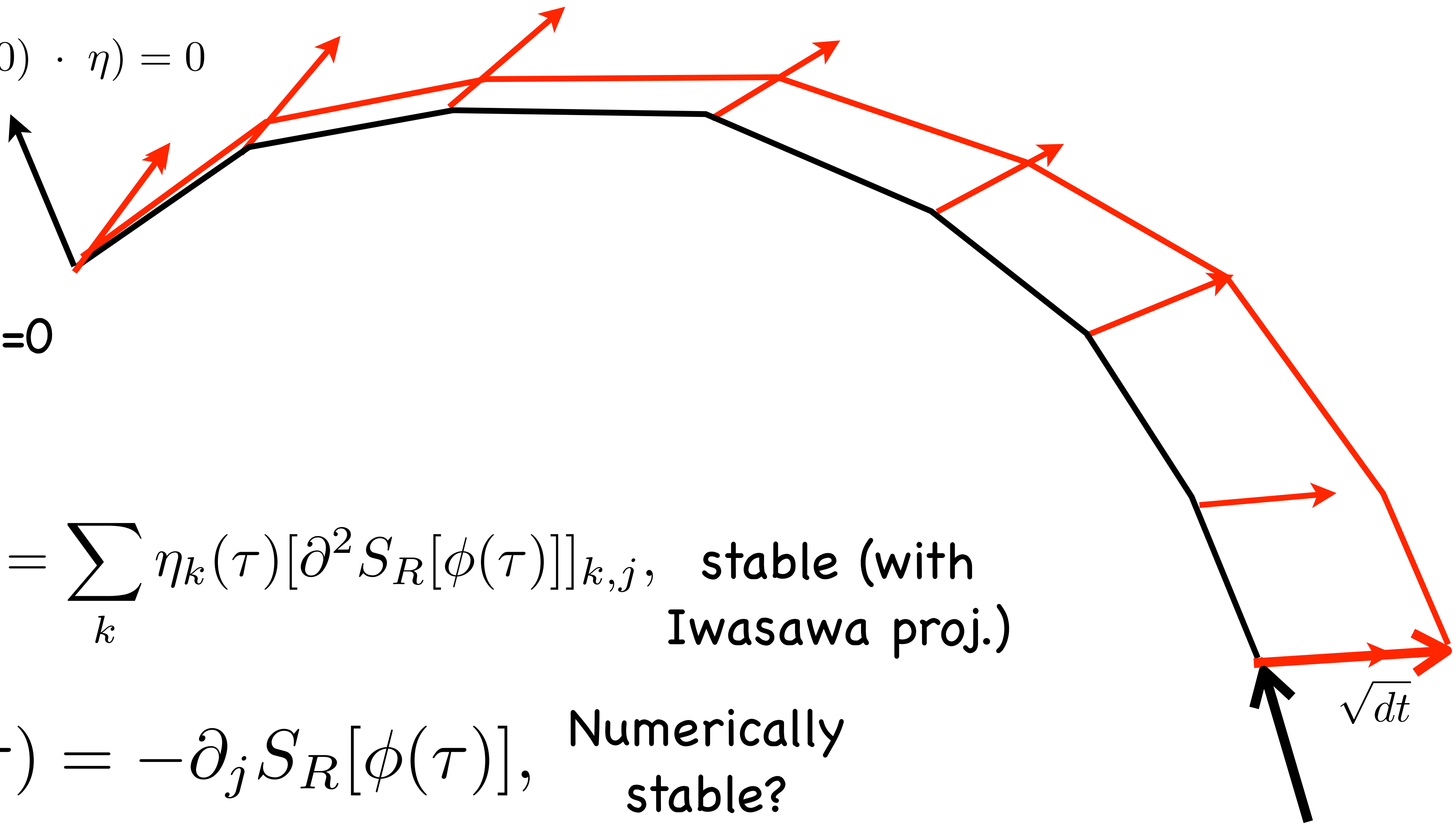

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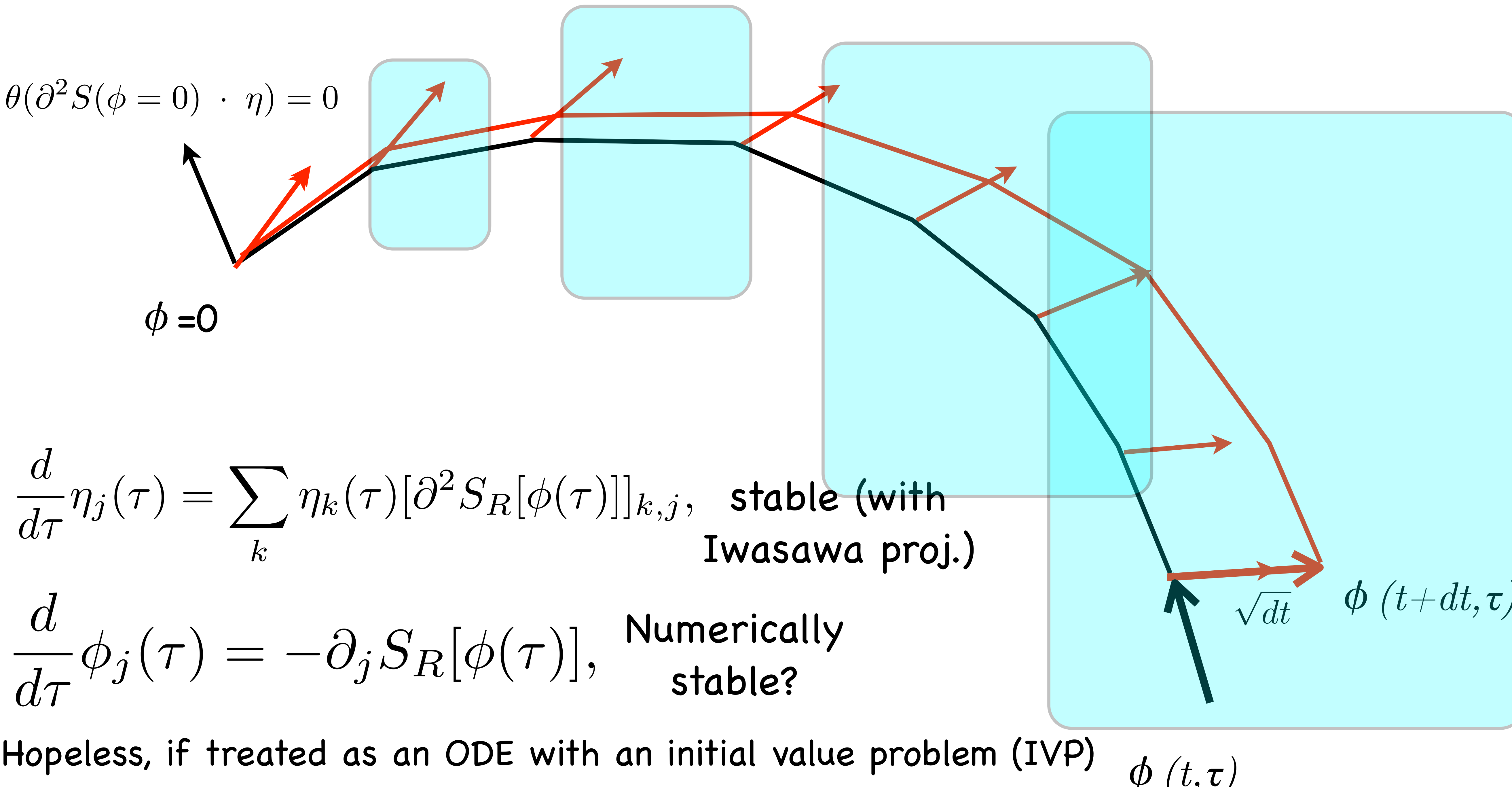

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But can be made stable if formulated as a 5D **BVP**

Residual phase

As noticed at the beginning, there is still a phase

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Does it lead to a "**sign problem**" ? (which means $\langle d\Phi\rangle \approx e^{-V}$)

We cannot "prove" it does not, BUT:

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But it should be computed and it is expensive.

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We don't know in general, but see next talk.

What about QCD ?!?

Complexification

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

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

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.

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

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:

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

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 <u>non-degenerate critical point</u> with that of <u>non-degenerate critical manifold</u> (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 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 $SL(3,\mathbb{C})$.

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

Proof of gauge invariance is now essentially identical to the proof of U(1) global symmetry for the scalar case.

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

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

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

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

Proof of gauge invariance is now essentially identical to the proof of U(1) global symmetry for the scalar case.

<u>Note 1</u>: This means that also Ward Identities are fulfilled.

Gauge Symmetry of the thimble

Consider the SD equation:

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Under gauge transformations it changes as:

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

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

Proof of gauge invariance is now essentially identical to the proof of U(1) global symmetry for the scalar case.

Note 1: This means that also Ward Identities are fulfilled.

Note 2: 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.

Algorithm

Only few difference w.r.t. the scalar case.

Langevin Eq:

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

Transport equation:

$$\frac{d}{d\tau}\eta_j(\tau) = \eta_{j'}(\tau)\nabla_{j'}\nabla_j S_R,$$

Conclusions

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- Our first applications will be discussed in Marco's talk.