The sign problem and the Lefschetz thimble

Luigi Scorzato

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"Heavy quarks and quarkonia in thermal QCD" — 2 April 2013

Let me review what the sign problem is.

Lattice simulations of QCD at finite density are hindered because

$$\langle \mathcal{O} \rangle = \frac{\mathrm{Tr}\ \left[\mathcal{O}\, e^{-(\mathcal{H}-\mu_B \mathcal{N}_q)/T}\right]}{\mathrm{Tr}\ \left[e^{-(\mathcal{H}-\mu_B \mathcal{N}_q)/T}\right]} = \frac{\int dU\, \mathcal{O}[U]\, e^{S_G[U]} \det(Q[U;\mu_B])^{N_f}}{\int dU\, e^{S_G[U]} \det(Q[U;\mu_B])^{N_f}}$$

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But, when $\det[Q]$ oscillates strongly, reweighting is not effective:
the cost is expected to scales as ~ e^V,
and even lattices as tiny as $V=4^4$ are unfeasible.

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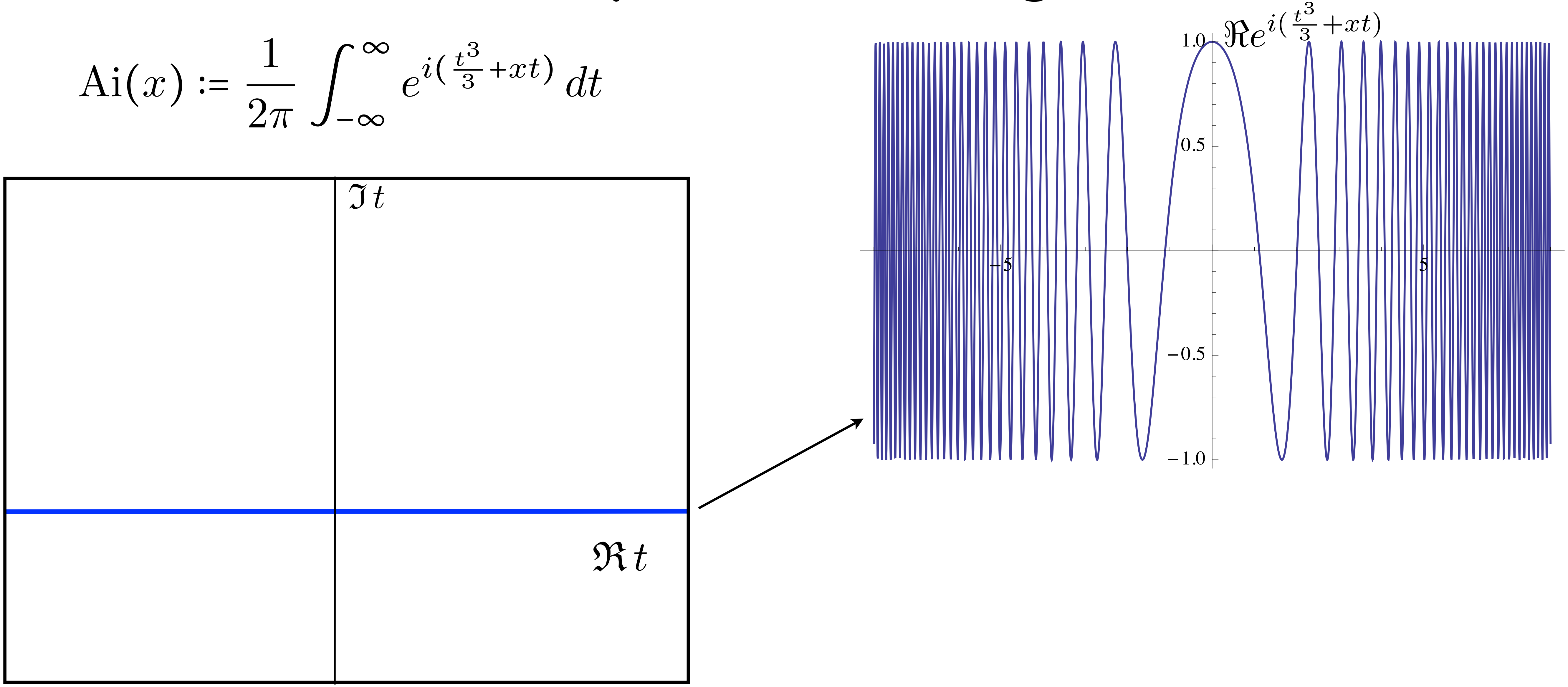

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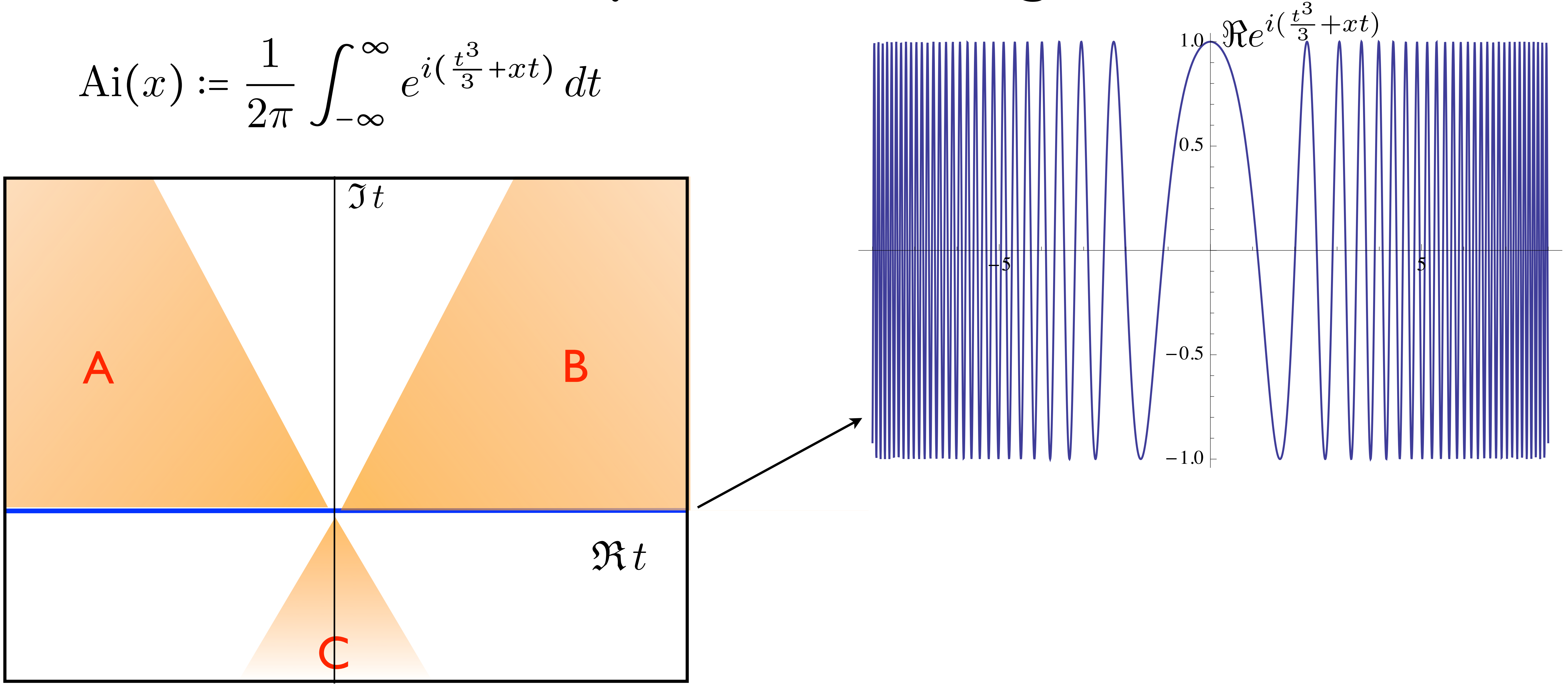

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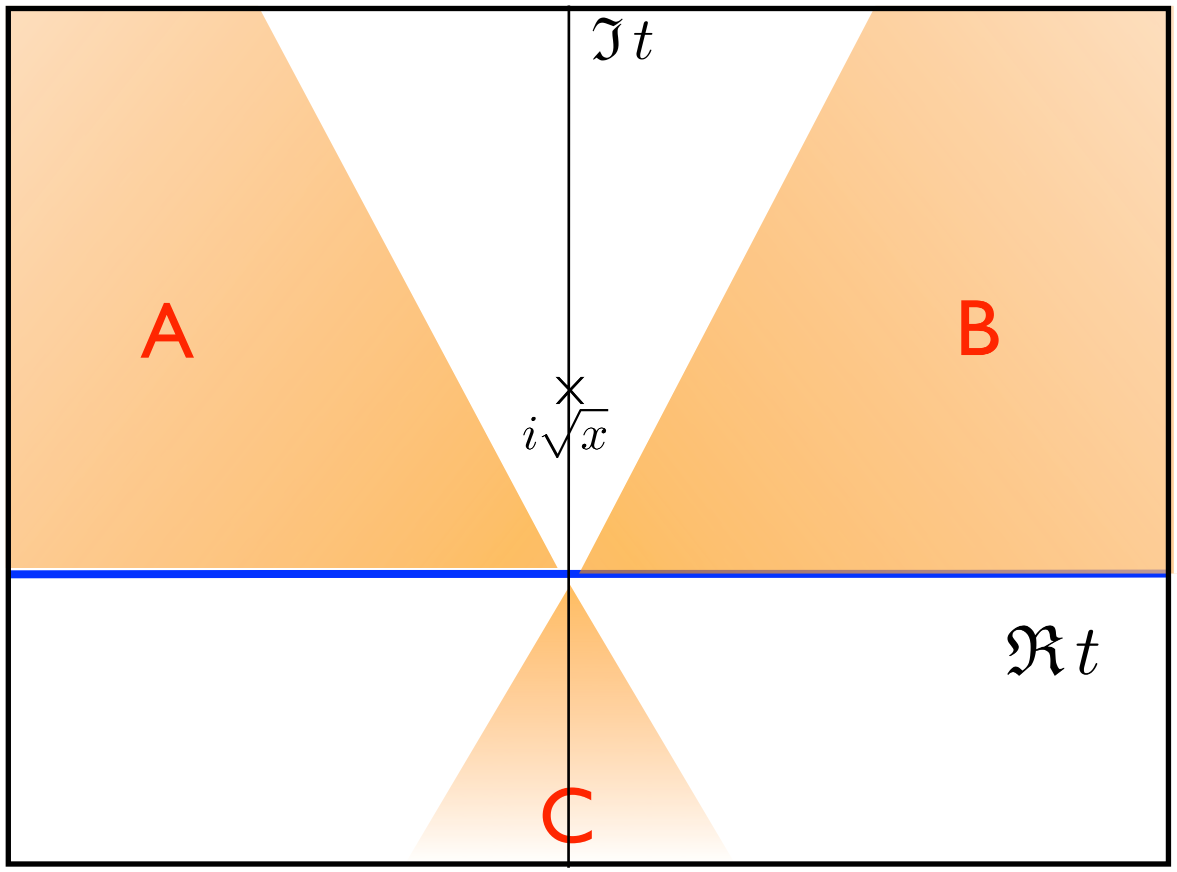

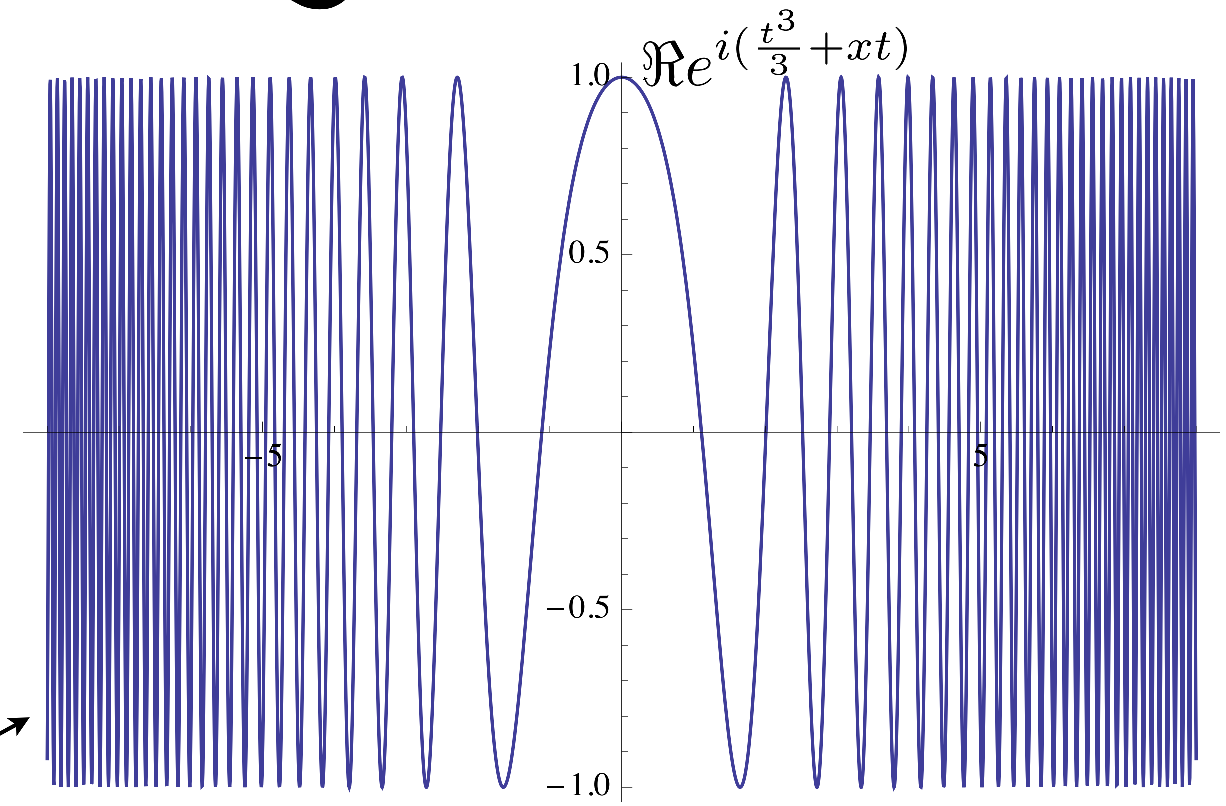

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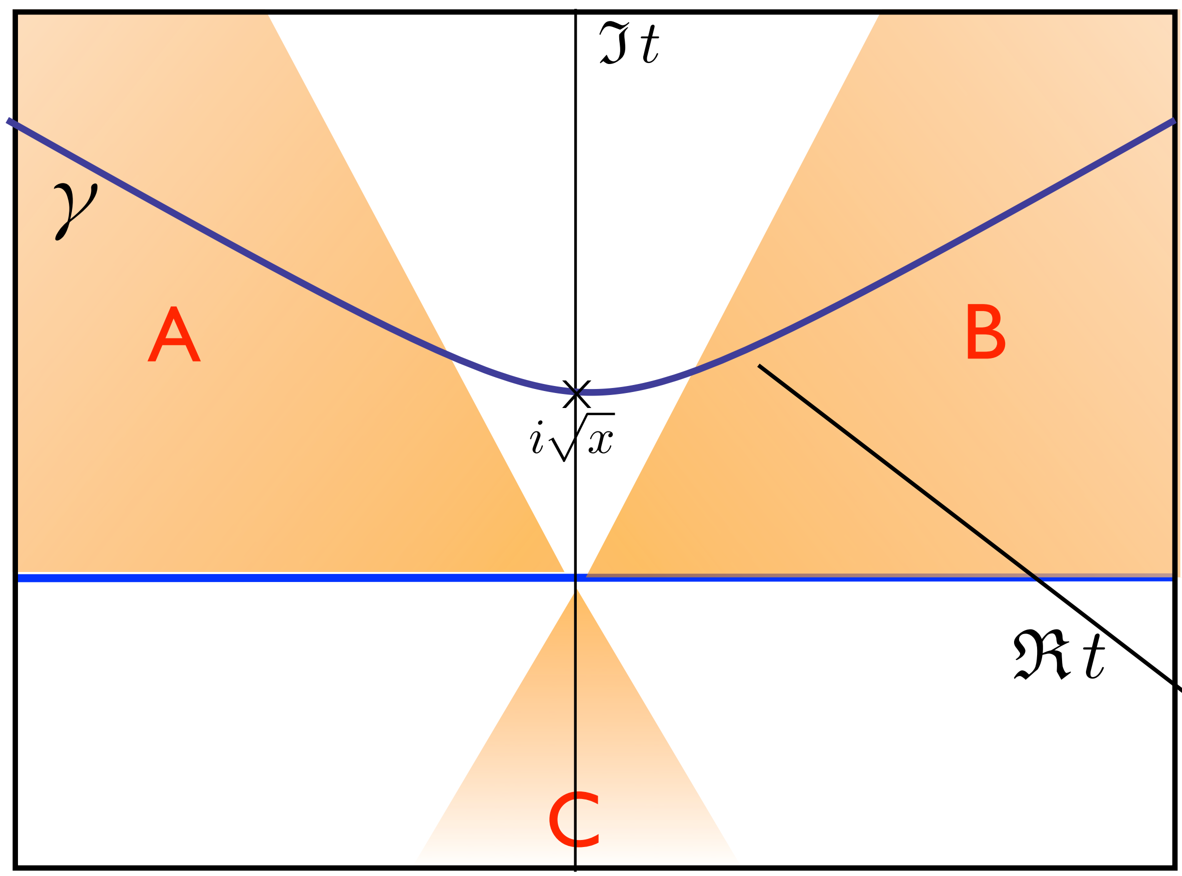

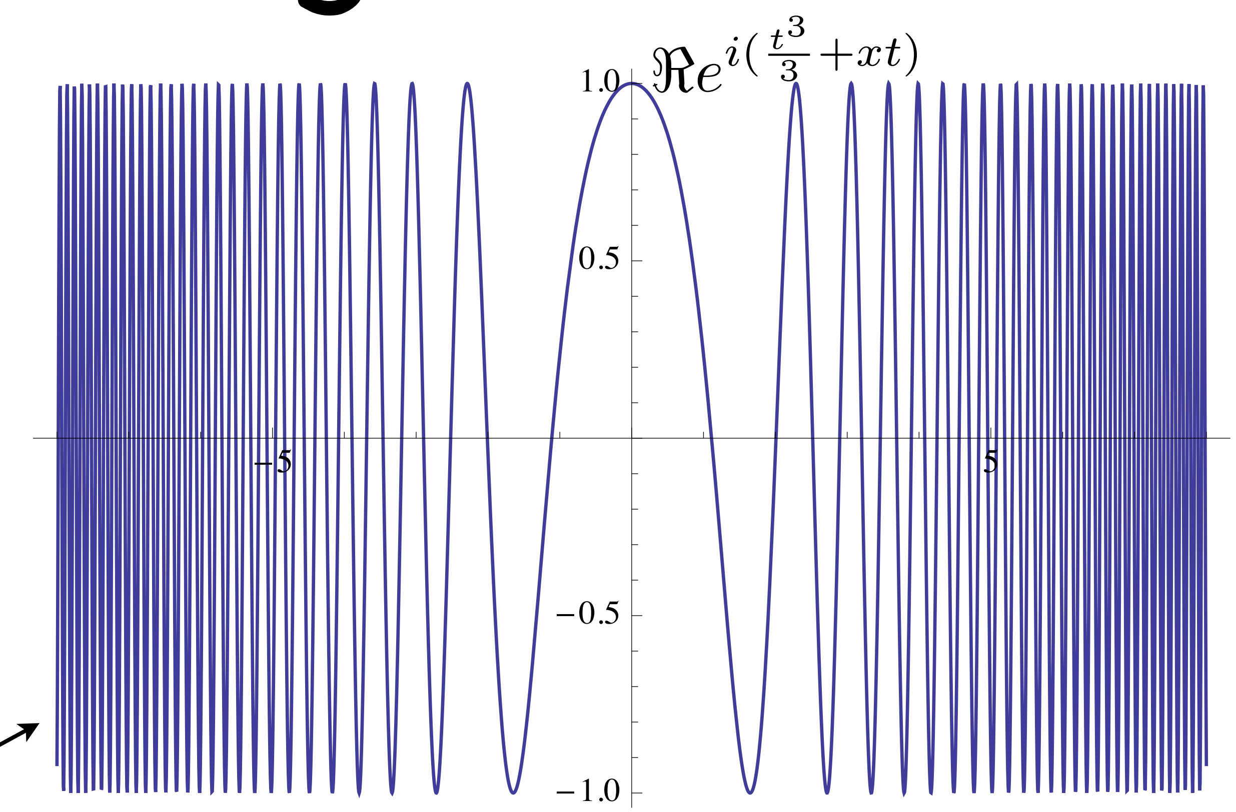

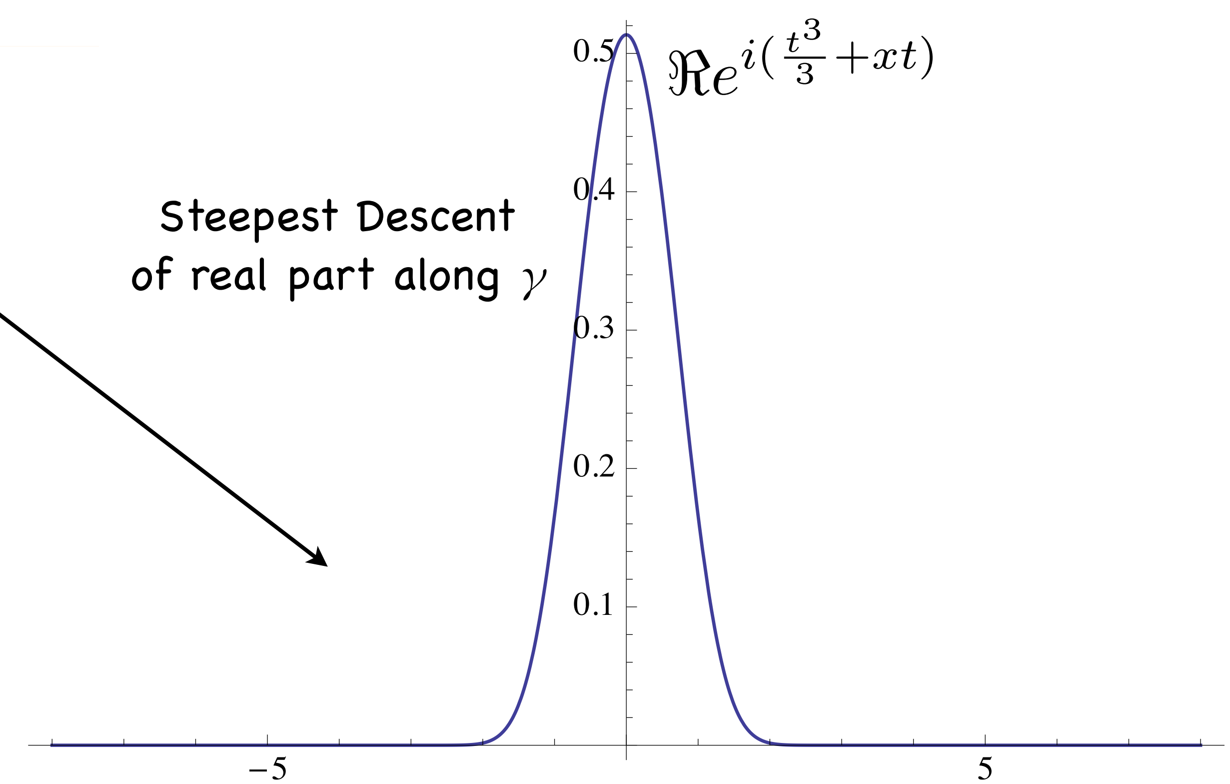

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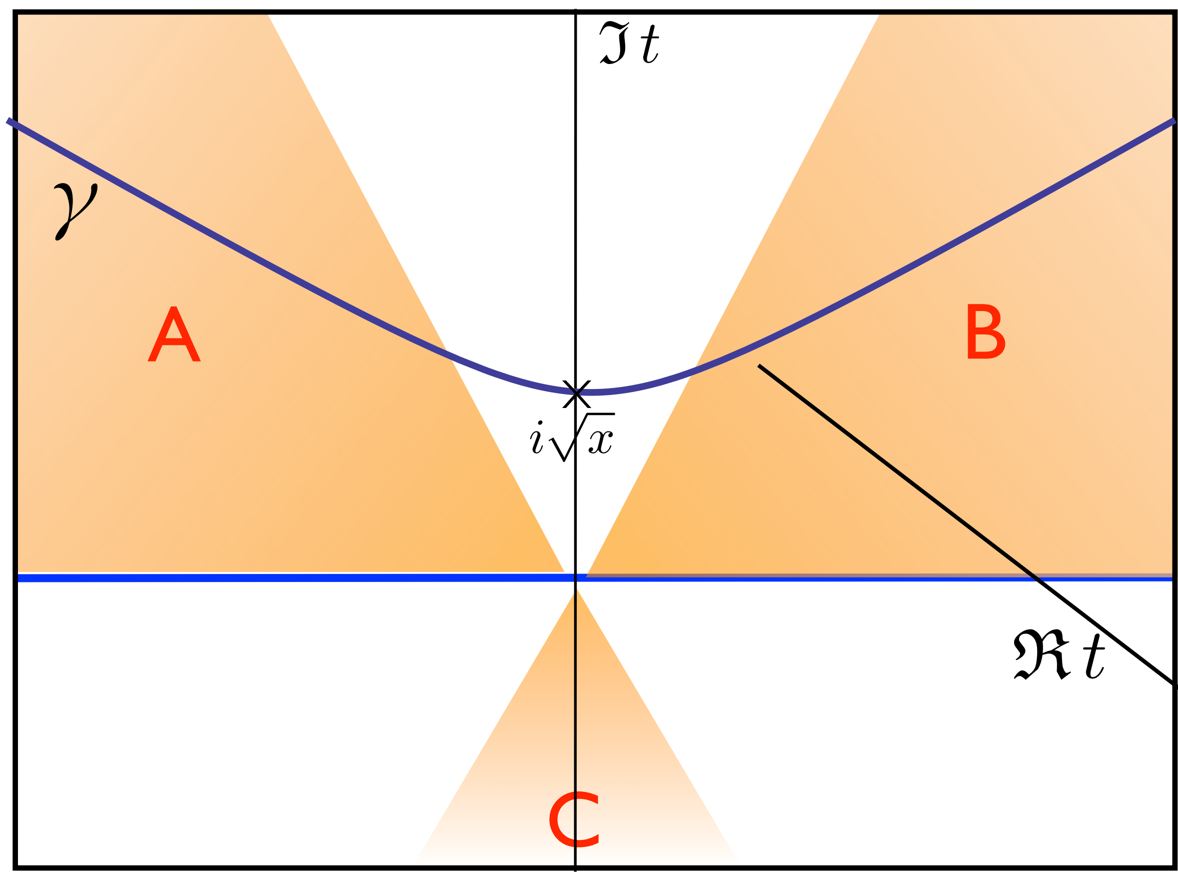
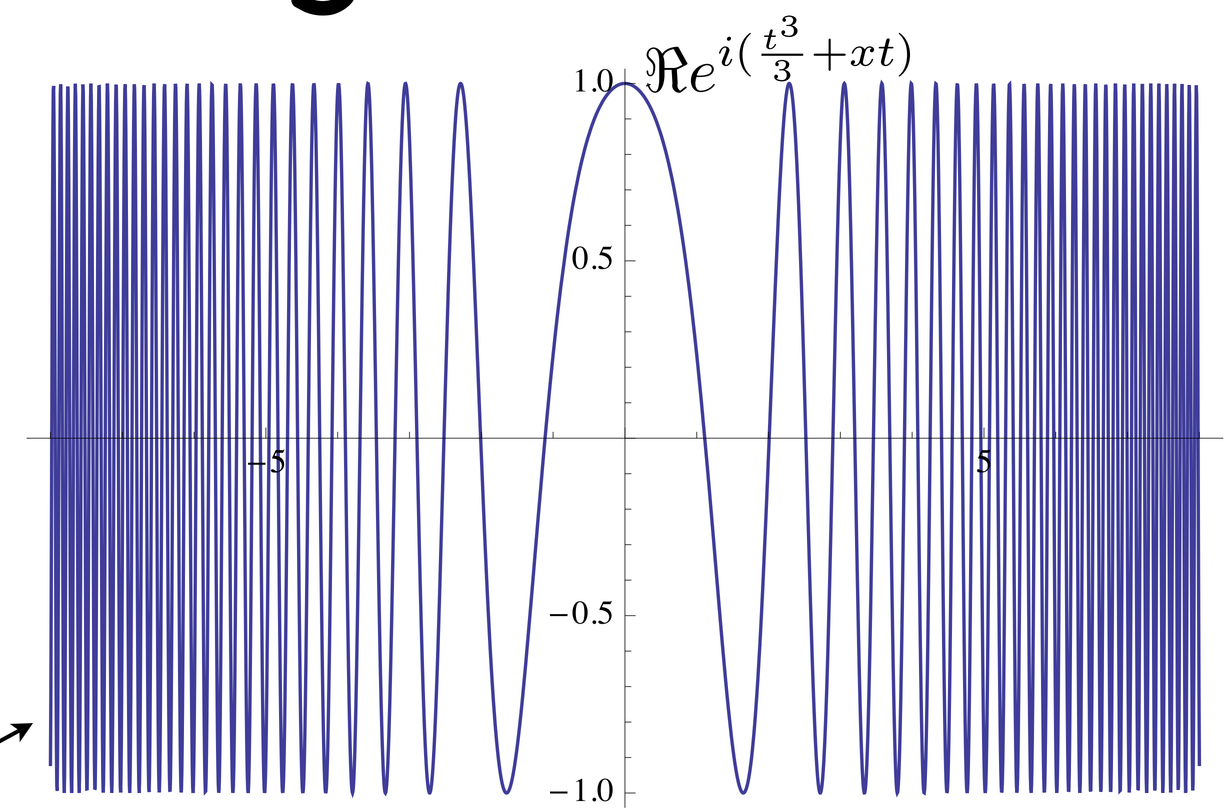
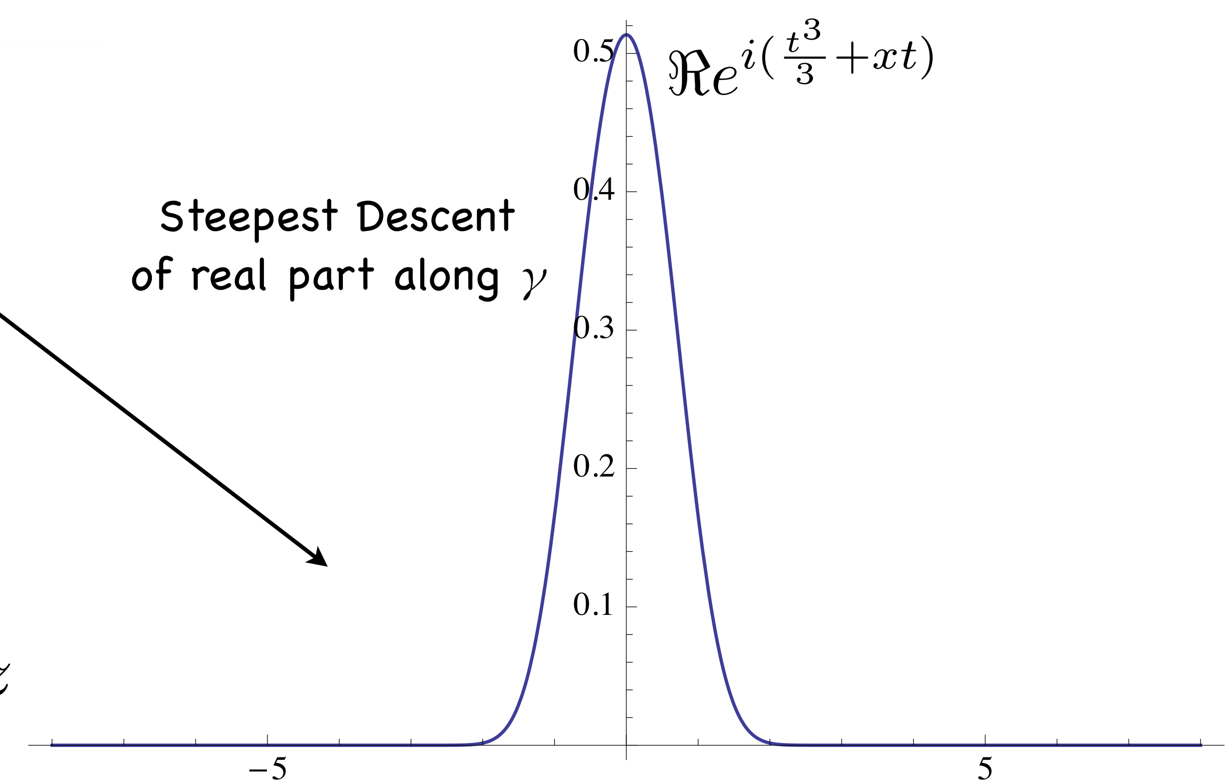




Steepest Descent of real part along γ



Stationary phase along γ

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

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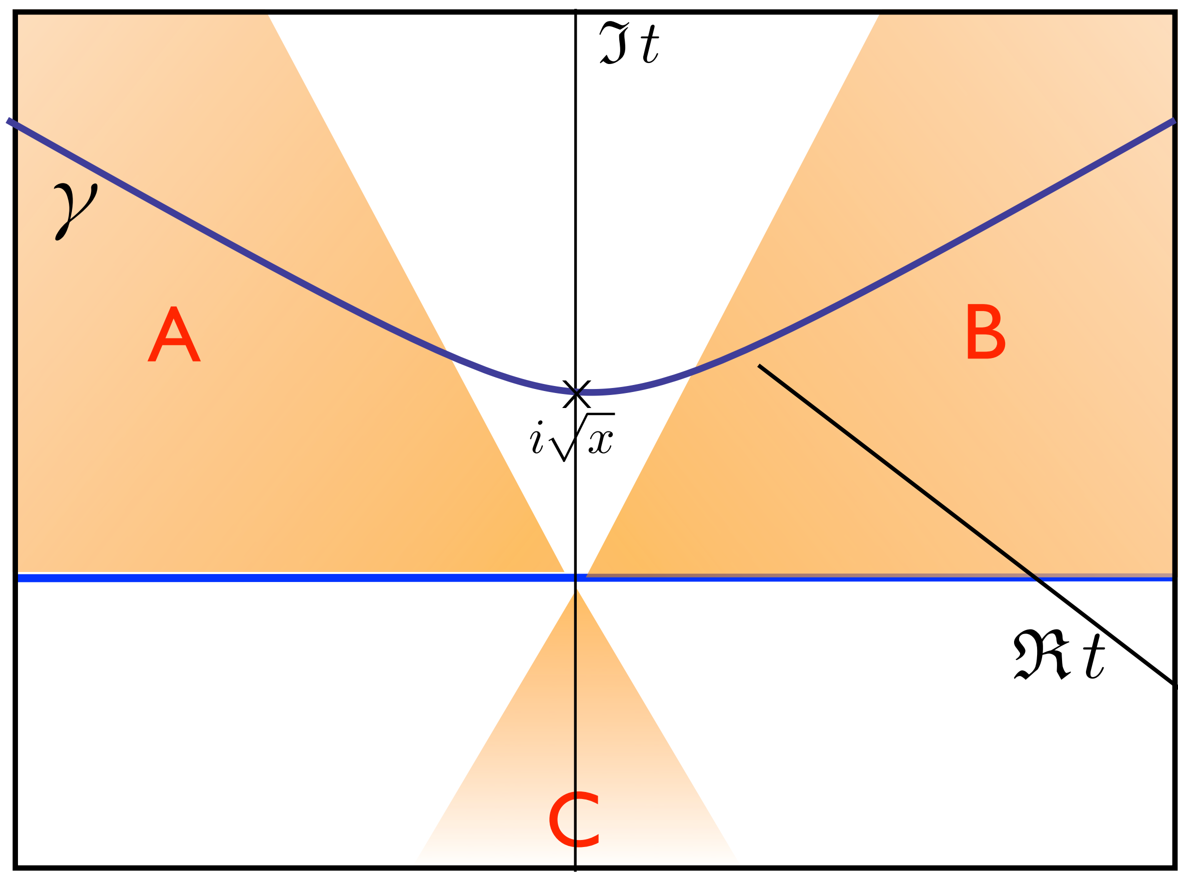

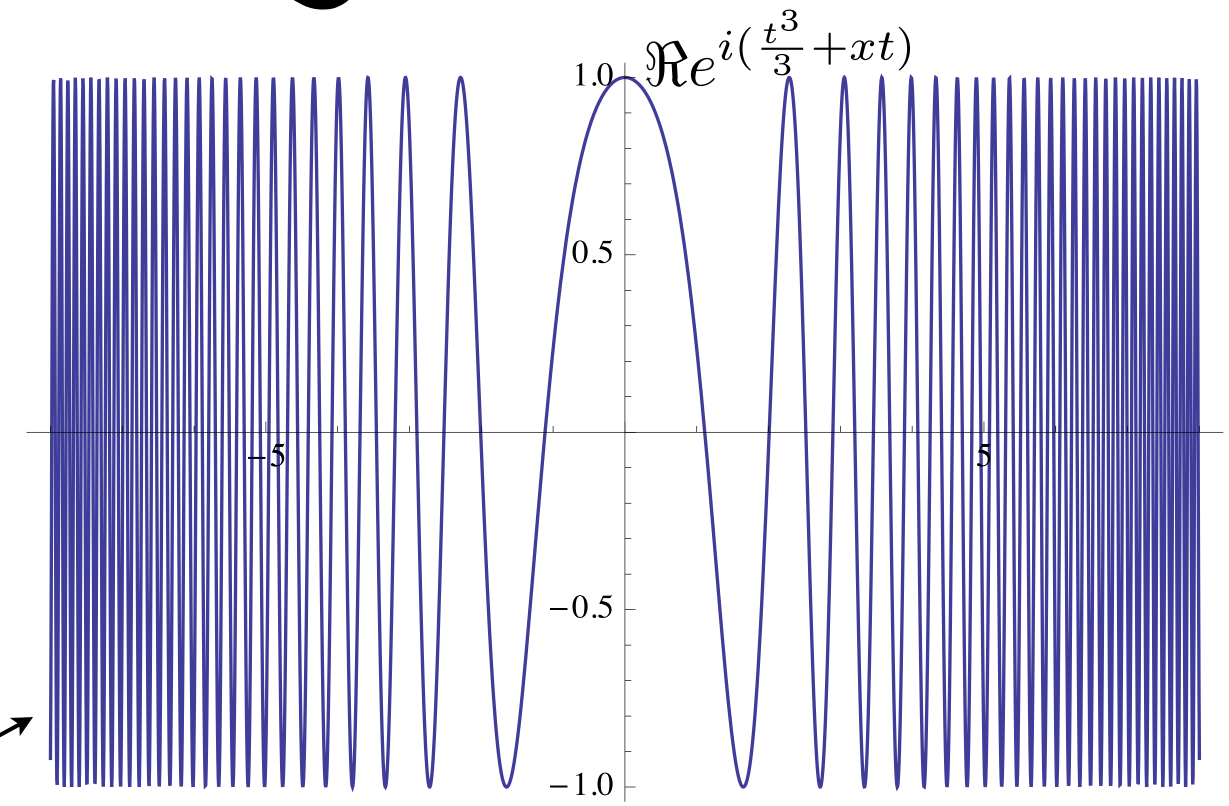

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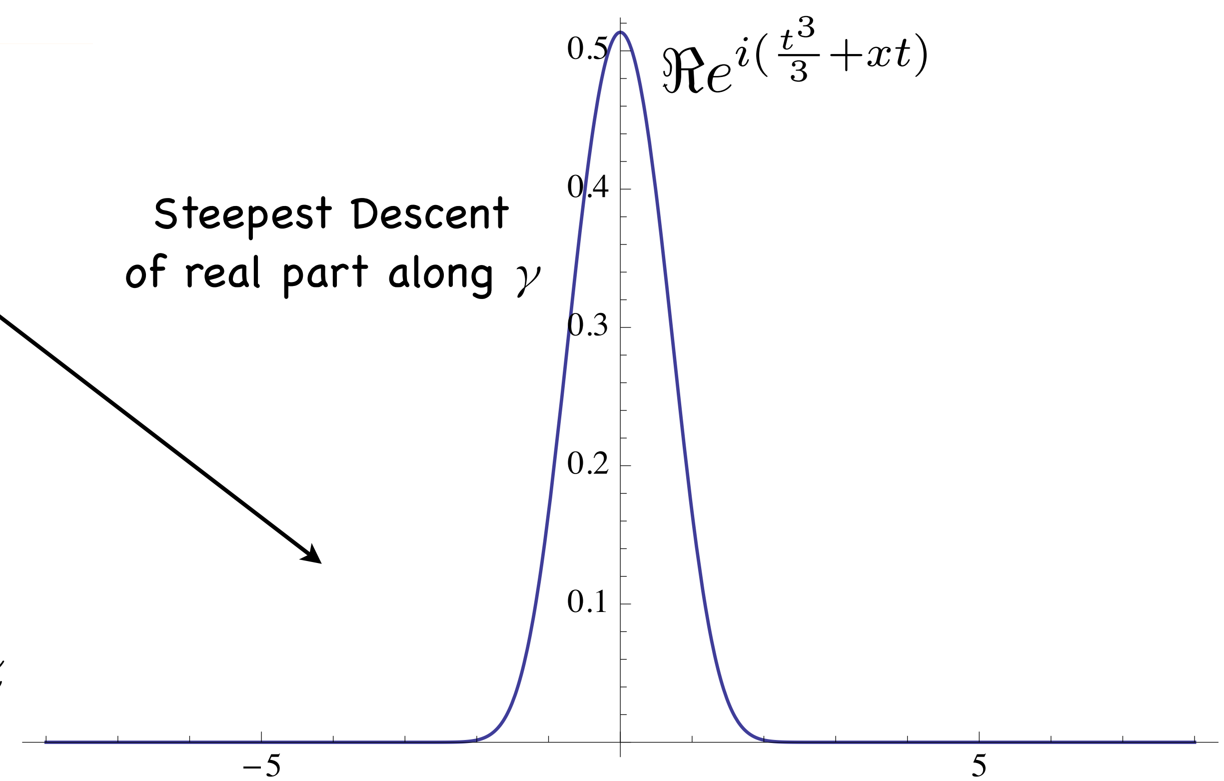

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NOTE γ' is not constant, but changes smoothly!

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- It is a classic and elementary tool that works extremely well for low dimensional oscillating integrals.
- It is usually combined with an **asymptotic expansion** around the stationary point.
  - But, that would correspond to some version of Perturbation Theory, which is not what we want.
- 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)?

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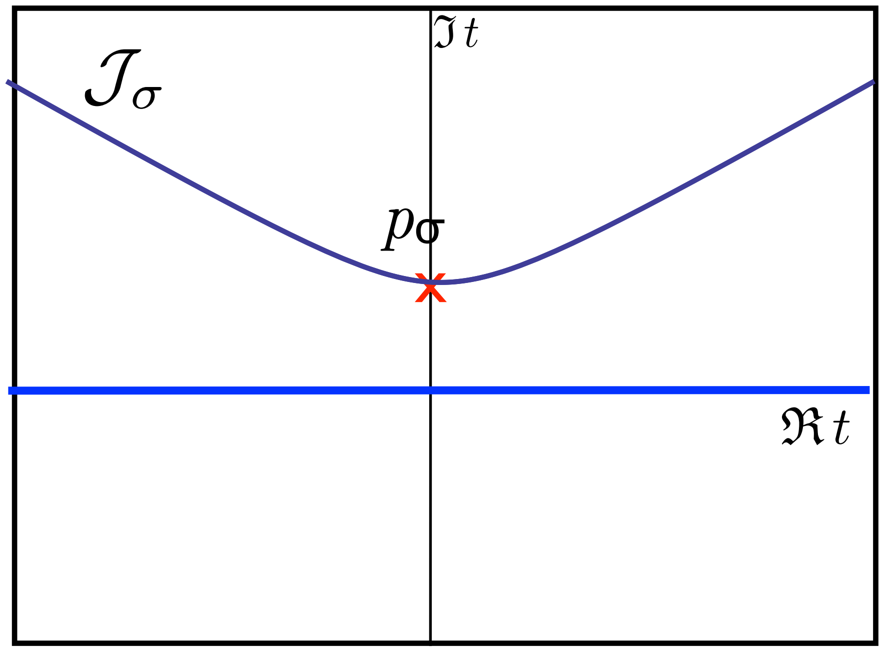

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For each stationary point p_σ of the complexified $f(z)$, $\mathcal{J}_\sigma$ is the union of the paths of SD that fall in p_σ at ∞.

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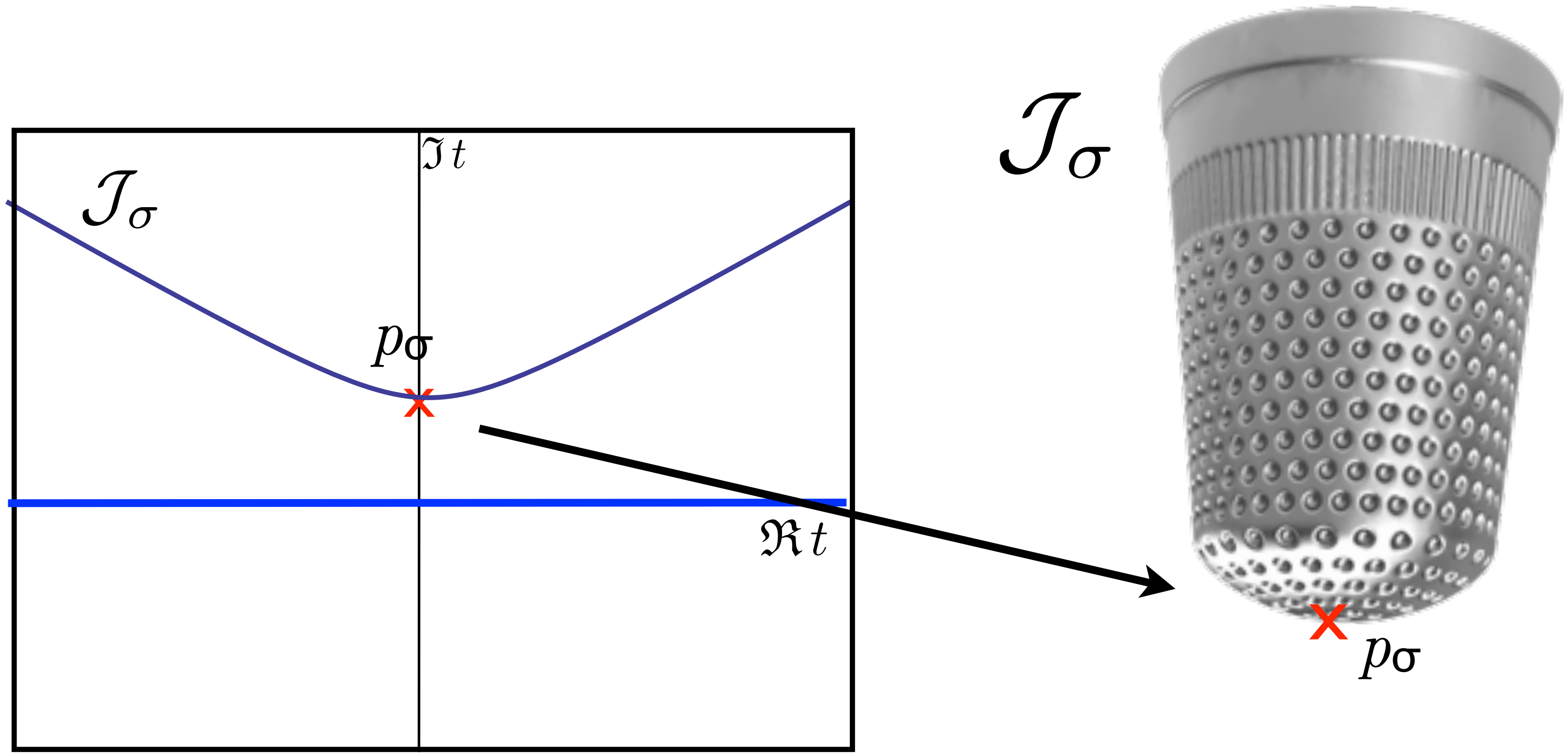

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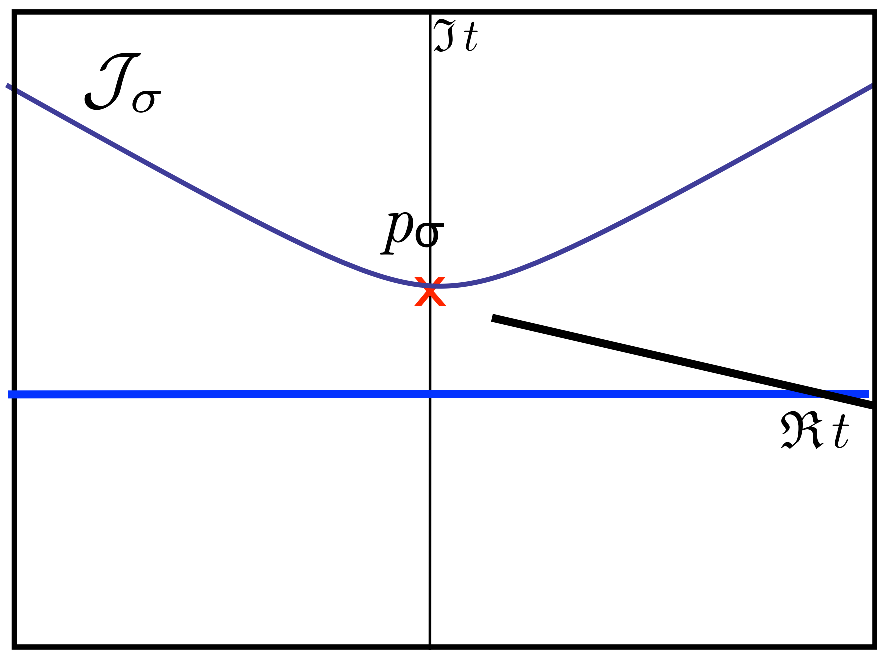

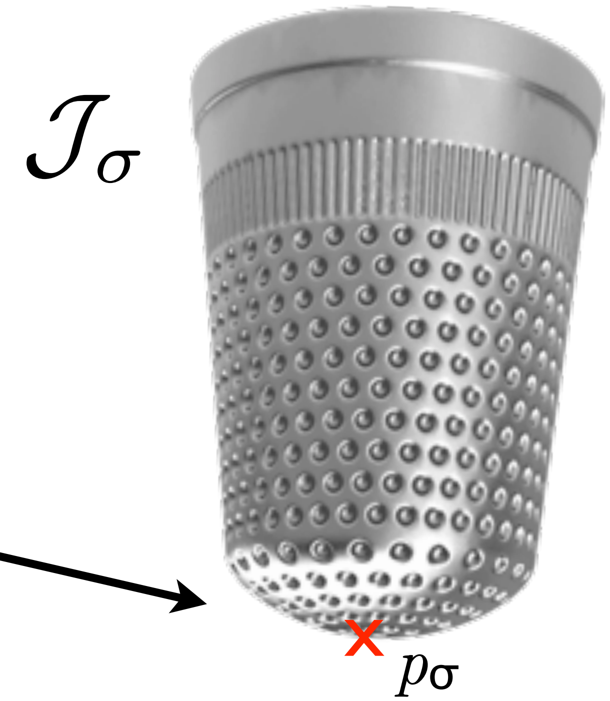

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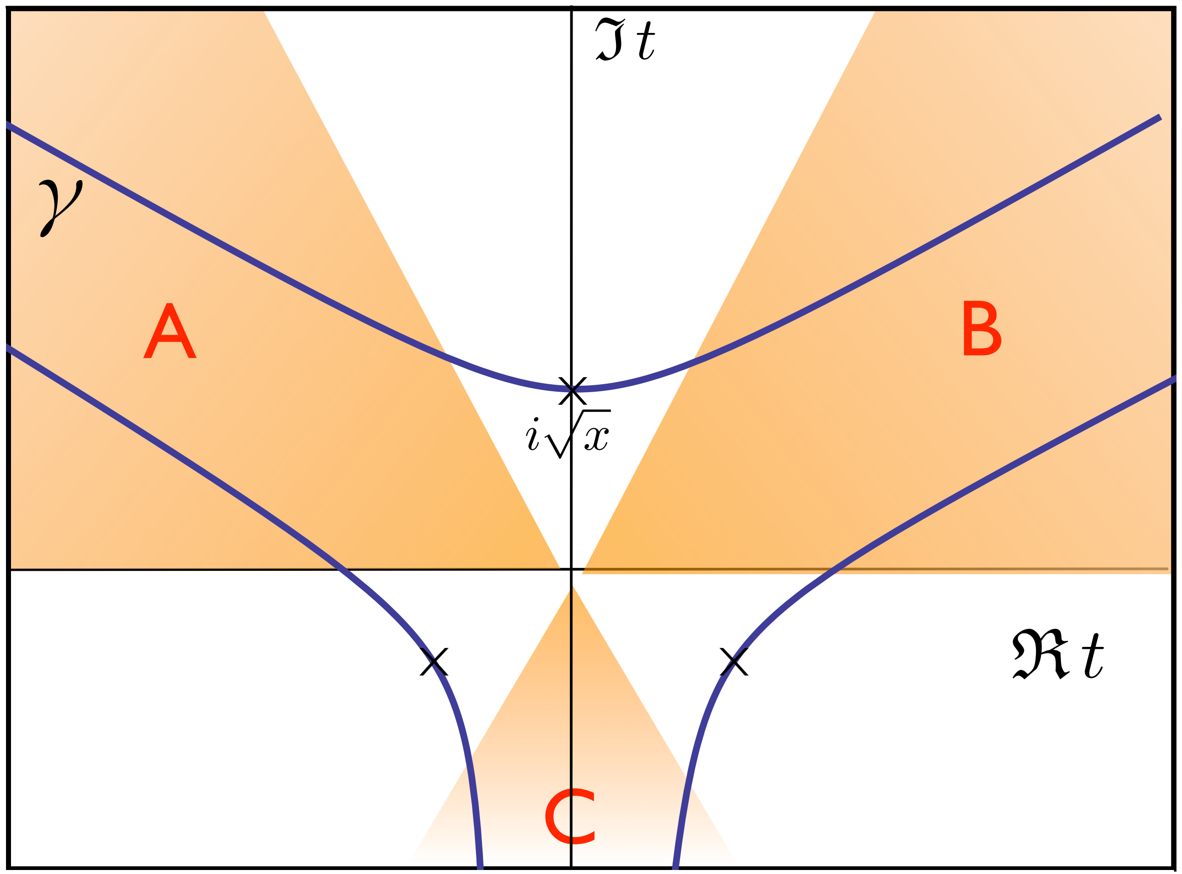
Under suitable conditions on $f(x)$ and $g(x)$, **Morse theory** (Pham '83, Vassiliev '02, Nicolaescu '11, Witten '10) tells us that the timbles $\mathcal{J}_\sigma$ are smooth manifolds of real dimension n immersed in $\mathbb{C}^n$, and, for each cycle C, where the integral converges:

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

$$\mathcal{C} = \sum_\sigma n_\sigma \mathcal{J}_\sigma$$ (in the homological sense)

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

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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- So, in principle, the original integral could be expressed as a sum of integrals over the thimbles $\mathcal{J}_\sigma$, where the integral is rapidly convergent and the phase of the integrand is constant (~stationary phase idea).
- Interesting, BUT, finding all the stationary points p_σ of the complexified action, computing the integer coefficient n_σ, is not feasible. And still we have to perform a Monte Carlo on each $\mathcal{J}_\sigma$.

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

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

thimble attached to the global minimum of S_R

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- Formulate on the thimble
- Check Symmetries
- Check Perturbation Theory
- Formulate a Monte Carlo algorithm

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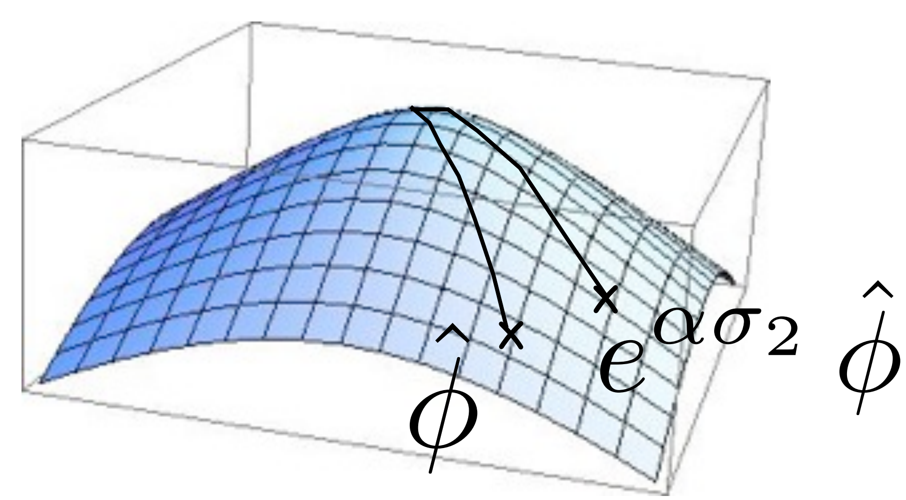

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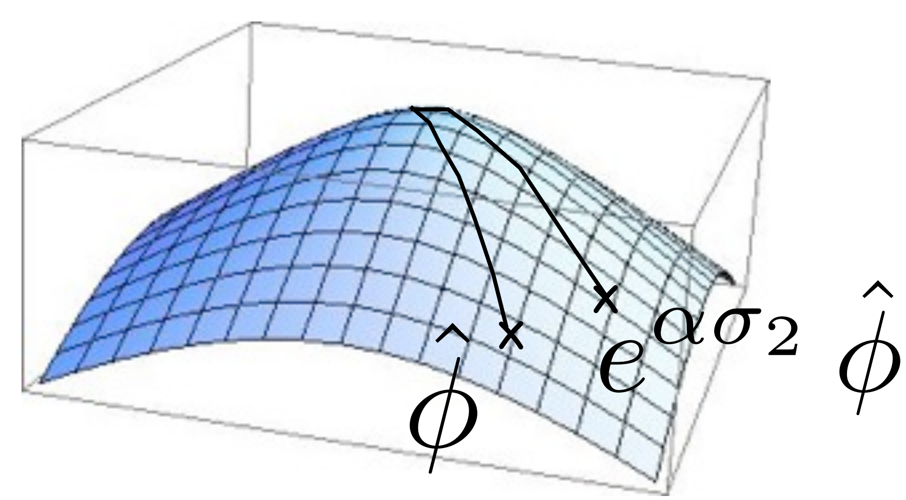
GREAT!!



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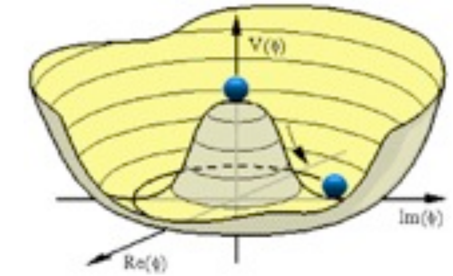
Spontaneous Symmetry Breaking with Mexican Hat Potential



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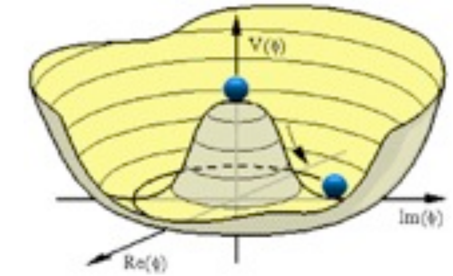

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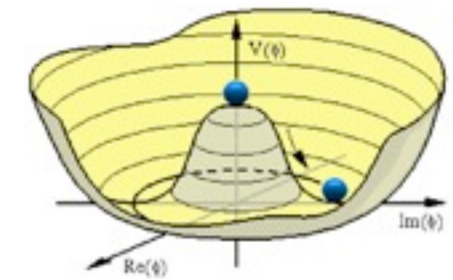

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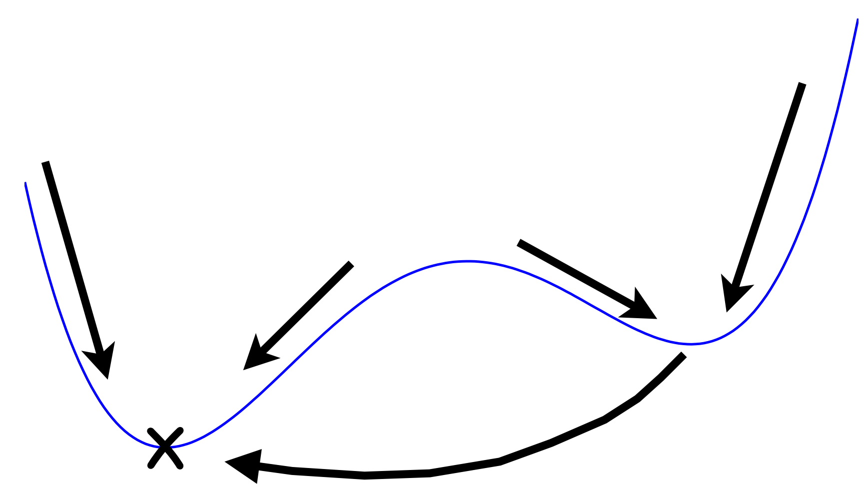

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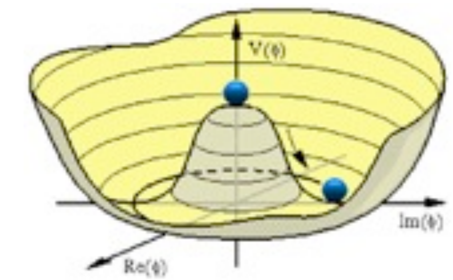

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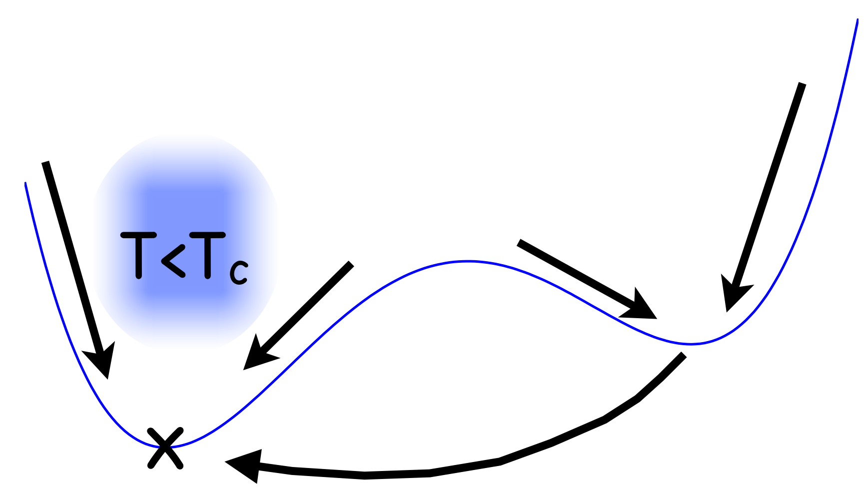

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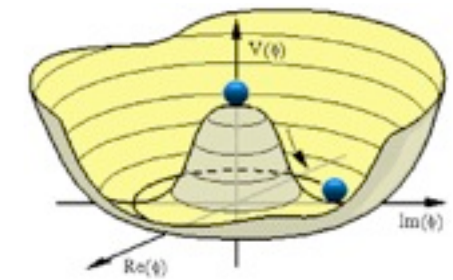

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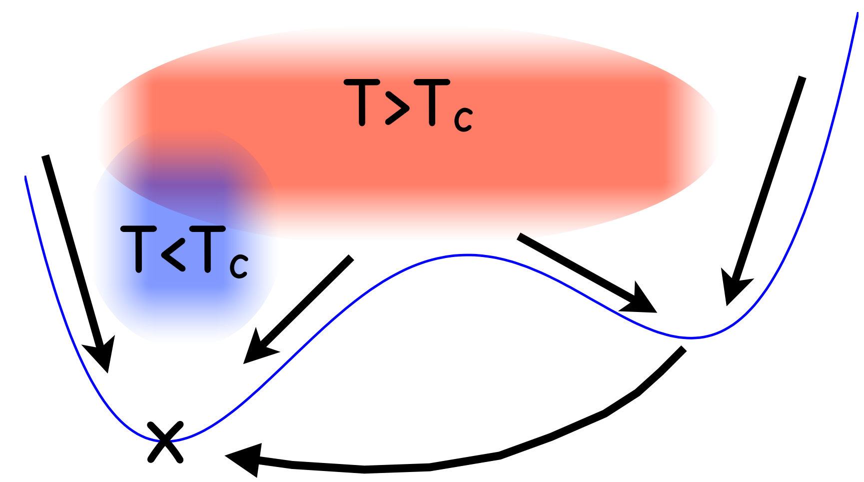

SSB is a dynamical question!

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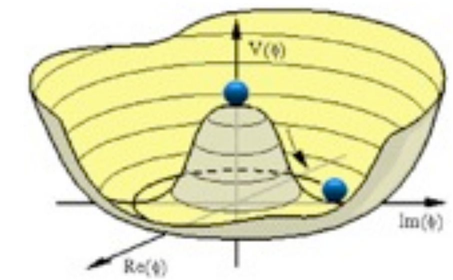

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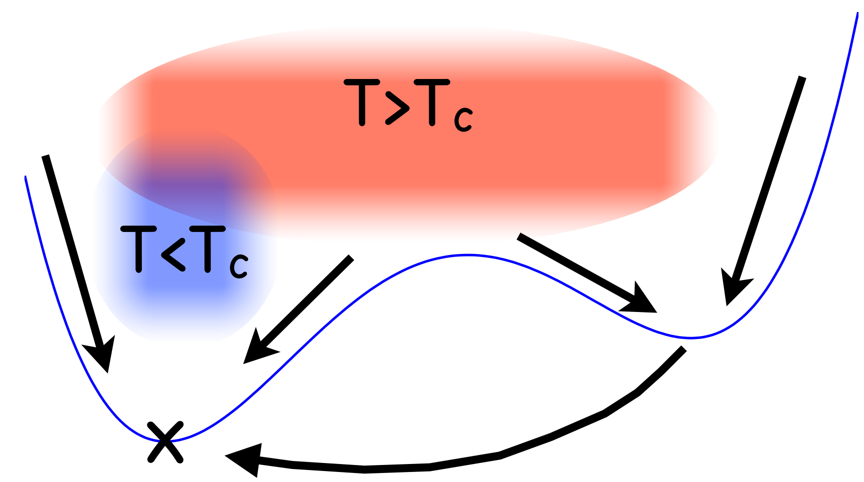

SSB is a dynamical question!

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

A Monte Carlo algorithm on a thimble?

The Aurora algorithm

review:

Langevin Algorithm

review:

Langevin Algorithm

I want to compute: $$\langle \mathcal{O} \rangle = \frac{1}{Z_0} \int \prod_x d\phi_x \, e^{-S[\phi]} \mathcal{O}[\phi]$$

S is real and bounded from below.

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This procedure is also called **stochastic quantization**

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Constant on $\mathcal{J}_0$!

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How can I compute the tangent space $T_\phi(\mathcal{J}_0)$ at ϕ ?

(How do we know which neighbors will eventually fall in ϕ =0 under SD...?)

... non local problem? go to 5D?

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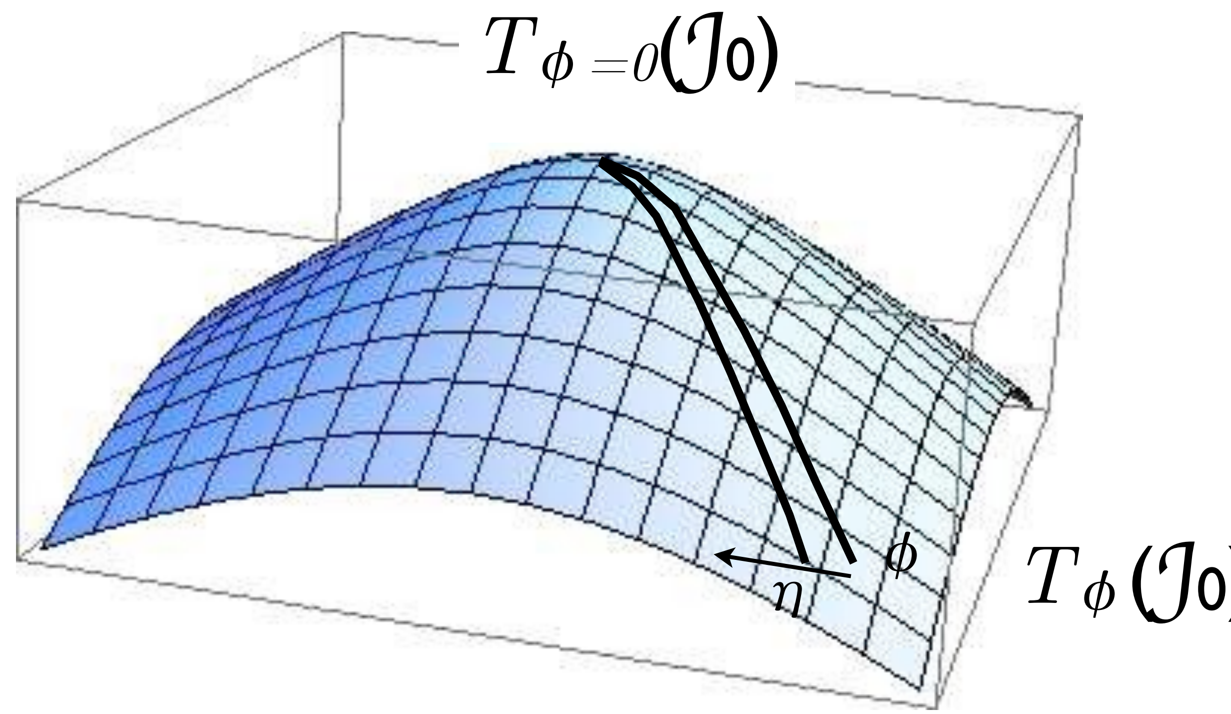

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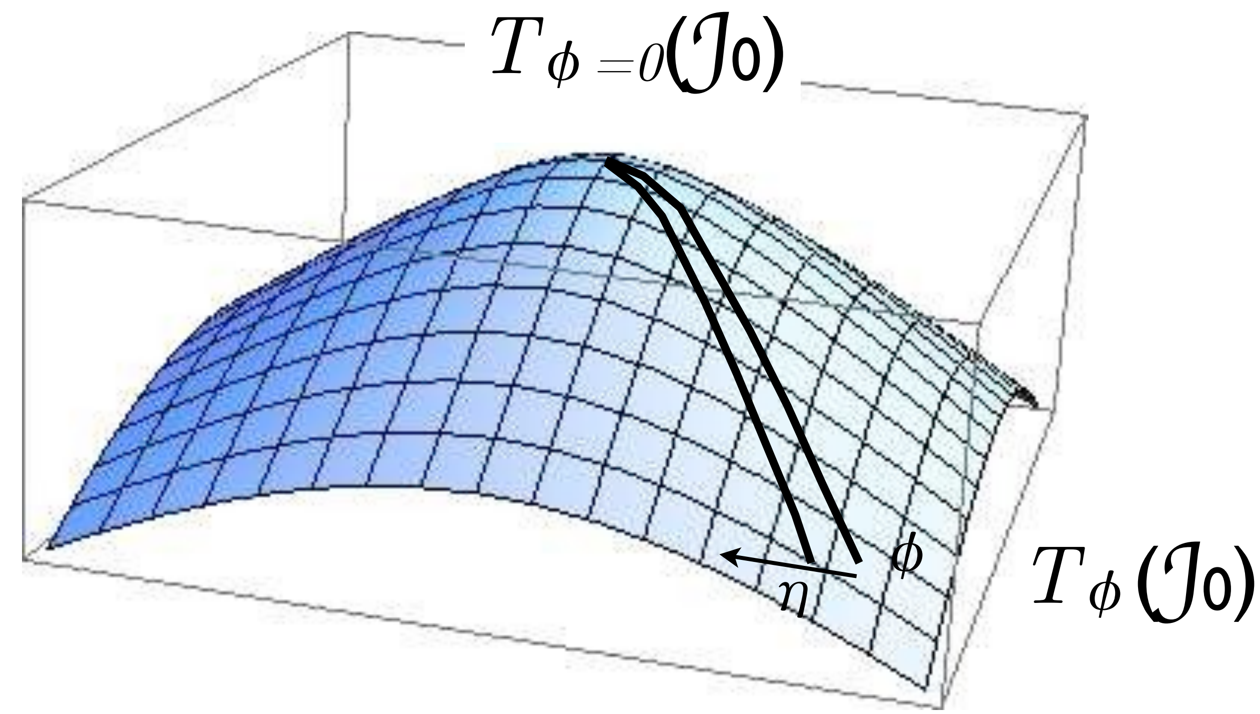

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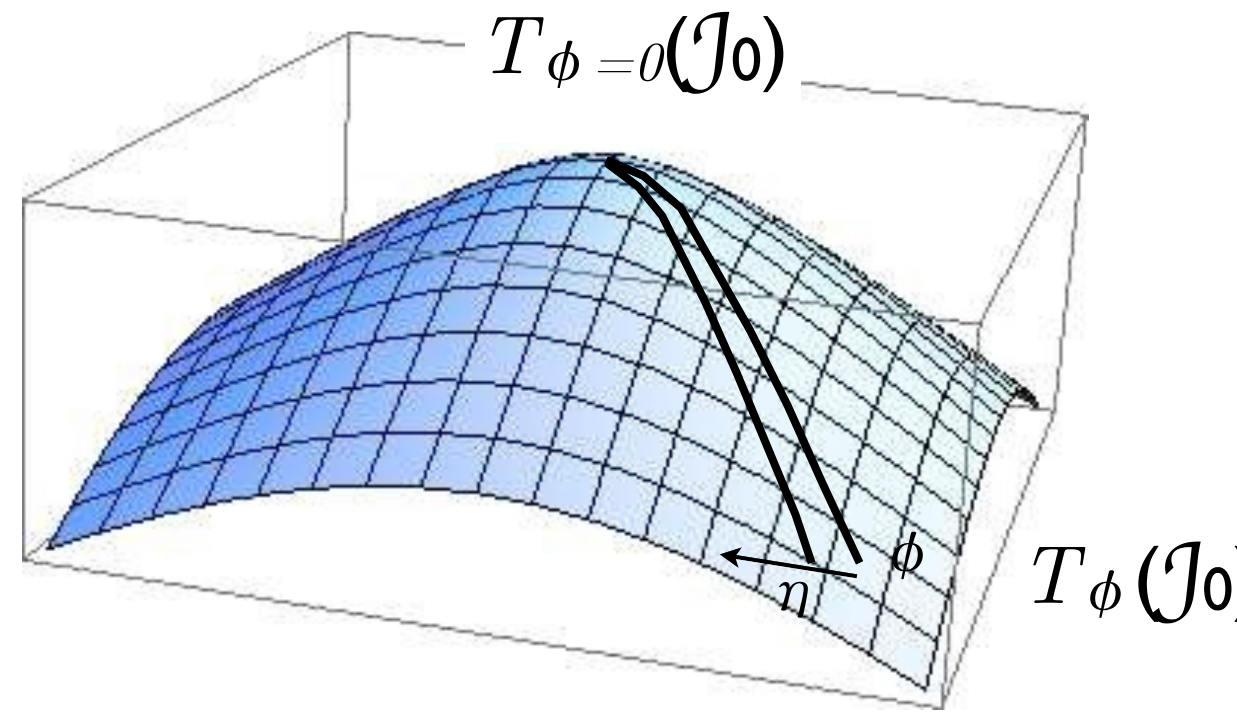

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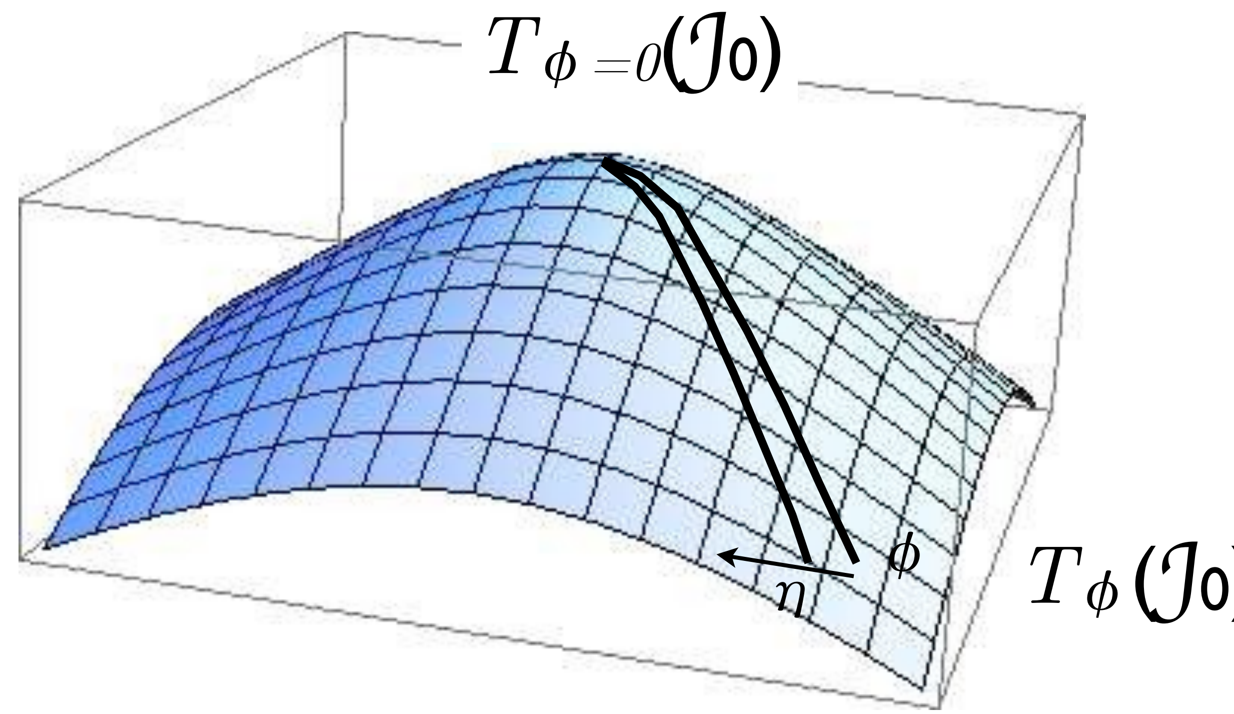

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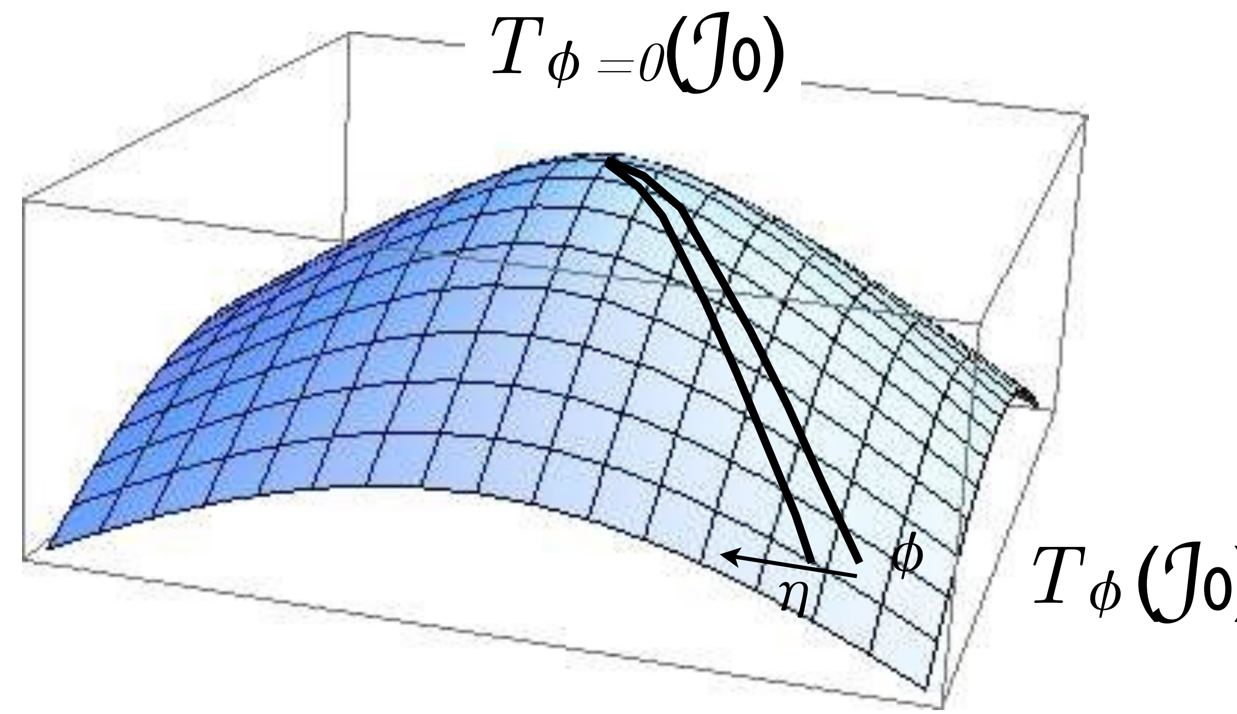

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compact (skew-symmetric)

abelian (diagonal)

nilpotent (upper triang.)

⇒ Very easy to implement!

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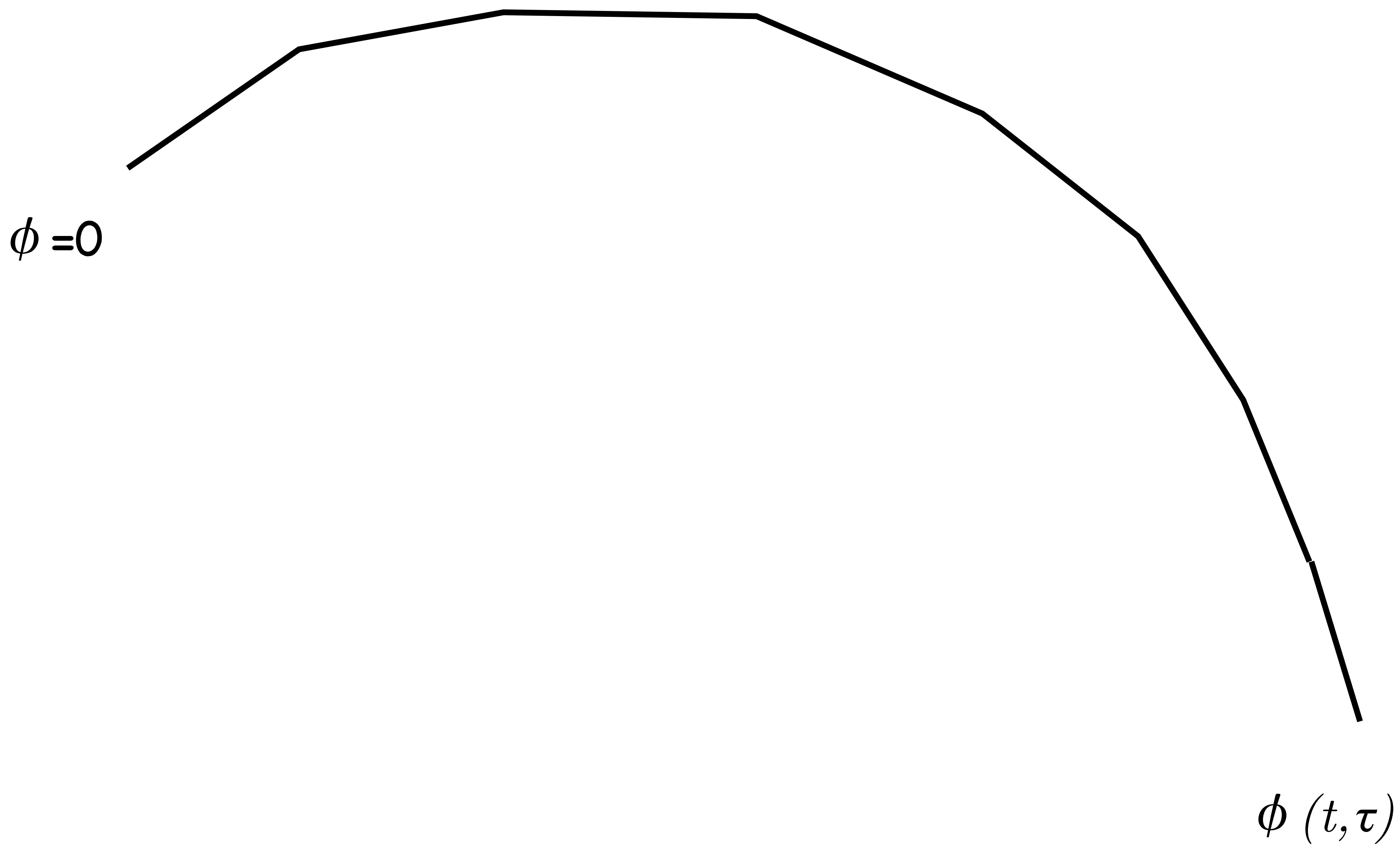
This is an **orthogonal flow** and it can be preserved also numerically (e.g. Implicit Midpoint Rule ⇒ solve a linear system of size $O(N_T V)$)

Graphical summary of a Langevin step



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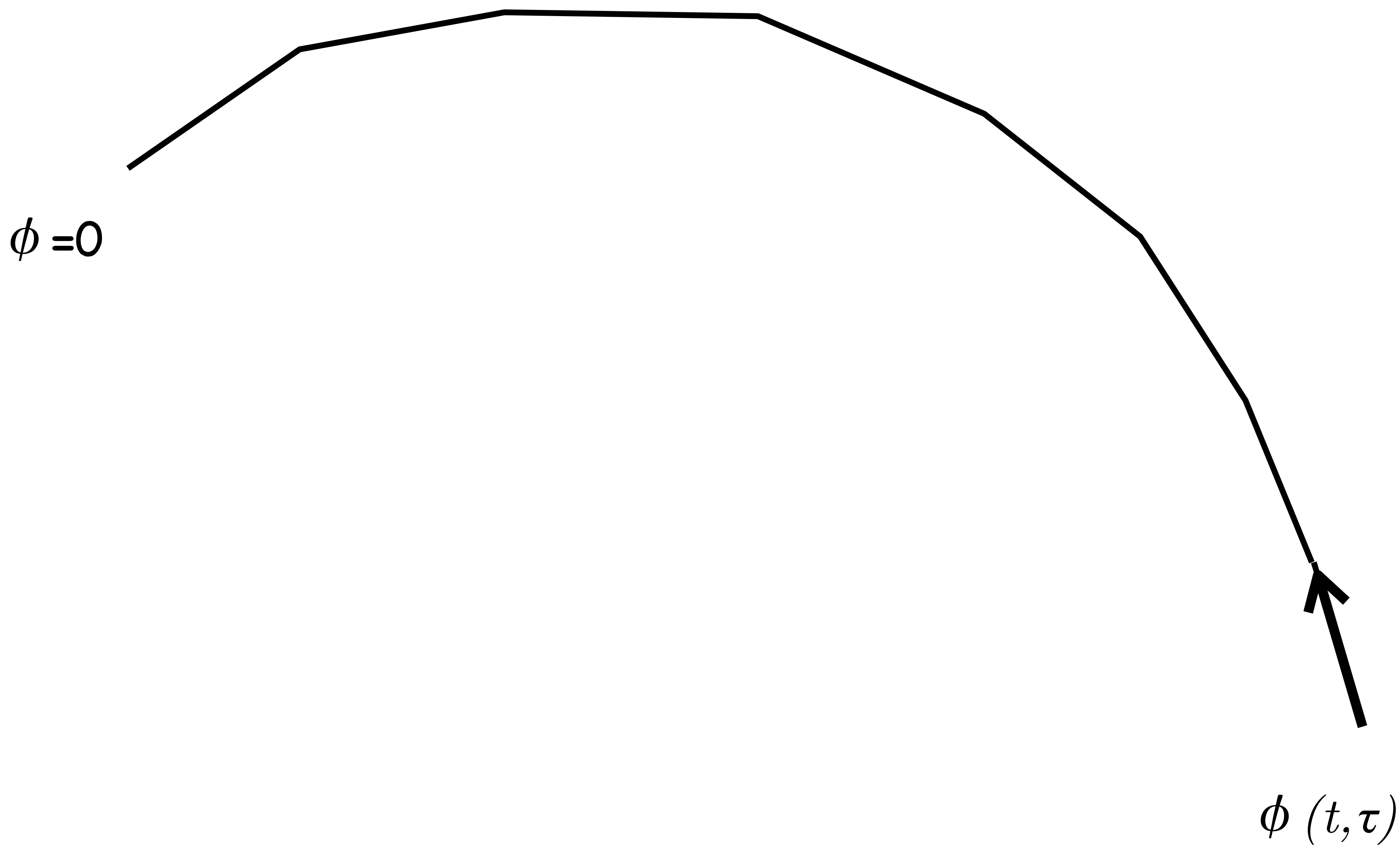

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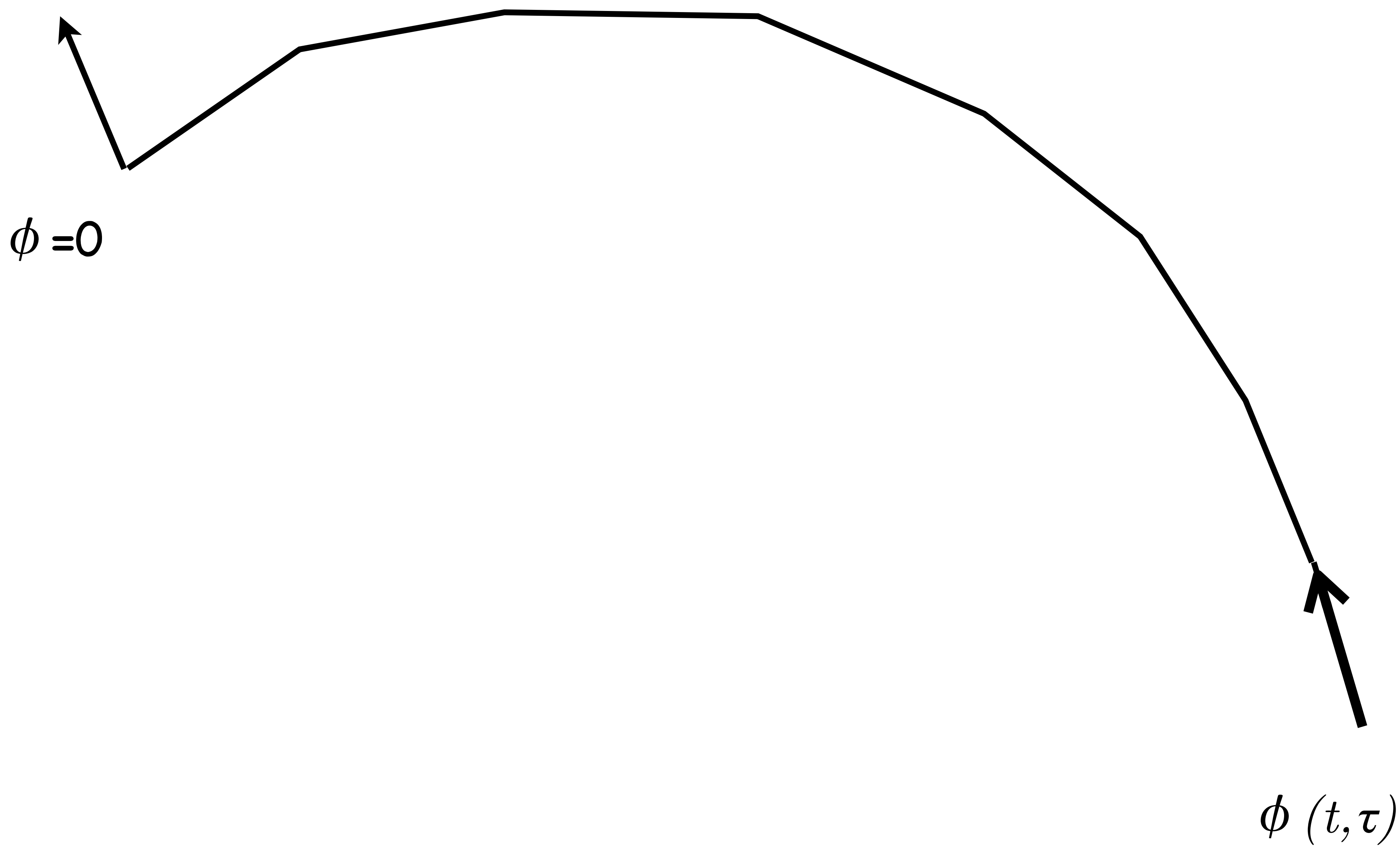

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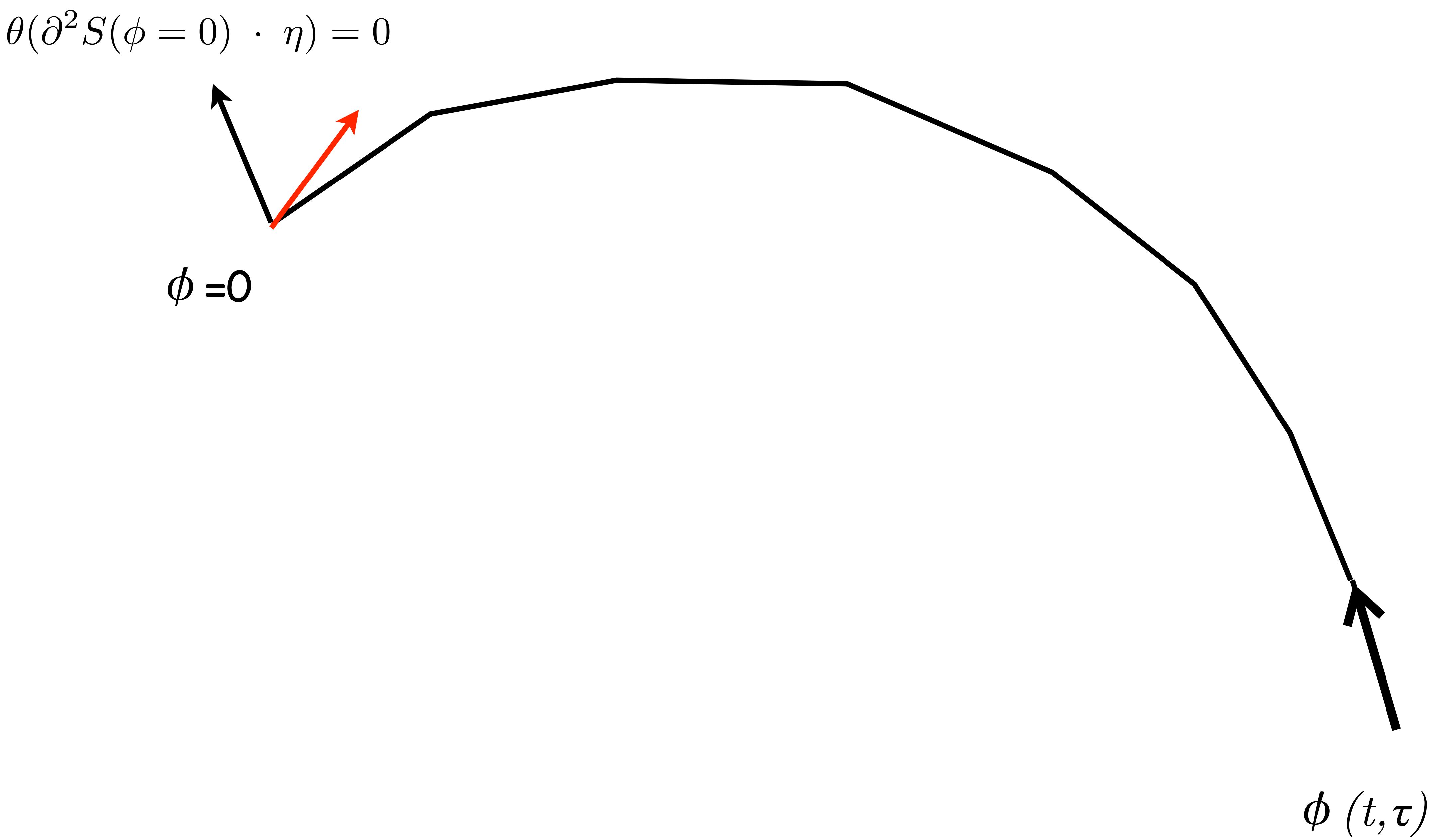

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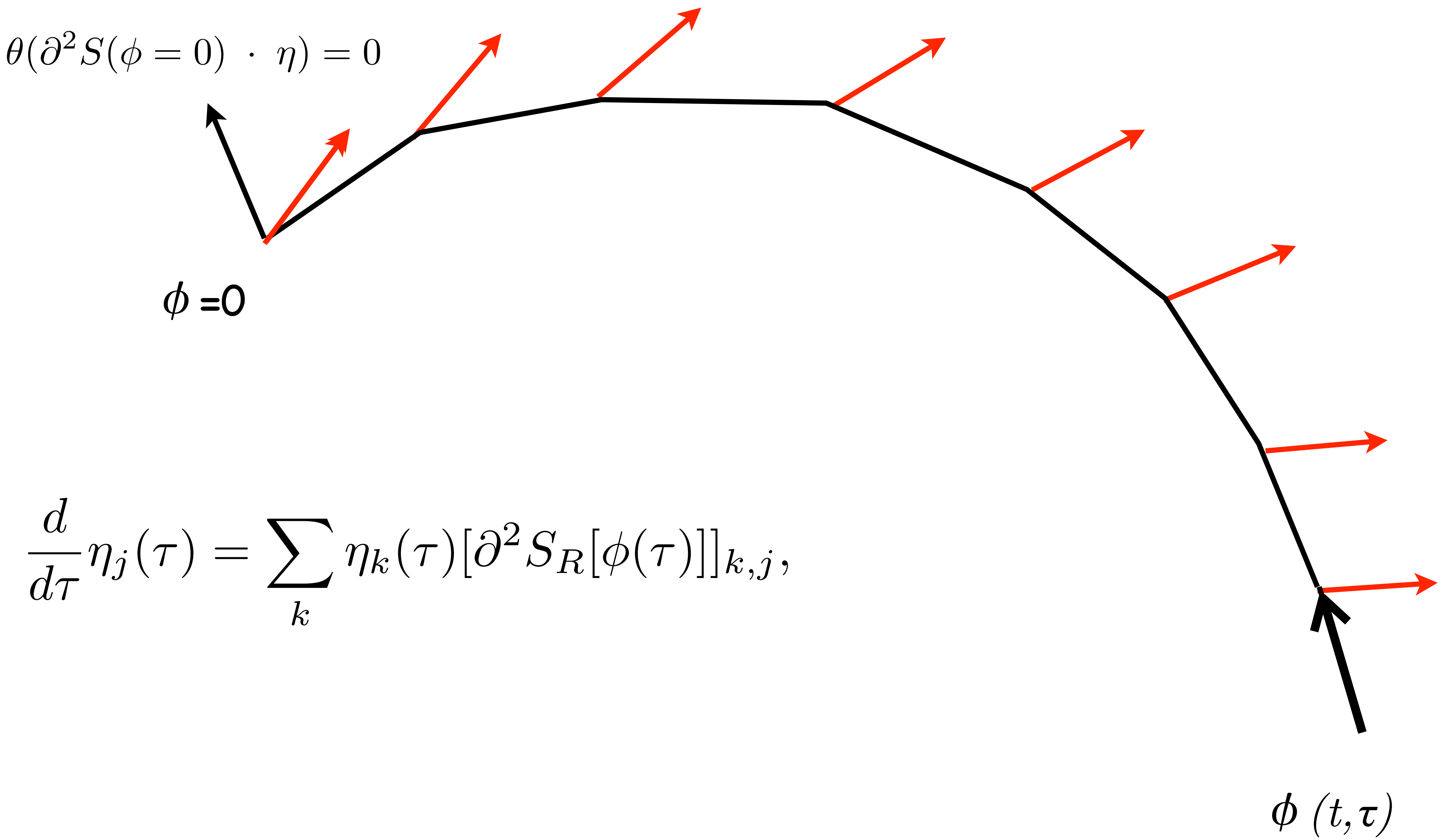

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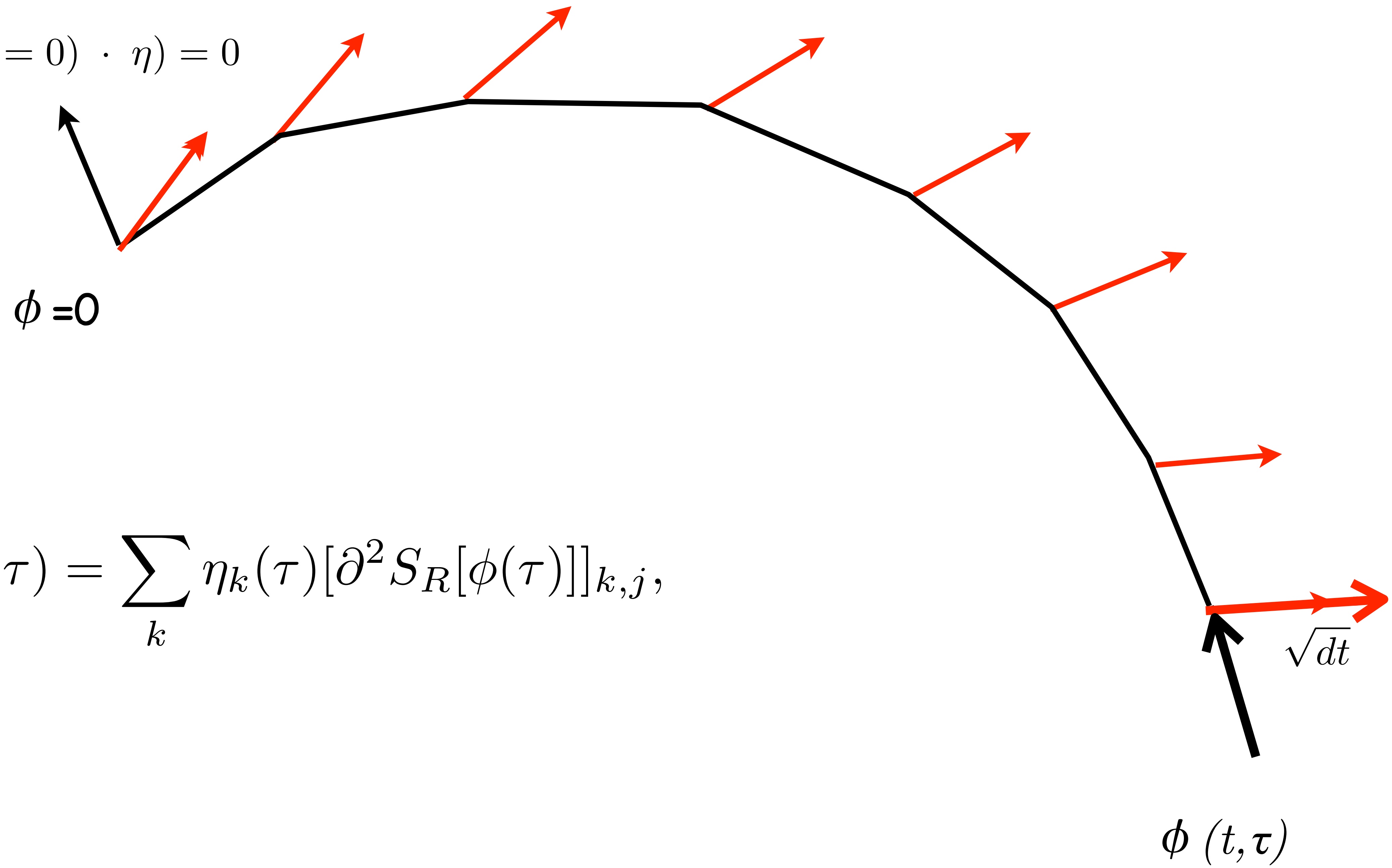
Graphical summary of a Langevin step

$$\theta(\partial^2 S(\phi = 0)\ \cdot\ \eta) = 0$$



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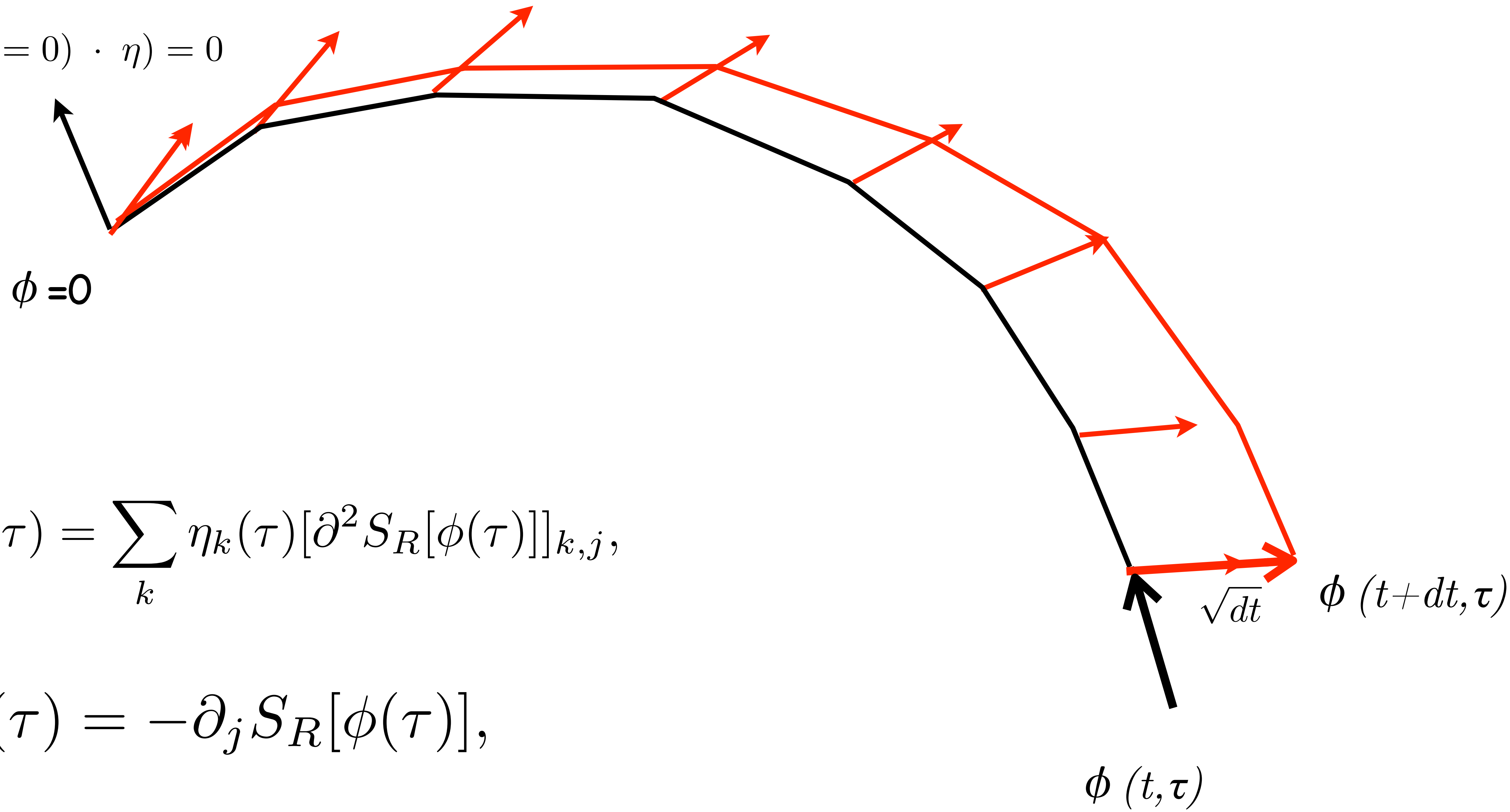

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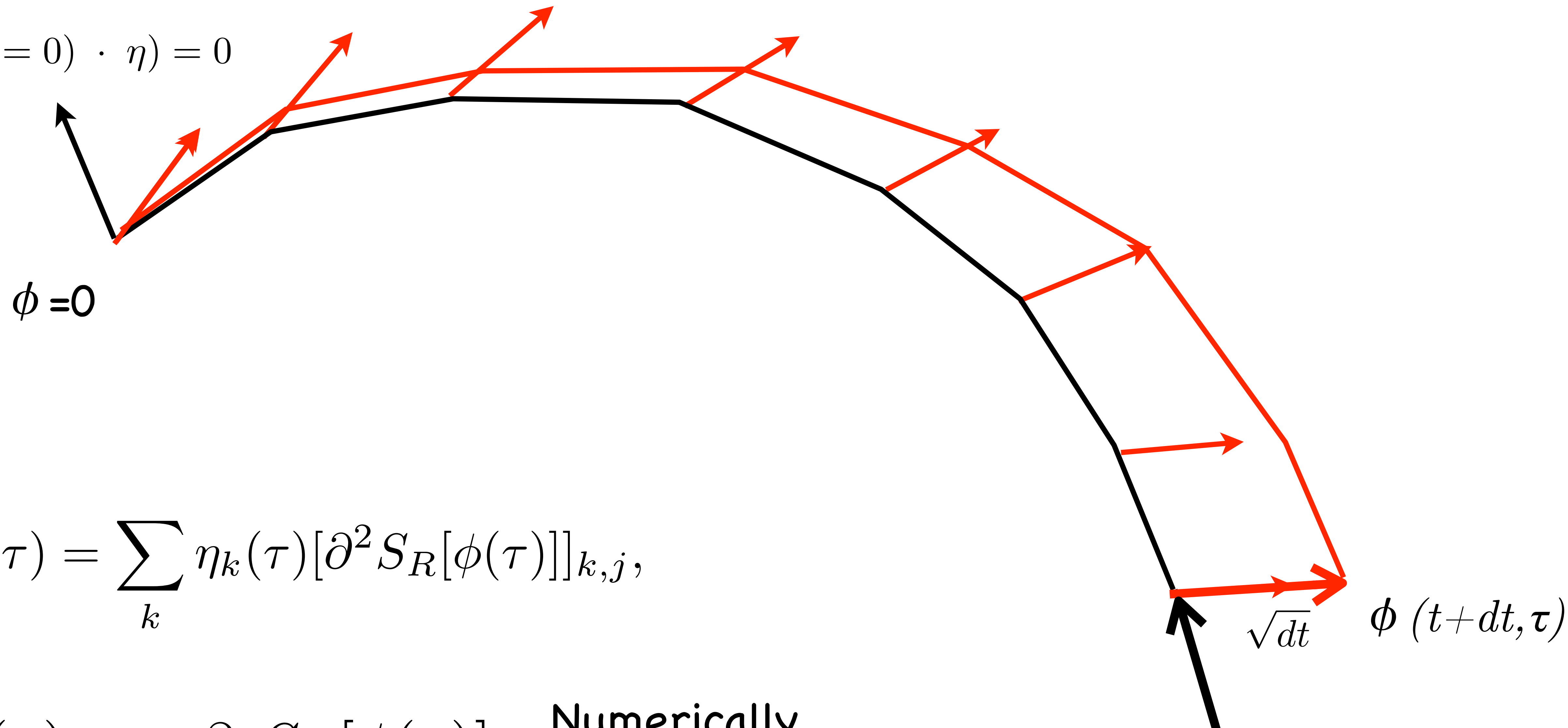

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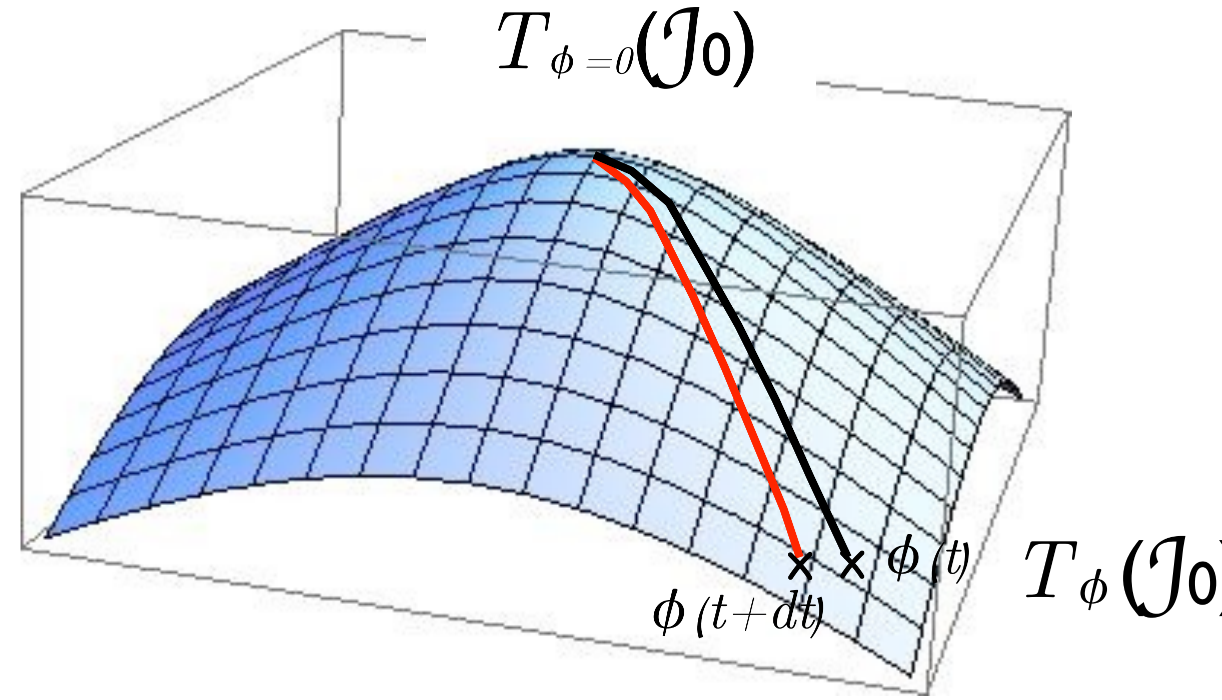
Numerically stable?

Hopeless, if treated as an ODE with an initial value problem (IVP)

Numerical stability of the SD step

This is a typical case that should be treated as a boundary value problem (BVP), by using the condition:

$lim_{\tau\to\infty}\ \phi\ (t+dt,\tau)\ =0.$



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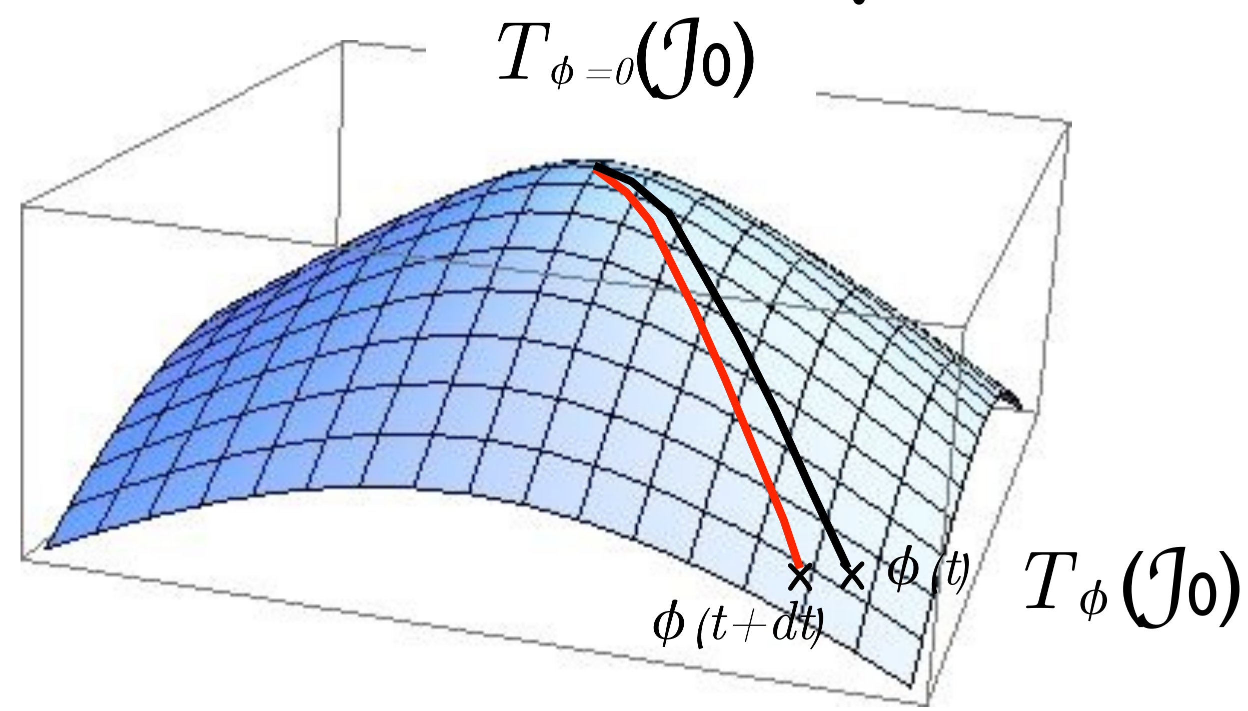

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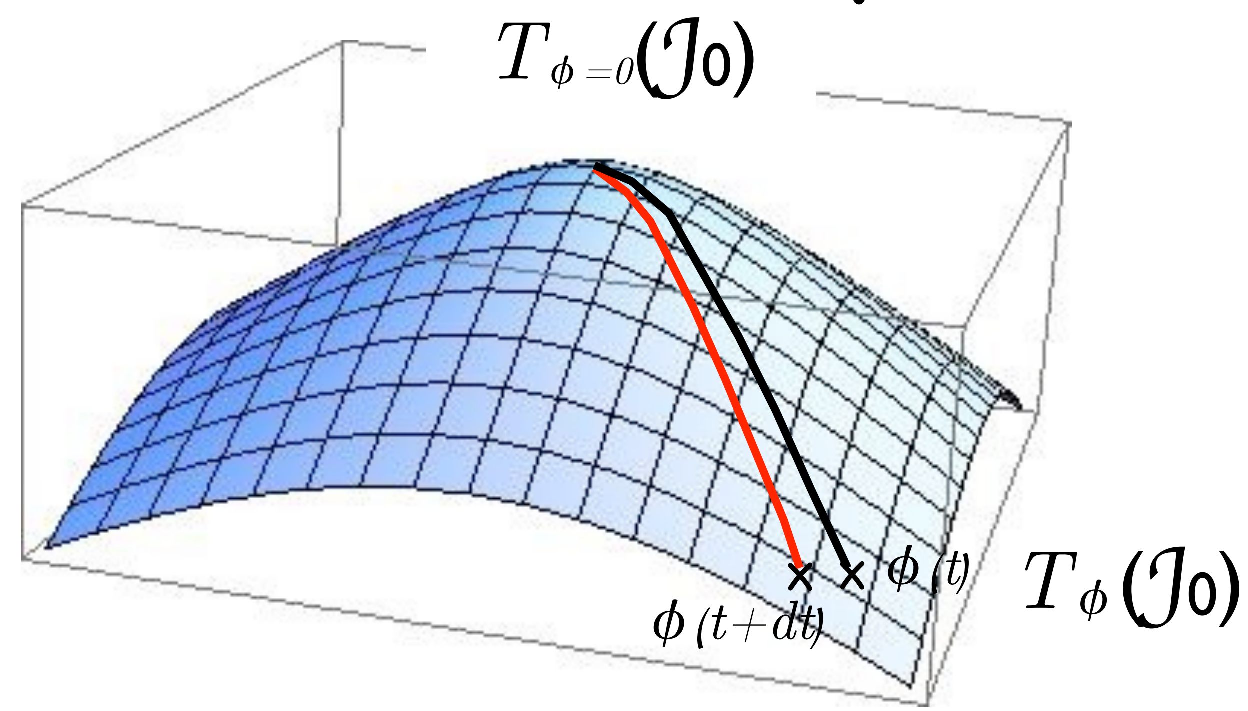

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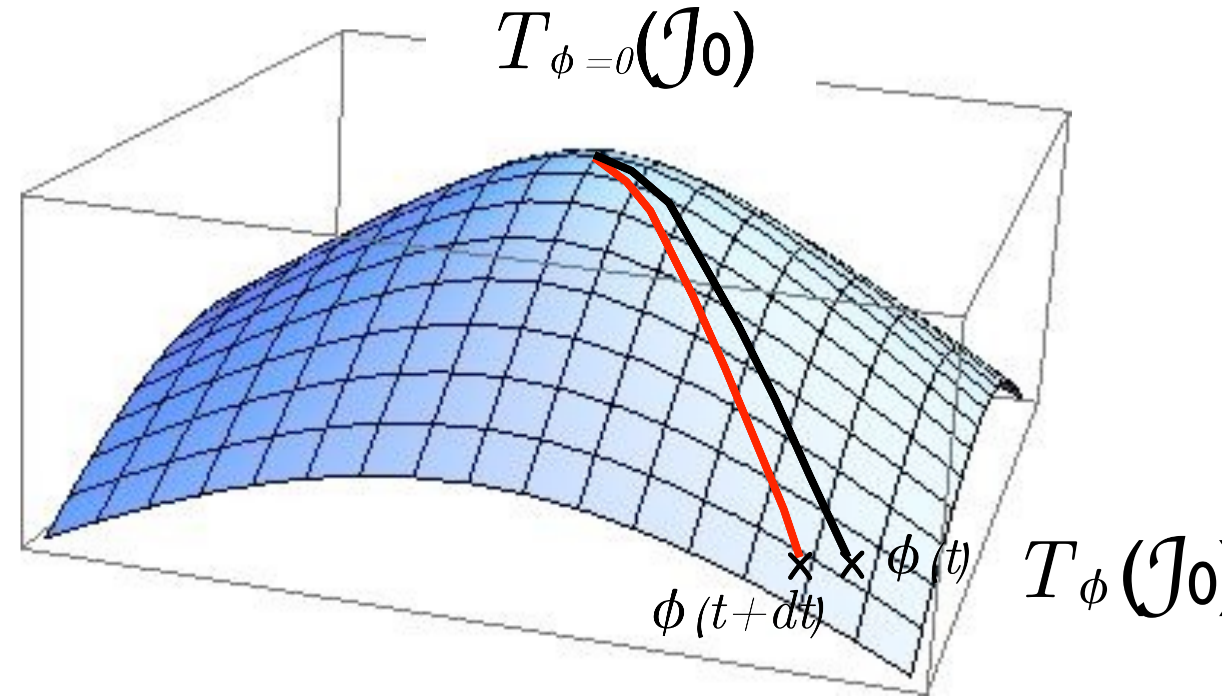

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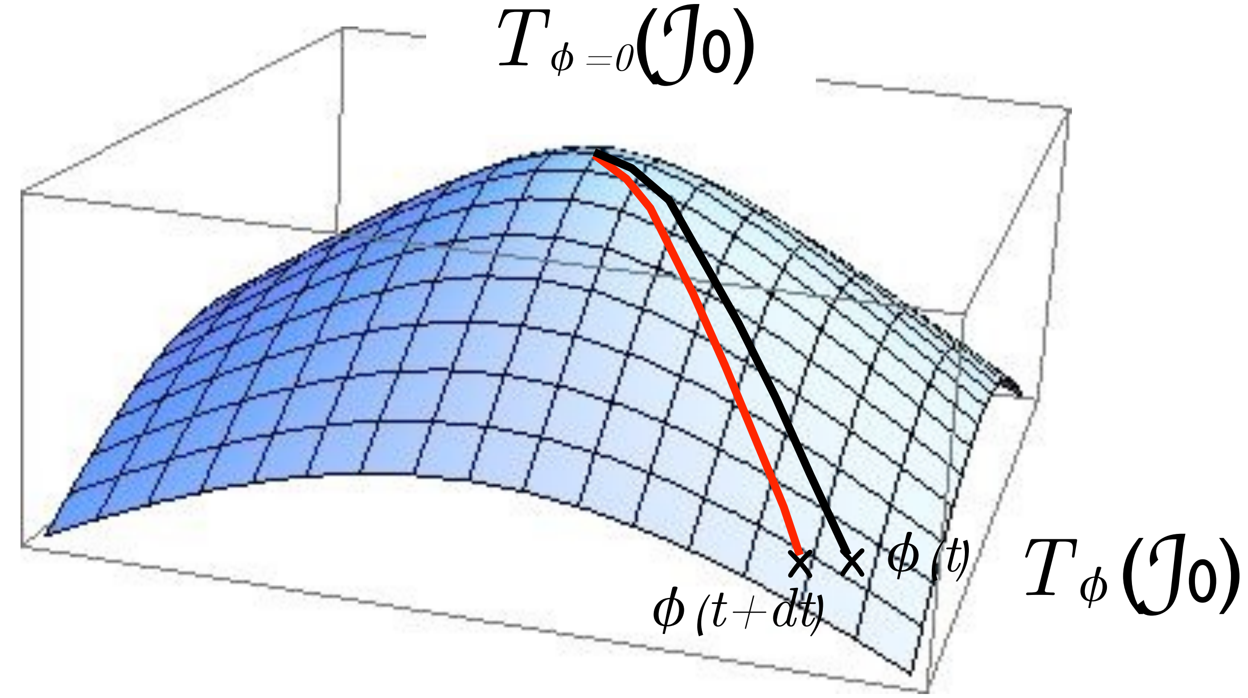

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Test it!

Residual phase

As noticed at the beginning, there is still a phase

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

$$\prod_x d\phi_x \longrightarrow \mathtt{det}(T_\phi)$$

T_ϕ is the tangent space to $\mathcal{J}_0$ in ϕ.

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In fact, such phase is neglected in the saddle point method.

Moreover, one expects this phase to change very smoothly...

We have good reasons to expect that it can be treated with reweighting,
but no a priori justification to ignore it!

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$\det(T_\phi)$

T_ϕ is the tangent space to $\mathcal{J}_0$ in ϕ.

The determinant can be evaluated as a sum of variations, that become traces:

$$\det(T_{\phi_\tau}) = -\int_\tau^\infty ds \, \mathrm{Tr}[\, T_{\phi_s}^{-1} \frac{d}{ds} T_{\phi_s} \,] \simeq \sum_{i=0}^{N_\tau} \mathrm{Tr}[\, T_{\phi_i}^{-1} \, \Delta T_{\phi_i} \,] =$$

and the traces can be computed with N_R noisy estimators (ξ).

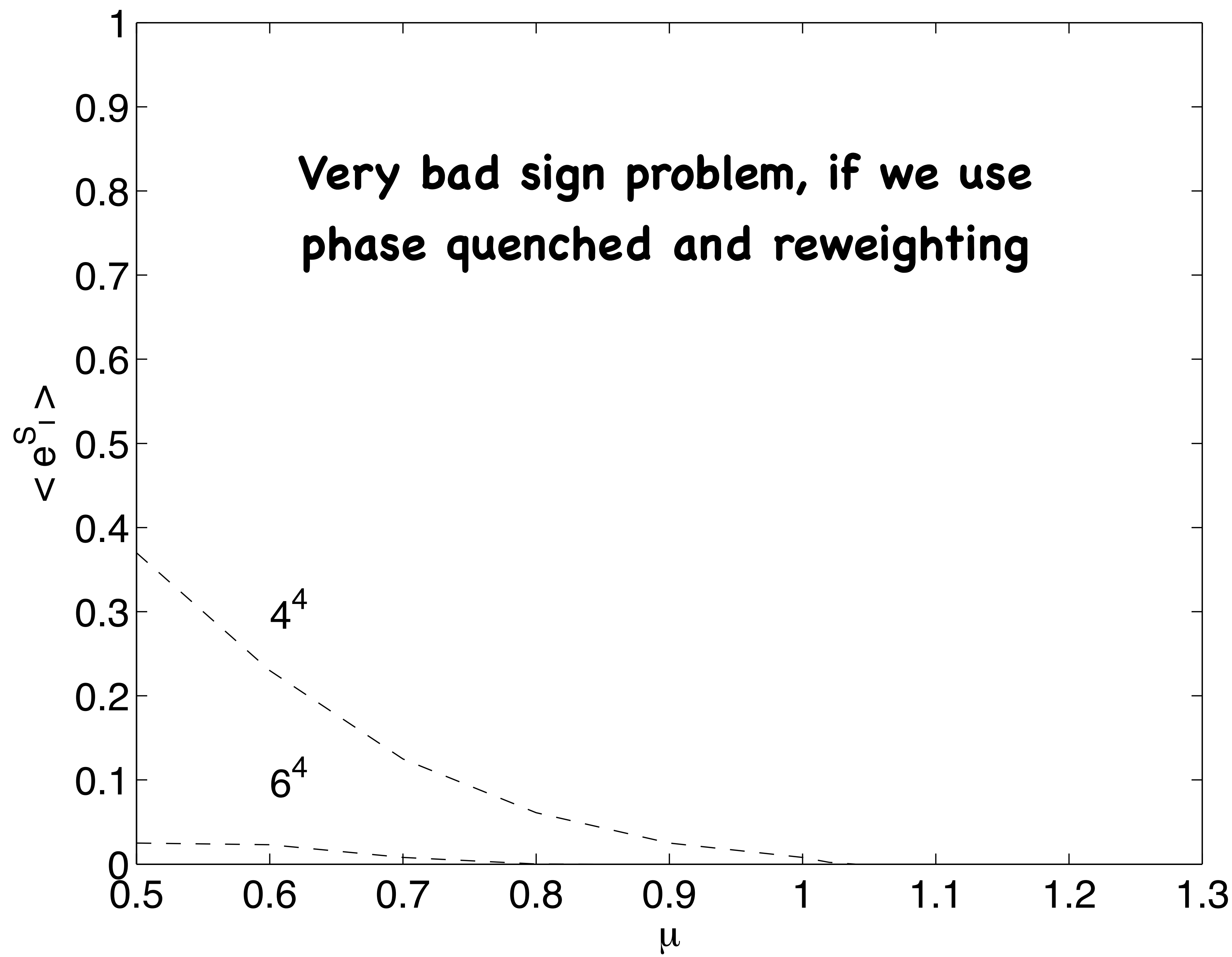
$$= \sum_{i=0}^{N_\tau} \sum_{k=1}^{N_R} {\xi^{(k)}}^T T_{\phi_i}^{-1} \Delta T_{\phi_i} \, \xi^{(k)} =$$

We have to evolve $N_R \, N^{CG}$ vectors, where each evolution costs O($N_\tau V$).

Does it work?

Bose gas on the thimble

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



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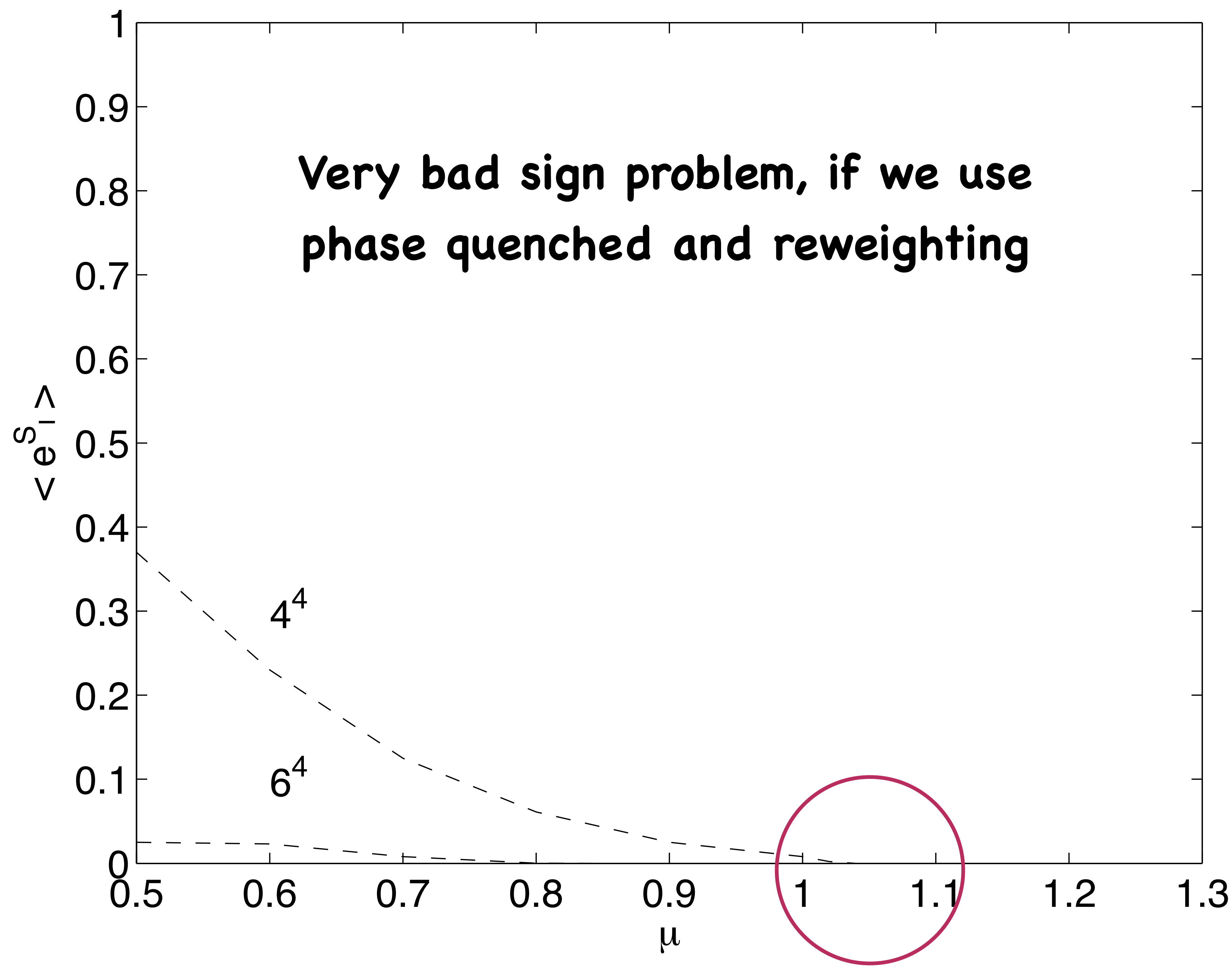

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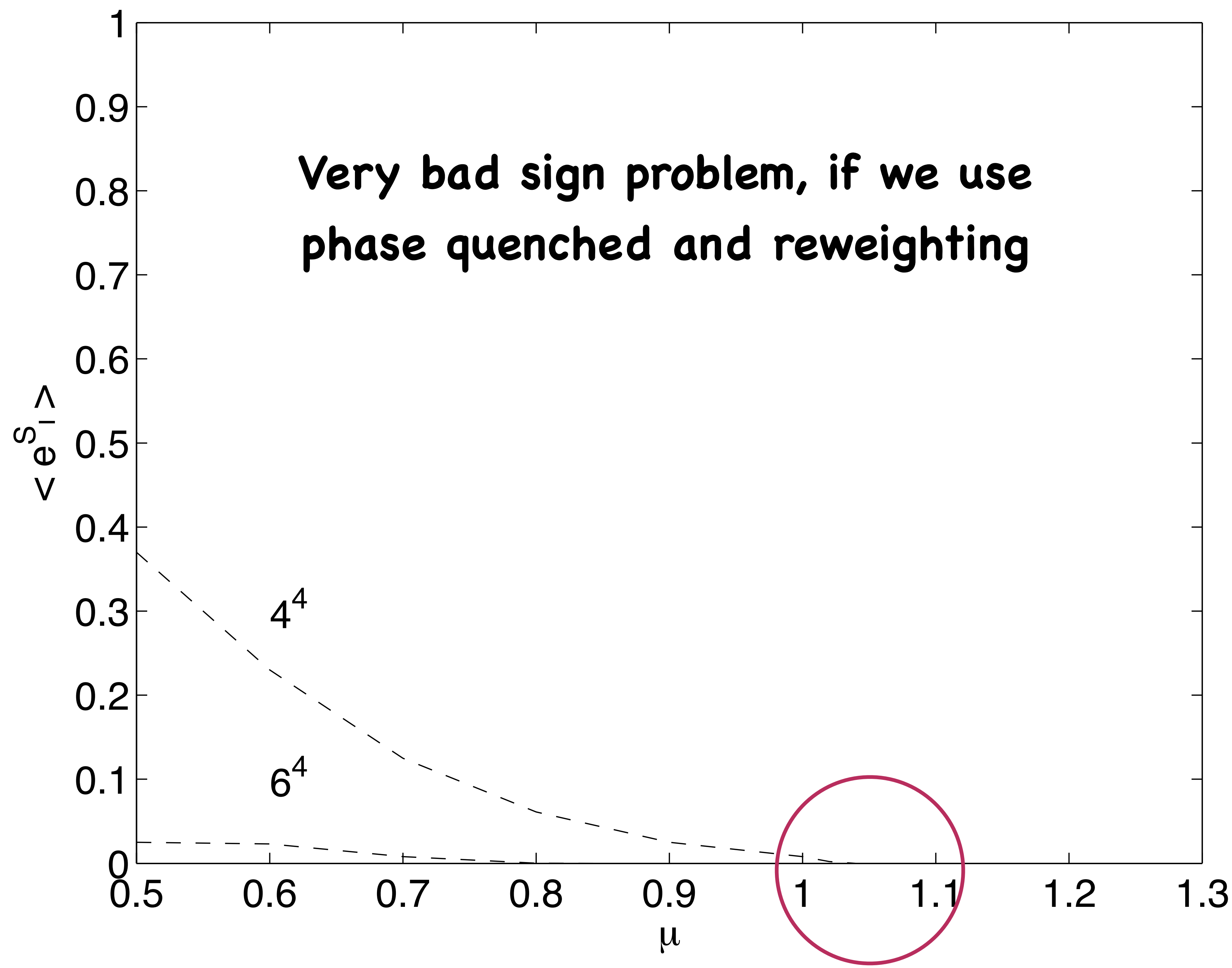
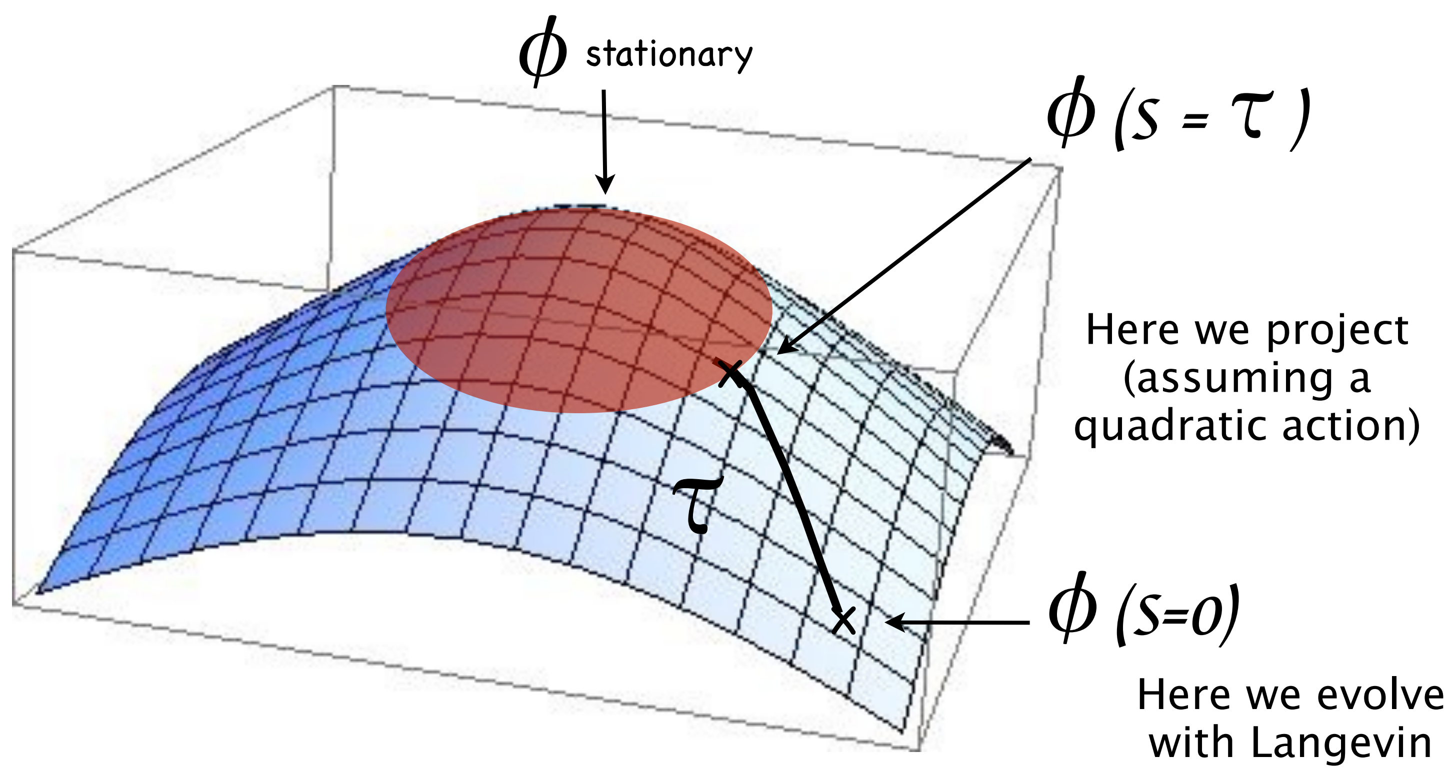


m=λ=1

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

How precisely should we approximate the thimble?



Equivalently: what is the minimal τ? i.e. the distance between the region where the system thermalizes and the region where the quadratic approximation is sufficient

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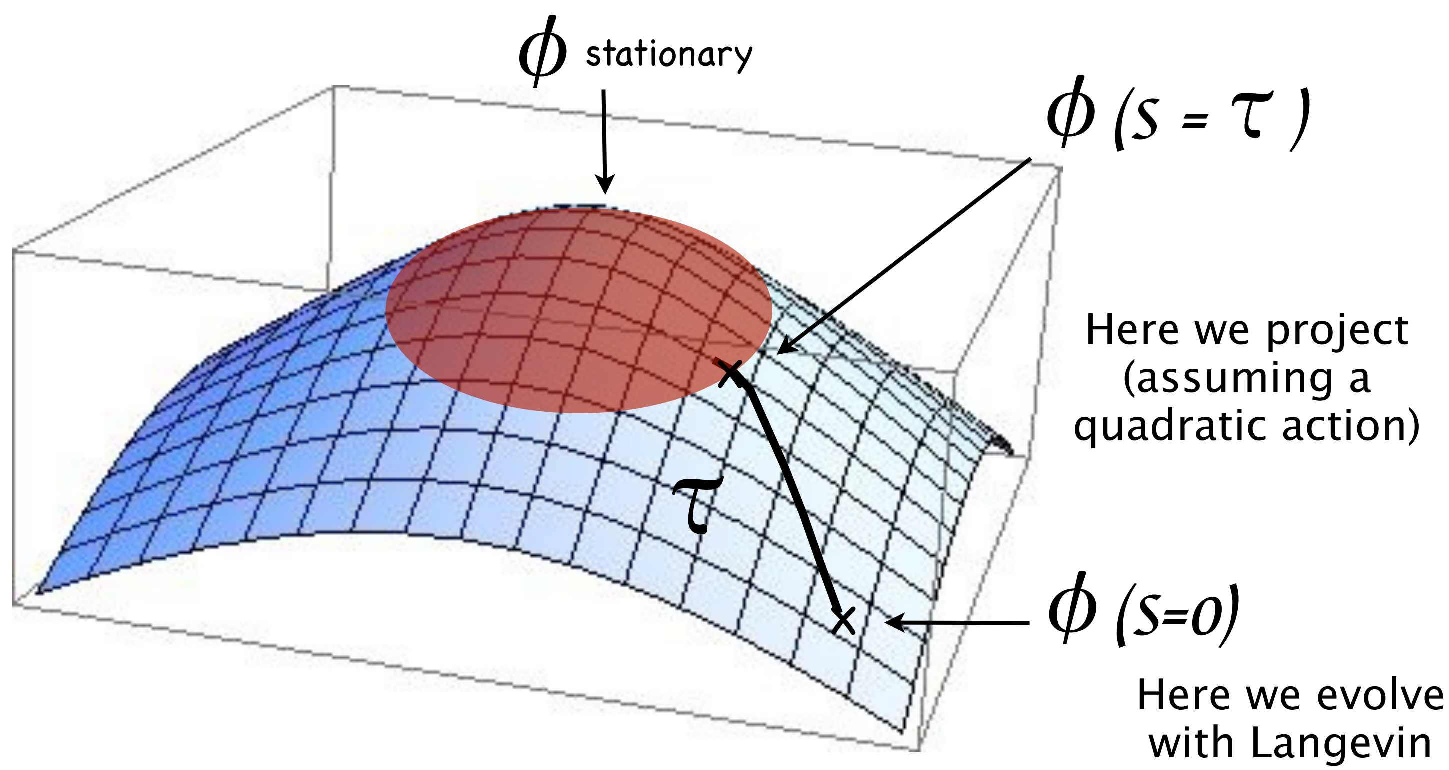

Equivalently: what is the minimal τ? i.e. the distance between the region where the system thermalizes and the region where the quadratic approximation is sufficient

It depends on two requirements:

1. The homology class of the thimble should be preserved.
2. The fluctuations in S_I should not produce a sign problem.

What about τ=0 ?

which corresponds to the vector space associated
to positive eigenvalues of the Hessian:

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

Project everywhere along the directions
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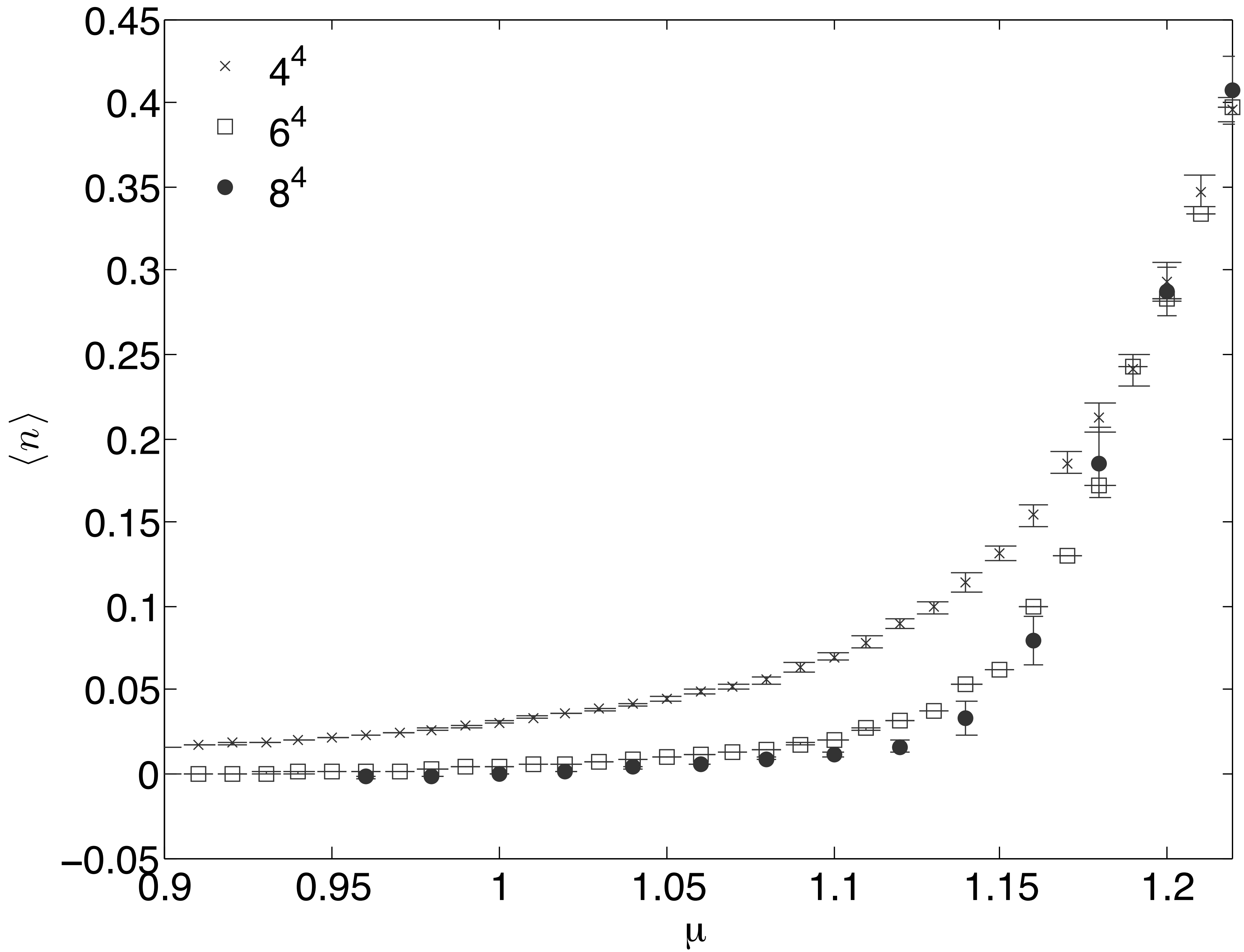
In practice, in this model for our choice of parameters we saw divergences only about 1% of the histories (almost 1M trajectories long),
which suggests that removing these histories might already be a good approximation.

Bose gas on the thimble

In fact, we find already excellent agreement with the known solution!



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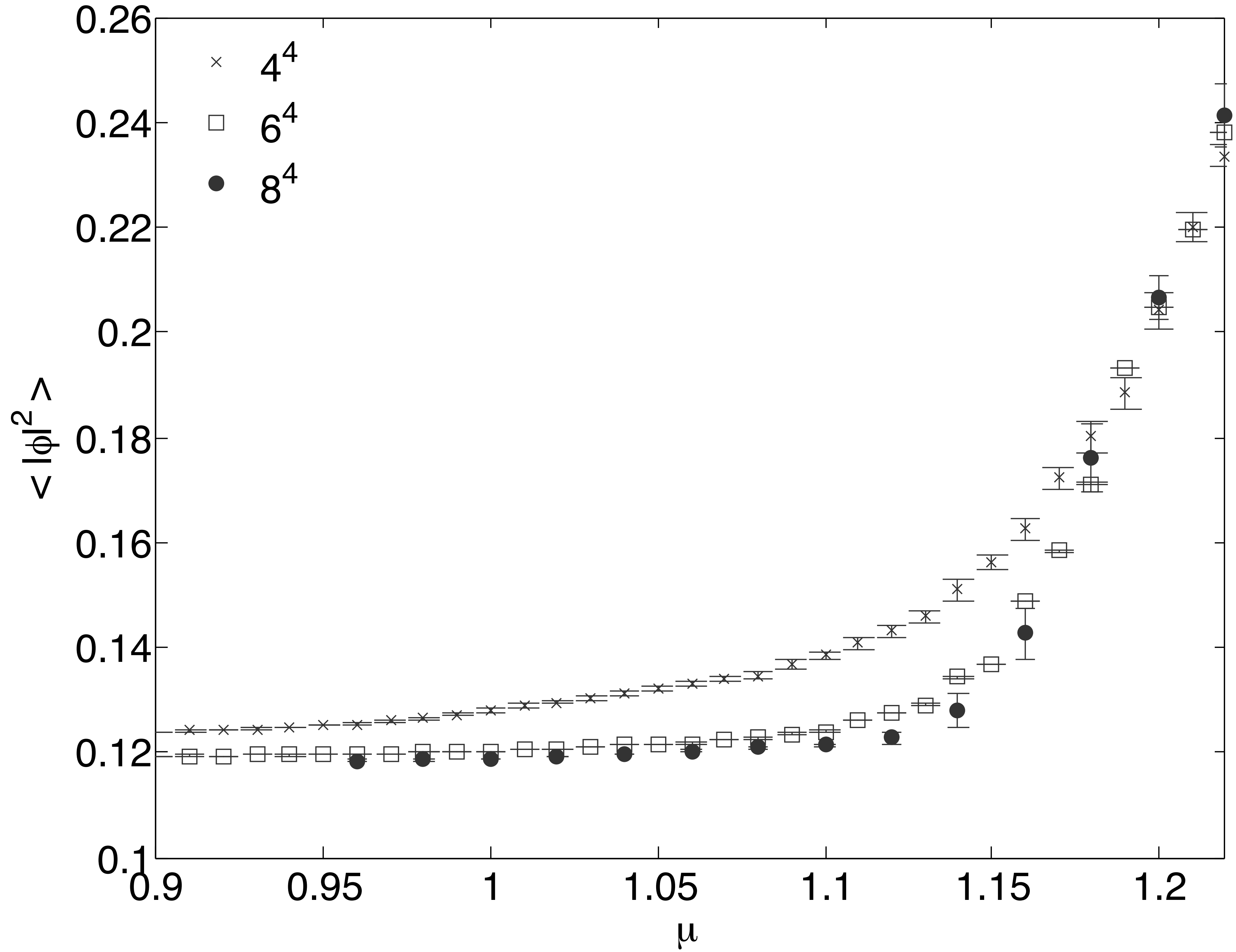
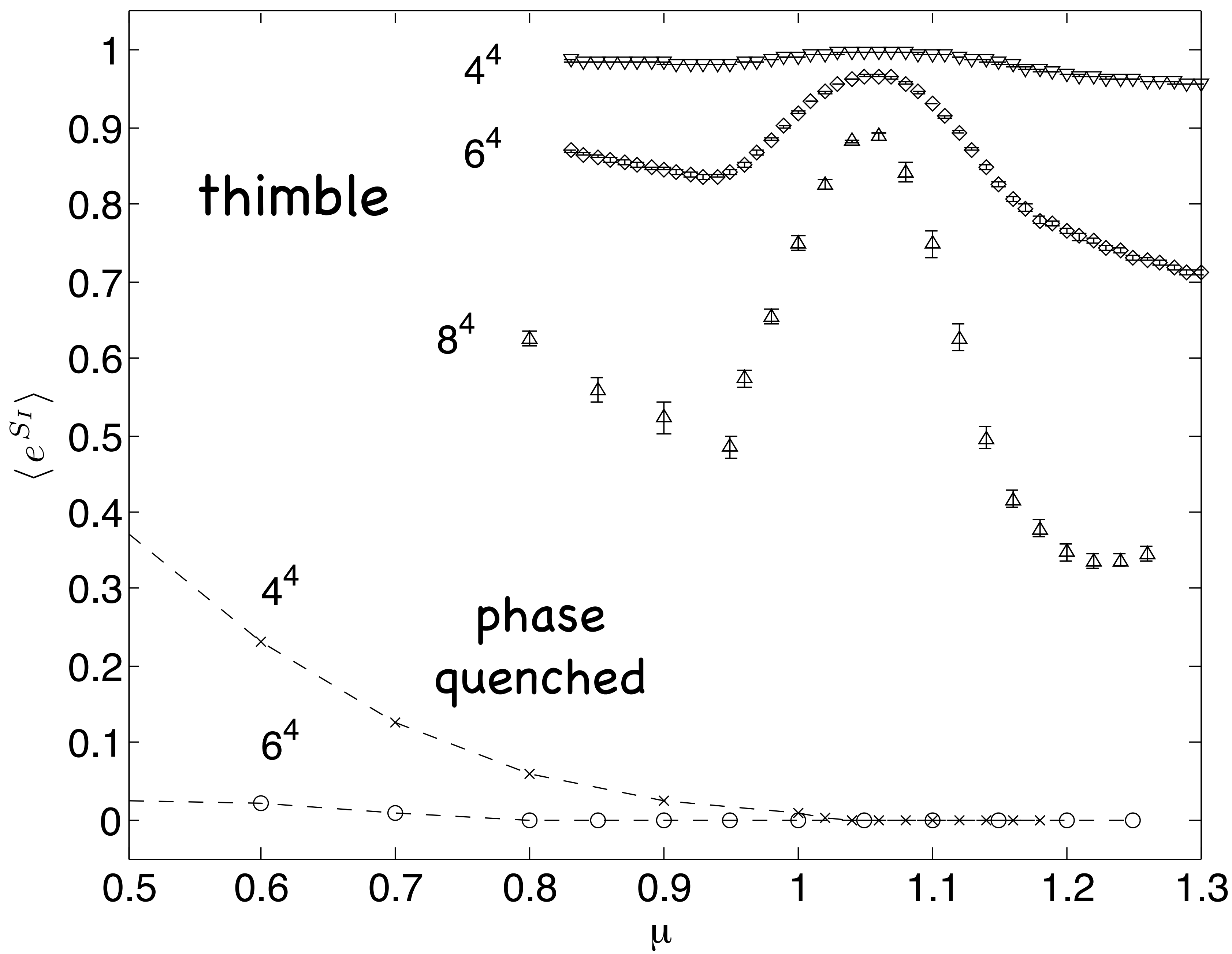


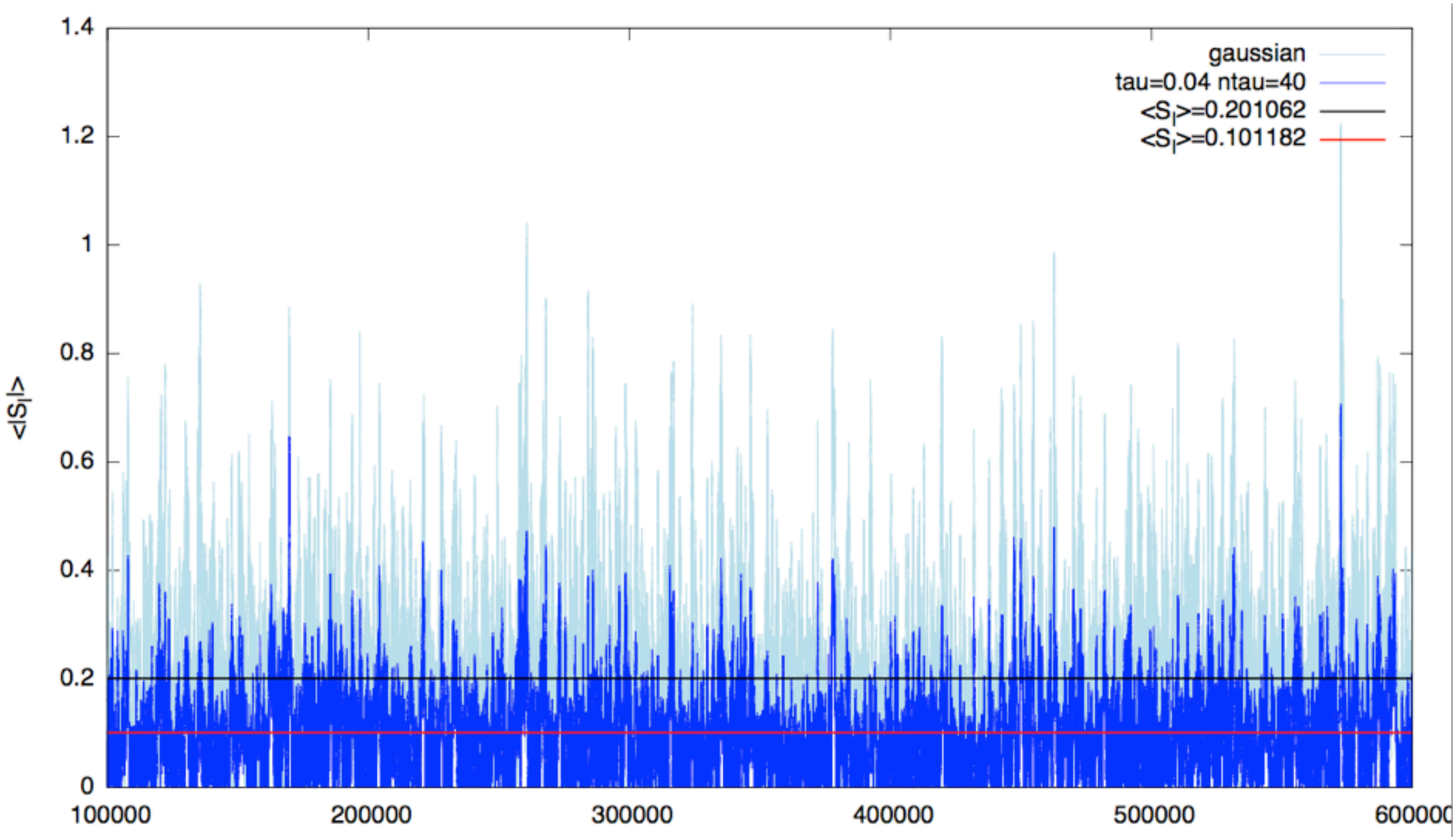
Bose gas on the thimble

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)

Bose gas on the thimble



Moreover, we can further approach the thimble by following the SD equations (measured by the reduced fluctuations on the imaginary part of the action).
This is necessary, in principle, to remove the unknown bias introduced by rejecting 1% of the histories

QCD ?

QCD Action

$$S[U] = \beta \sum_{x,\mu<\nu} \left[1 - \frac{1}{3} \Re \, \mathrm{Tr} \, U_{\mu,\nu}(x) \right] + N_f \, \mathrm{Tr} \log Q[U]$$

$$U_{\mu,\nu}(x) = U_\mu(x) U_\nu(x+\hat{\mu}) U_\mu(x+\hat{\nu})^{-1} U_\nu(x)^{-1}$$

Wilson Plaquette

$$Q[U]_{xy} = (m+4)\delta_{xy} - \frac{1}{2} \sum_{\nu=0,3} (1-\gamma_\nu)\delta_{x+\hat{\nu},y} e^{\mu\,\delta_{0,\nu}} U_\nu(x) - \frac{1}{2} \sum_{\nu=0,3} (1+\gamma_\nu)\delta_{x-\hat{\nu},y} e^{-\mu\,\delta_{0,\nu}} U_\nu(x-\hat{\nu})^{-1}$$

Wilson Fermion Matrix

Complexification

$$A^a_\nu(x) \to A^{a,R}_\nu(x) + i A^{a,I}_\nu(x) \qquad a = 1 \ldots N_c^2 - 1.$$

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

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.

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

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: $[T_a, T_b] = if_{abc}T_c$

Note that the Hessian is still well defined and symmetric in the stationary points.

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).

Strictly speaking no stationary point can be non-degenerate
(the Hessian has zero eigenvalues corresponding to the gauge d.o.f.)

Solution: Substitute the concept of <u>non-degenerate critical point</u>
with the one of <u>non-degenerate critical manifold</u> (Bott 1956)

A manifold $\mathcal{N} \subset$ D is a <u>non-degenerate critical sub-manifold</u> of D for the function F : D $\rightarrow \mathbb{R}$ if:

1. $dF = 0$, along $\mathcal{N}$.
2. The Hessian $\partial^2 F$ is non-degenerate on the normal bundle $\nu(\mathcal{N})$.

Under these conditions the normal bundle decomposes in $\nu(\mathcal{N}) = \nu^+(\mathcal{N}) + \nu^-(\mathcal{N})$
associated to positive and negative eigenvalues of $\partial^2 F$.

In the case of QCD the manifold $\mathcal{N}$ corresponds to a gauge orbit. $n_G := dim_{\mathbb{R}} \mathcal{N} = (V-1) \times (N_c^2 - 1)$

In the case of the thimble $\mathcal{J}_0$, it is the gauge orbit generated from $A = 0$.

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:

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

The thimble $\mathcal{J}_0$ can now be defined as:

$$\mathcal{J}_0 := \left\{U \in (SL(3,\mathbb{C}))^{4V} \mid \exists U(\tau) \ \ \text{solution of SD Eq} \mid U(0) = U \ \ \& \ \ \lim_{\tau\to\infty} U(\tau) \in \mathcal{N}^{(0)}\right\}$$

which has dimension: $(n\text{-}n_G)+n_G=n$.

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.

(This means that also Ward Identities are fulfilled).

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:

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

Minimum

A=0 is always a stationary point for the complexified action.

A=0 is a local minimum, when the (Wilson) fermions have
anti-periodic boundary conditions in all directions.
(the other two Z_3 brothers are saddle points)

Sufficiently near to the continuum limit,
A=0 is also a global minimum (for any μ).

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- The residual phase should not give a sign problem and hence should be manageable with reweighting, the Bose gas provides the first confirmation of this expectation.
- Our first application on a nontrivial model is very encouraging…

Backup

Topology

With Wilson fermions there are no disconnected topological sectors.
There are gauge configurations with some topological content (apprx. instantons),
If we smooth them (SD~cooling), they initially reveal their topological content
but eventually fall in the zero topological sector.

i.e. the thimble includes topologically nontrivial configurations.

To compute the tangent, we want to reach the zero charge sector fast.
Thanks to the choice of the thimbles, the configurations near A=0 should be
much more important; Moreover, Fourier acceleration might help.

Even in presence of disconnected topological sectors (e.g. overlap) one
thimble is restricted to one topological sector,
but the local physics is the same, up to finite volume corrections.

Similar remarks for vortices, since they are saddle points, and not minima.