Going with the flow: sign problem, thimbles and beyond

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(A. Alexandru, G. Basar, N. Warrington, G. Ridgway)

Sign problem

Standard field theoretical Monte Carlo:

$$\langle \mathcal{O} \rangle = \frac{\int D\phi \; e^{-S[\phi]} \mathcal{O}[\phi]}{\int D\phi \; e^{-S[\phi]}} \approx \frac{1}{\mathcal{N}} \sum_a \mathcal{O}[\phi_a]$$

configurations with $P[\phi] = \frac{e^{-S[\phi]}}{\int D\phi \; e^{-S[\phi]}}$

What if S is not real ?

That’s what happens :

- QCD at finite chemical potential (quark or nuclear matter) matter
- most theories with a finite chemical potential
- Hubbard model away from half filling
- real time dynamics
- QCD with a θ term
- …

Sign problem

Reweighting:

$$\langle \mathcal{O} \rangle = \frac{\int D\phi \; e^{-S_R[\phi]} e^{-iS_I[\phi]} \mathcal{O}}{\int D\phi \; e^{-S_R[\phi]} e^{-iS_I[\phi]}}$$

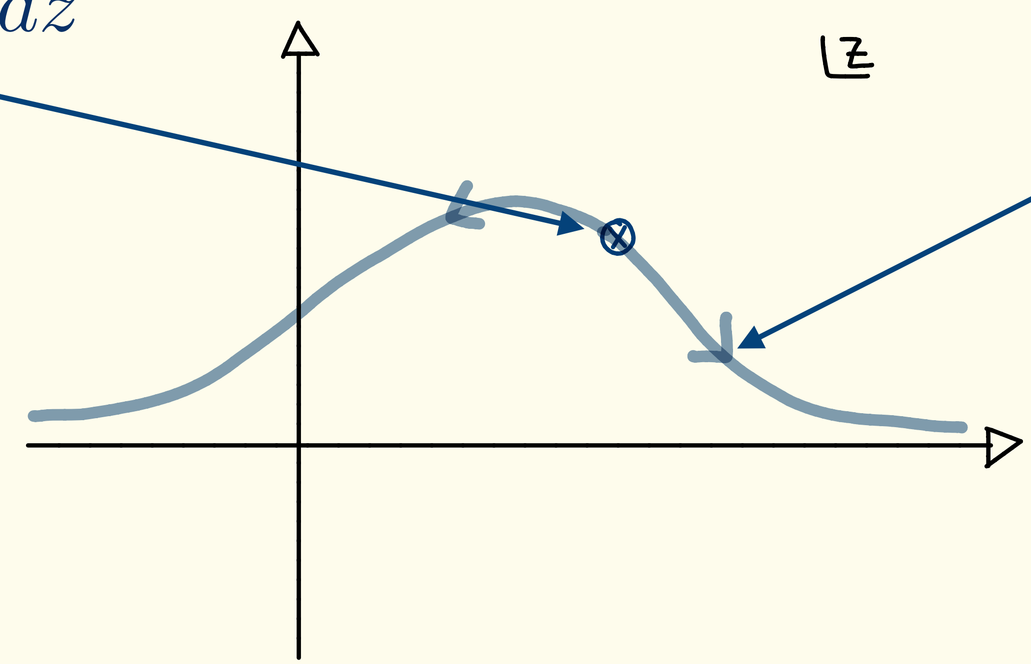
$$= \frac{\int D\phi \; e^{-S_R[\phi]} e^{-iS_I[\phi]} \mathcal{O}}{\int D\phi \; e^{-S_R[\phi]}} \frac{\int D\phi \; e^{-S_R[\phi]}}{\int D\phi \; e^{-S_R[\phi]} e^{-iS_I[\phi]}}$$

$$= \frac{\langle e^{-iS_I[\phi]} \mathcal{O} \rangle_{S_R}}{\langle e^{-iS_I[\phi]} \rangle_{S_R}}$$

average phase $\sim e^{-\# \beta L^3}$

The shortest path between two truths in the real domain passes through the complex domain, J.Hadamard

critical point: $\dfrac{dS}{dz} = 0$

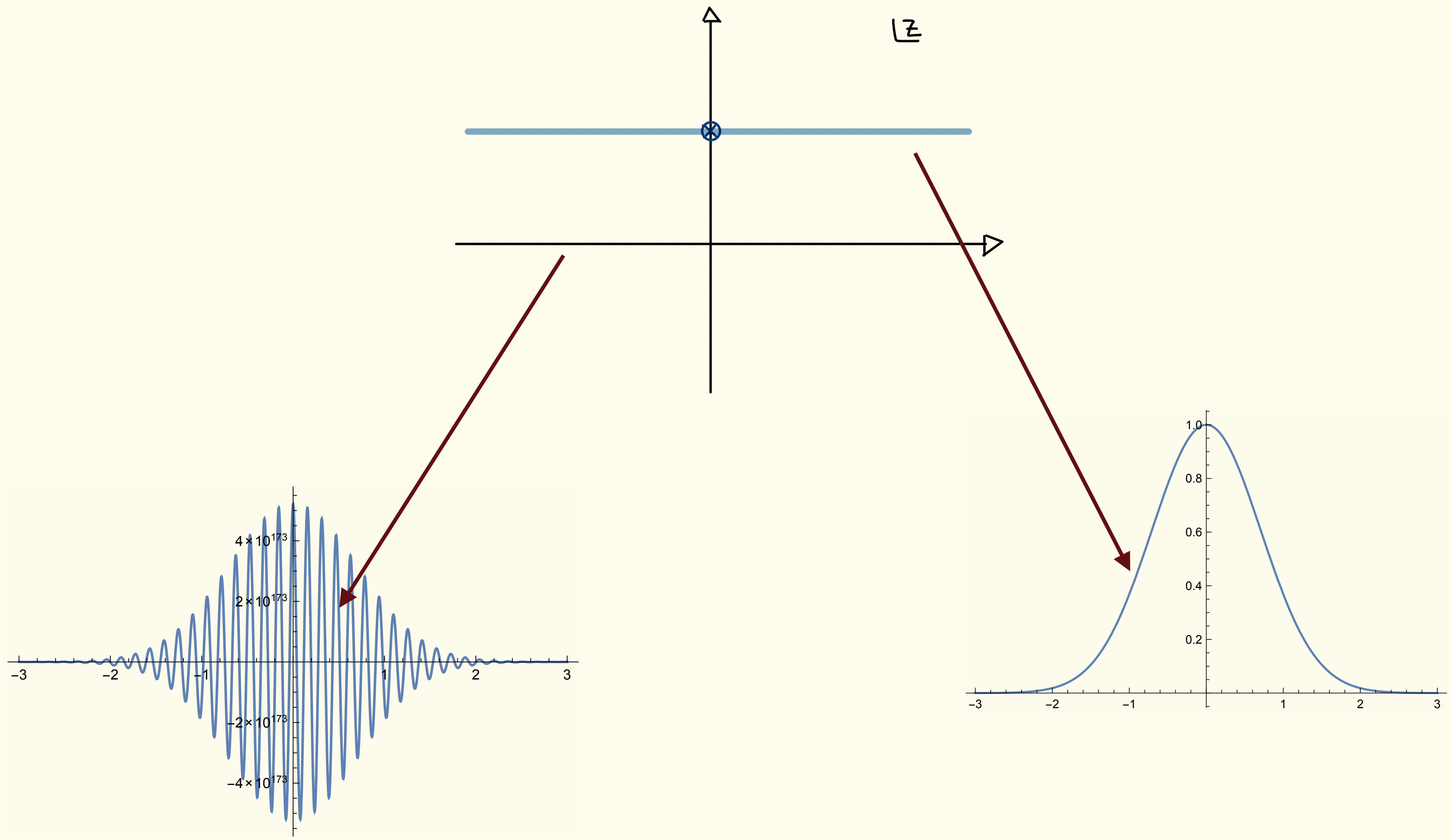


steepest descent
=
stationary phase

$$\int_{\mathbb{R}} dz\ e^{-S(z)} f(z) = e^{-iS_I} \int_C dz\ e^{-S_R(z)} f(z)$$

no sign problem

$$\int dz\ e^{-(x-i20)^2} = \sqrt{\pi}$$

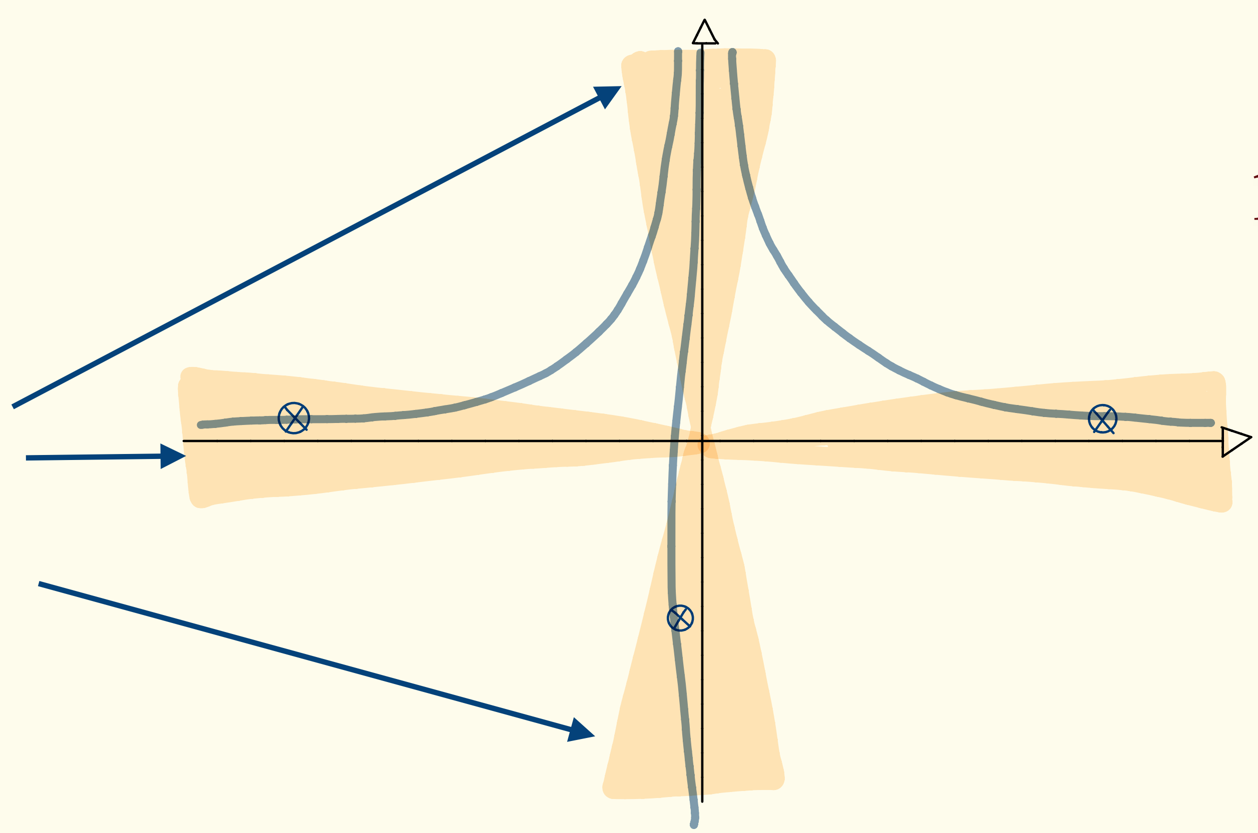


Cristoforetti, DiRenzo,Scorzato, ‘12

Sometimes two or more stationary phase paths are needed:

$$\int dz\ e^{-(hz+z^2+z^4)}$$

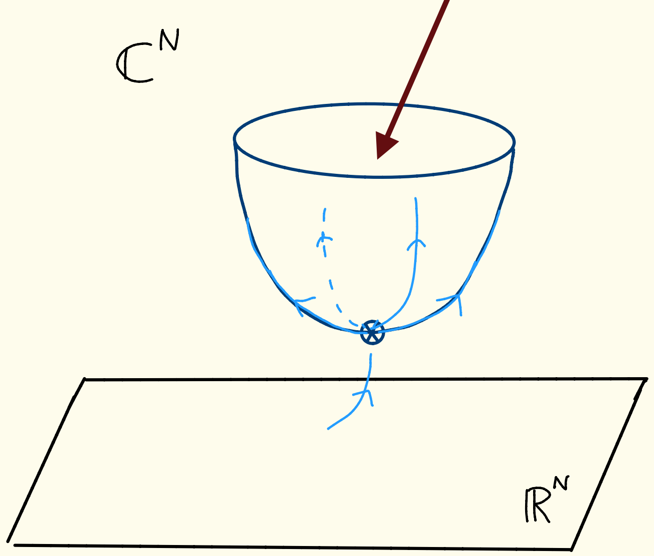
good asymptotic directions



integral depends only on initial and final directions: homological classes

How to generalize this idea to the many dimensional case ?

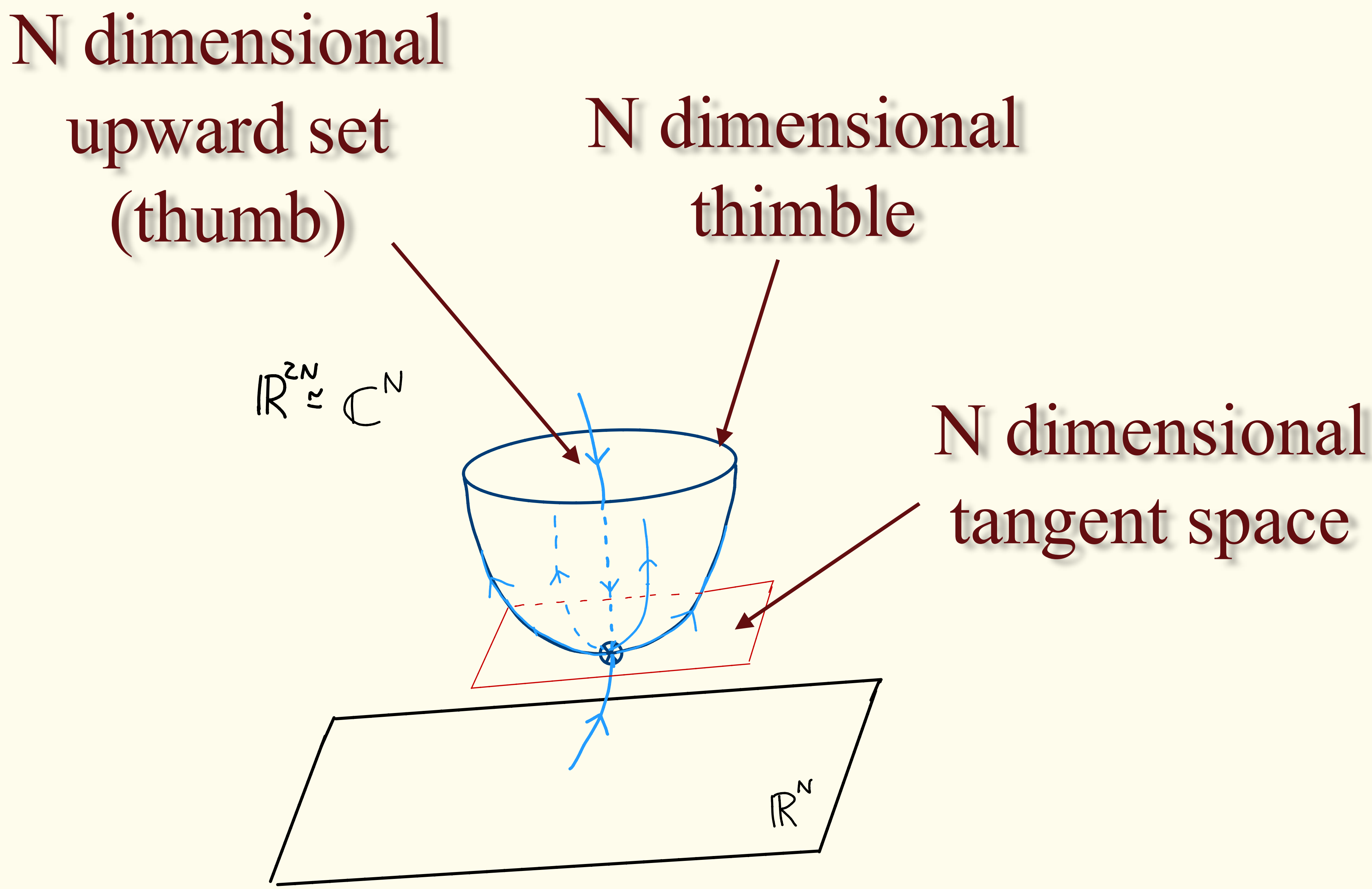
thimble



$$\frac{dz_i}{dt} = \overline{\frac{\partial S}{\partial z_i}} \Rightarrow \begin{array}{l} \dfrac{dx_i}{dt} = \dfrac{\partial S_R}{\partial x_i} = \dfrac{\partial S_I}{\partial y_i} \\ \dfrac{dy_i}{dt} = \dfrac{\partial S_R}{\partial y_i} = -\dfrac{\partial S_I}{\partial x_i} \end{array}$$

gradient flow of S_R

hamiltonian flow of S_I



N dimensional upward set (thumb)
N dimensional thimble
N dimensional tangent space
$\mathbb{R}^{2N} \simeq \mathbb{C}^N$
$\mathbb{R}^N$

in general:

$$\langle\mathcal{O}\rangle = \frac{n_1 e^{-iS_{I1}} \int_1 d\phi\; e^{-S_R}\mathcal{O} + n_2 e^{-iS_{I1}} \int_2 d\phi\; e^{-S_R}\mathcal{O} + \cdots}{n_1 e^{-iS_{I1}} \int_1 d\phi\; e^{-S_R} + n_2 e^{-iS_{I1}} \int_2 d\phi\; e^{-S_R} + \cdots}$$

integer coefficients
(determined by how the
thumbs cross the thimble)

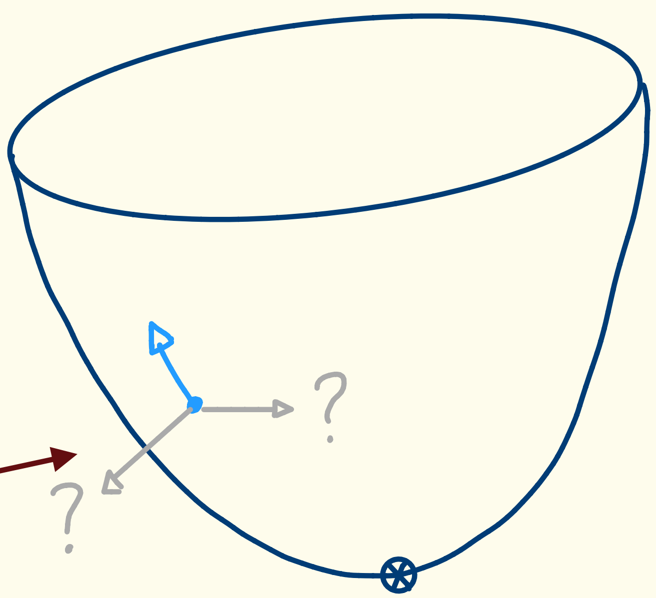
Things I'm not sure I believe:

1) $\Delta S_R \to \infty$ as $V \to \infty$ so only one thimble contributes in the thermodynamic limit

2) Path integral over one thimble has same symmetries as the path integral over real fields: yadda, yadda, universality, ... one thimble is enough.

more about multi-thimbles later ….

difficulty in the Monte Carlo:



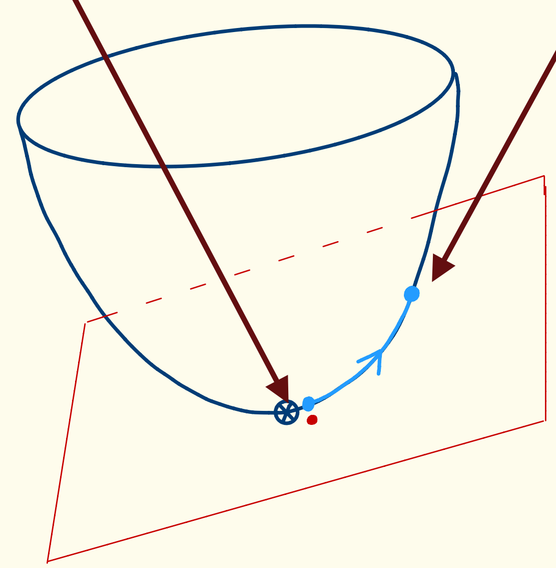
where to
go from here ?

There is no local characterization of the thimble

One thimble computation: contraction algorithm

$$\frac{dz_i}{dt} = \overline{\frac{\partial S}{\partial z_i}} \quad \Rightarrow \quad z_i(T)$$

$$z_i(0) = \tilde{z}$$

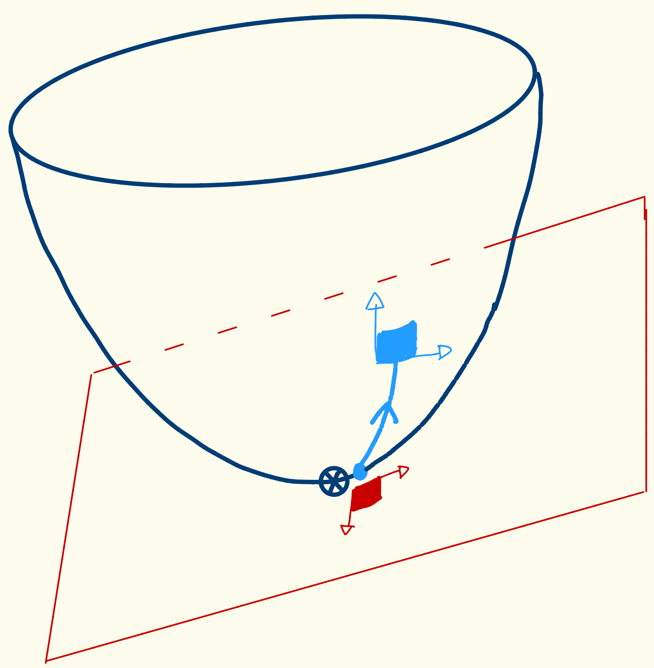


tangent space parametrizes the thimble

One thimble computation: contraction algorithm

$$\langle \mathcal{O} \rangle = \frac{\int dz_i \; \mathcal{O} e^{-S_R}}{\int dz_i \; e^{-S_R}} = \frac{\int d\tilde{z}_i \; \mathcal{O} \, \overbrace{\det\left(\frac{\partial z_i}{\partial \tilde{z}_j}\right)}^{J} e^{-S_R}}{\int d\tilde{z}_i \; \det\left(\frac{\partial z_i}{\partial \tilde{z}_j}\right) e^{-S_R}}$$

$$= \frac{\int d\tilde{z}_i \; e^{i\mathbb{I}m(lnJ)} e^{-\overbrace{(S_R - \mathbb{R}e(lnJ))}^{S_{eff}}} \mathcal{O}}{\int d\tilde{z}_i \; e^{i\mathbb{I}m lnJ} e^{-(S_R - \mathbb{R}e lnJ)}} = \frac{\langle e^{i\mathbb{I}m(lnJ)} \mathcal{O} \rangle_{S_{eff}}}{\langle e^{i\mathbb{I}m(lnJ)} \rangle_{S_{eff}}}$$



$$\frac{dJ_{ij}}{dt} = \overline{\frac{\partial^2 S}{\partial z_i \partial z_k} J_{jk}}$$

$$J_{ij}(0) = \mathbb{I}$$

$$\Rightarrow \quad J = \det J(T)$$

this is the expensive part

One thimble computation: contraction algorithm

$$\langle \mathcal{O} \rangle = \frac{\int dz_i \; \mathcal{O} e^{-S_R}}{\int dz_i \; e^{-S_R}} = \frac{\int d\tilde{z}_i \; \mathcal{O} \overbrace{\det\left(\frac{\partial z_i}{\partial \tilde{z}_j}\right)}^{J} e^{-S_R}}{\int d\tilde{z}_i \; \det\left(\frac{\partial z_i}{\partial \tilde{z}_j}\right) e^{-S_R}}$$

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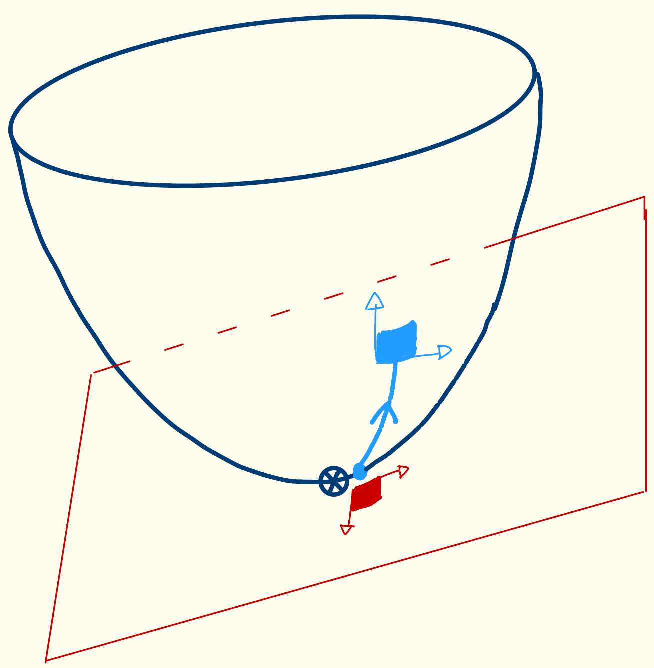


contraction algorithm

=

Metropolis in the tangent space,

action S_{eff} and

reweighted phase $e^{i \, \mathrm{Im}(\ln J)}$

Test it out on a model: 0+1 D Thirring model

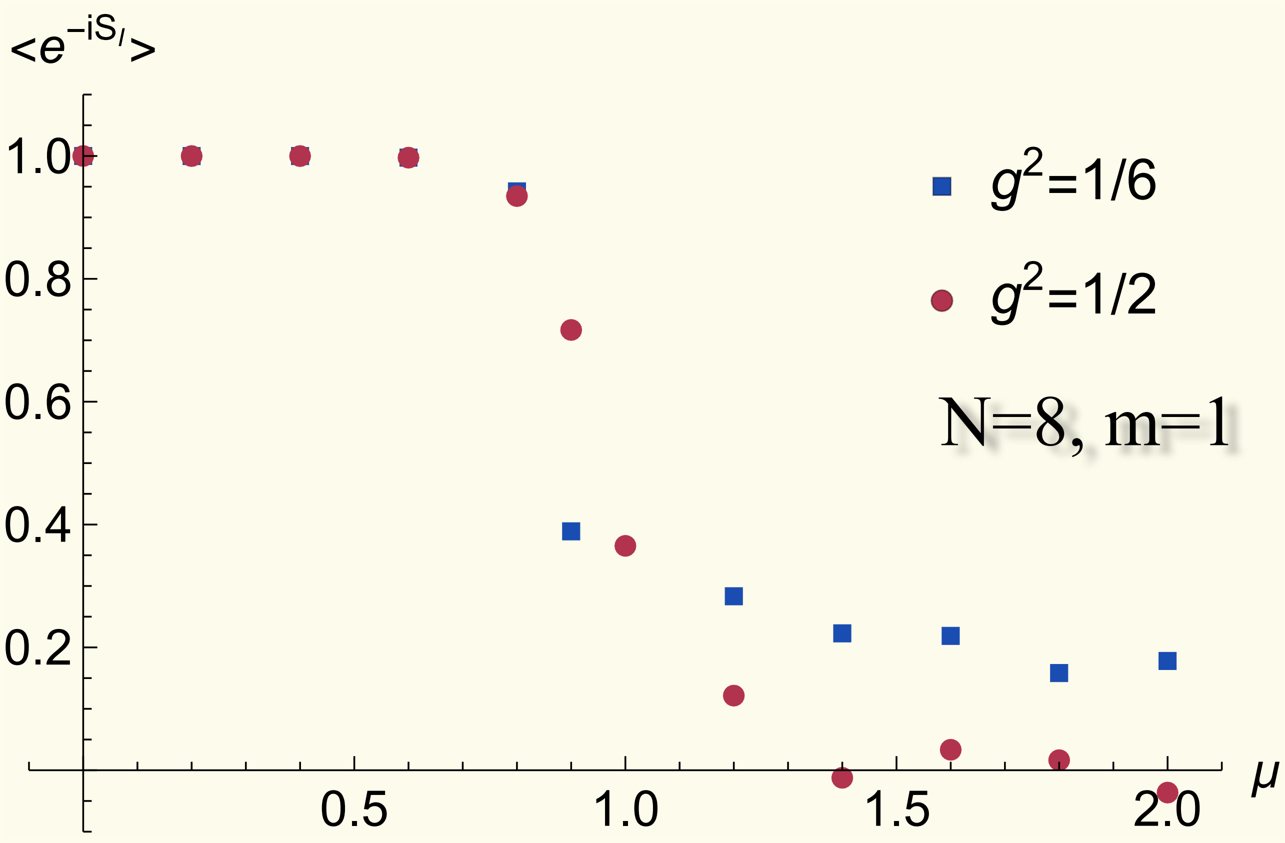
$$S = \int dt\ \bar{\chi}\left(\gamma^0 \frac{d}{dt} + m + \mu\gamma^0\right)\chi + \frac{g^2}{2}(\bar{\chi}\gamma^0\chi)^2$$

↑
just a 4-level system

discretize (staggered),
Hubbard-Stratanovich

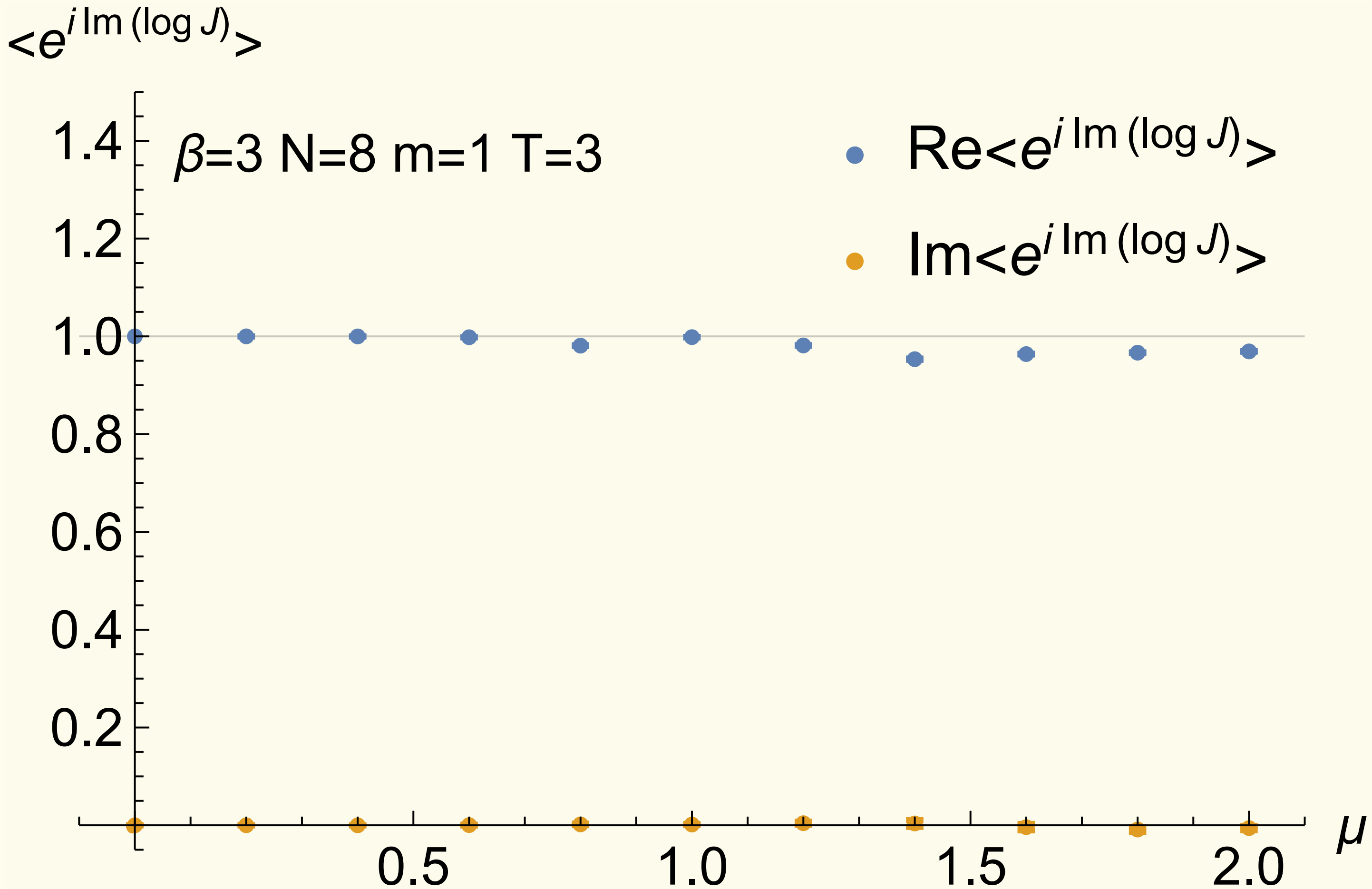
$$\begin{aligned} S[\phi] &= \frac{1}{g^2}\sum_t (1-\cos\phi_t) - \log det D[\phi] \\ D_{tt'} &= \frac{1}{2}(e^{\mu+i\phi_t}\delta_{t+1t'} - e^{-\mu-i\phi_t}\delta_{t-1t'} + e^{\mu-i\phi_t}\delta_{tN}\delta_{t'1}) + m\delta_{tt'} \end{aligned}$$

Is there a sign problem ?



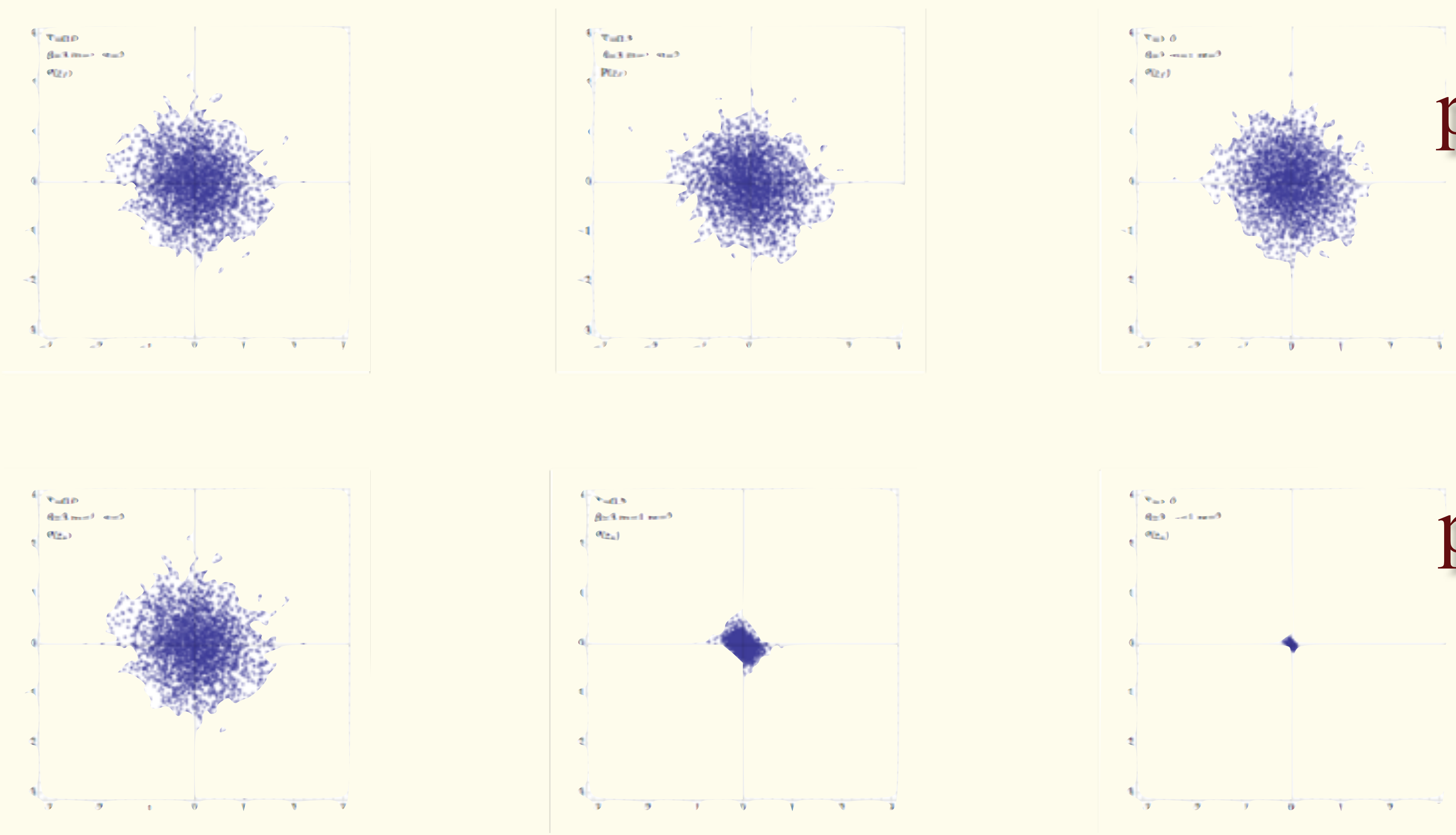
Yes, at μ>1 and specially at strong coupling.

Is there a remaining sign problem with the contraction algorithm ?



Nope, not on this model with these parameters.

Does it look like the algorithm is doing what is supposed to do ?

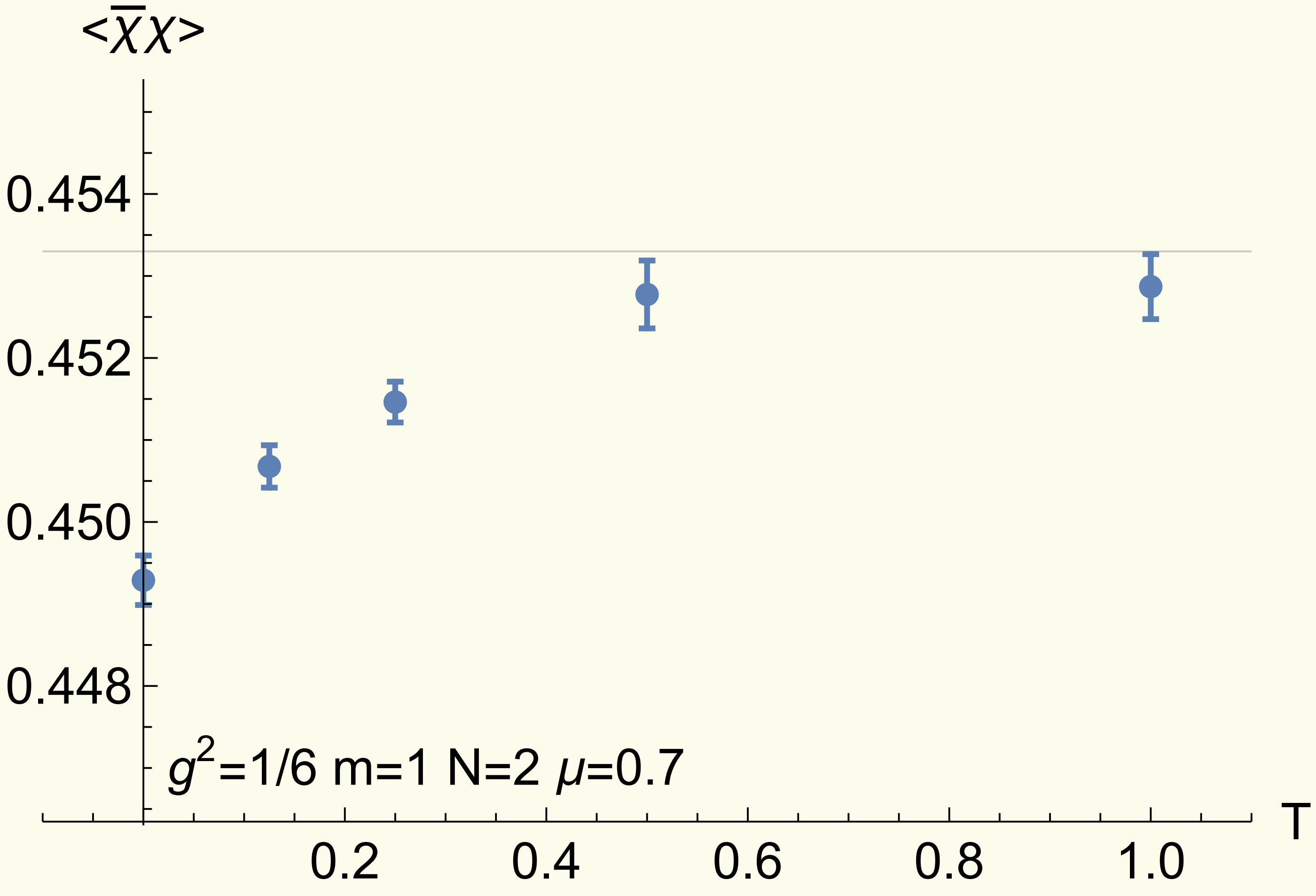


points on the thimble

points on the tangent space

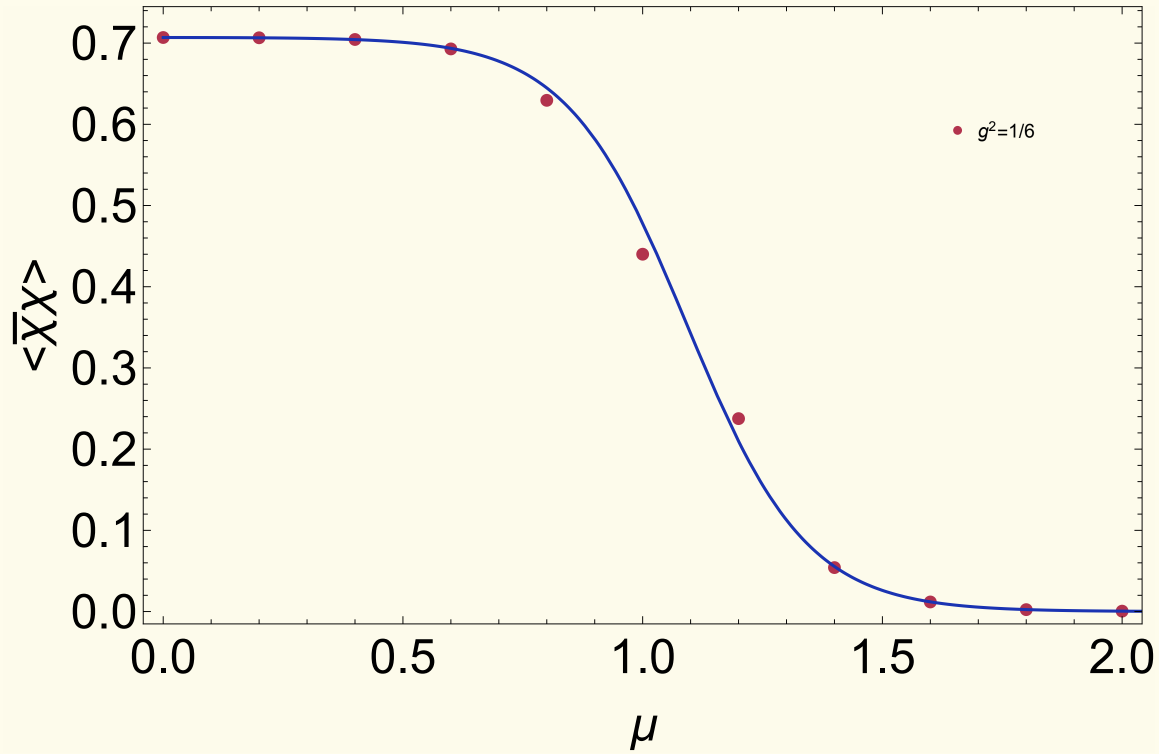
T=0 T=0.5 T=1

Does it look like the algorithm is doing what is supposed to do ?



Finally, the results:

$N=8$, $g^2=1/6$, $T=2$



Fujii, Kamata, Kikukawa, '15

Alexandru, Basar, Bedaque, '15

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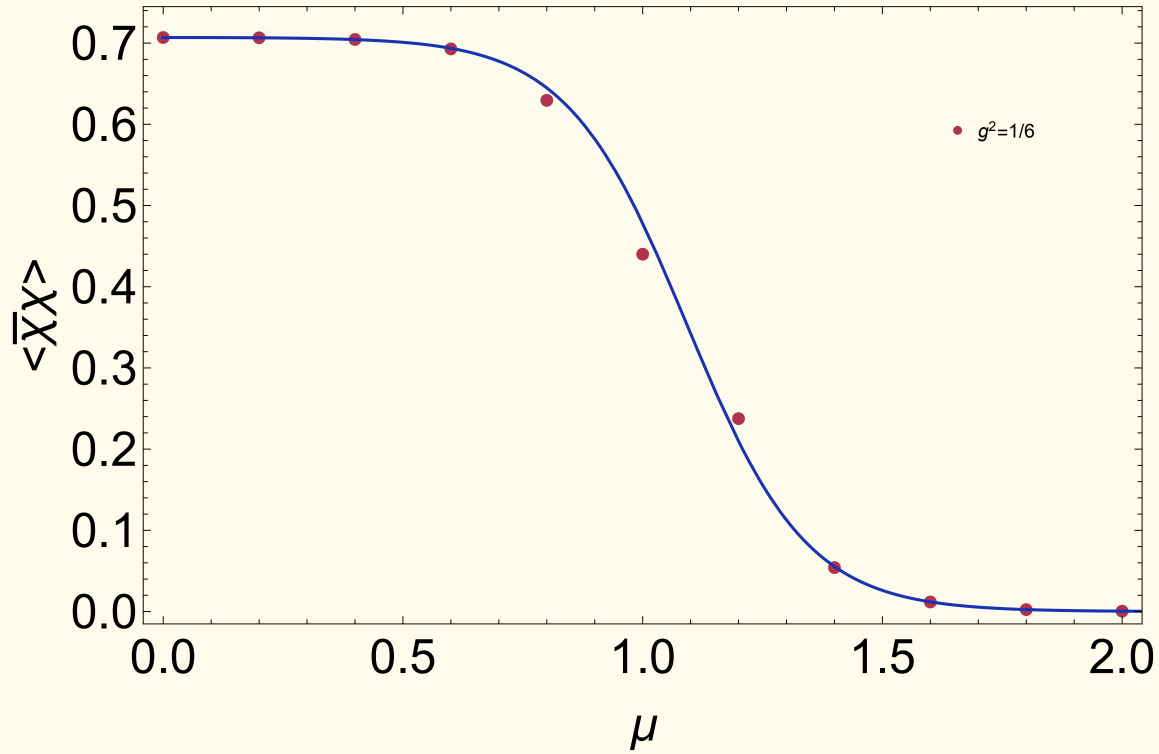
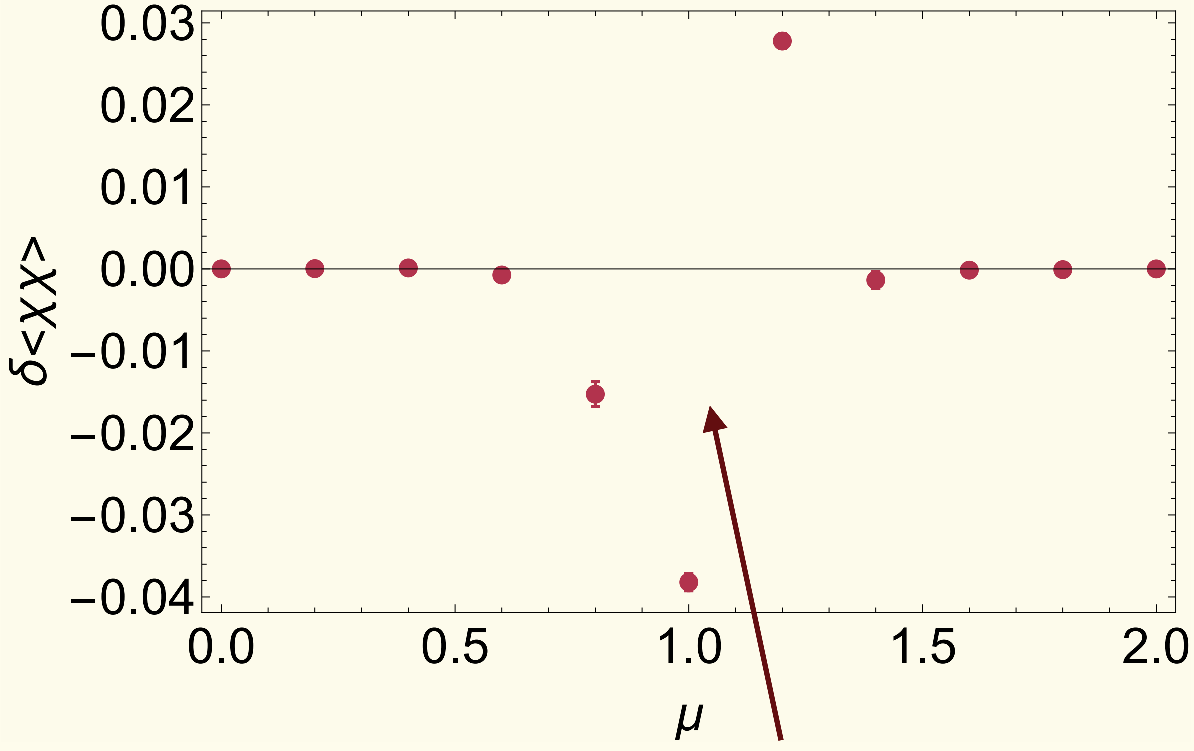


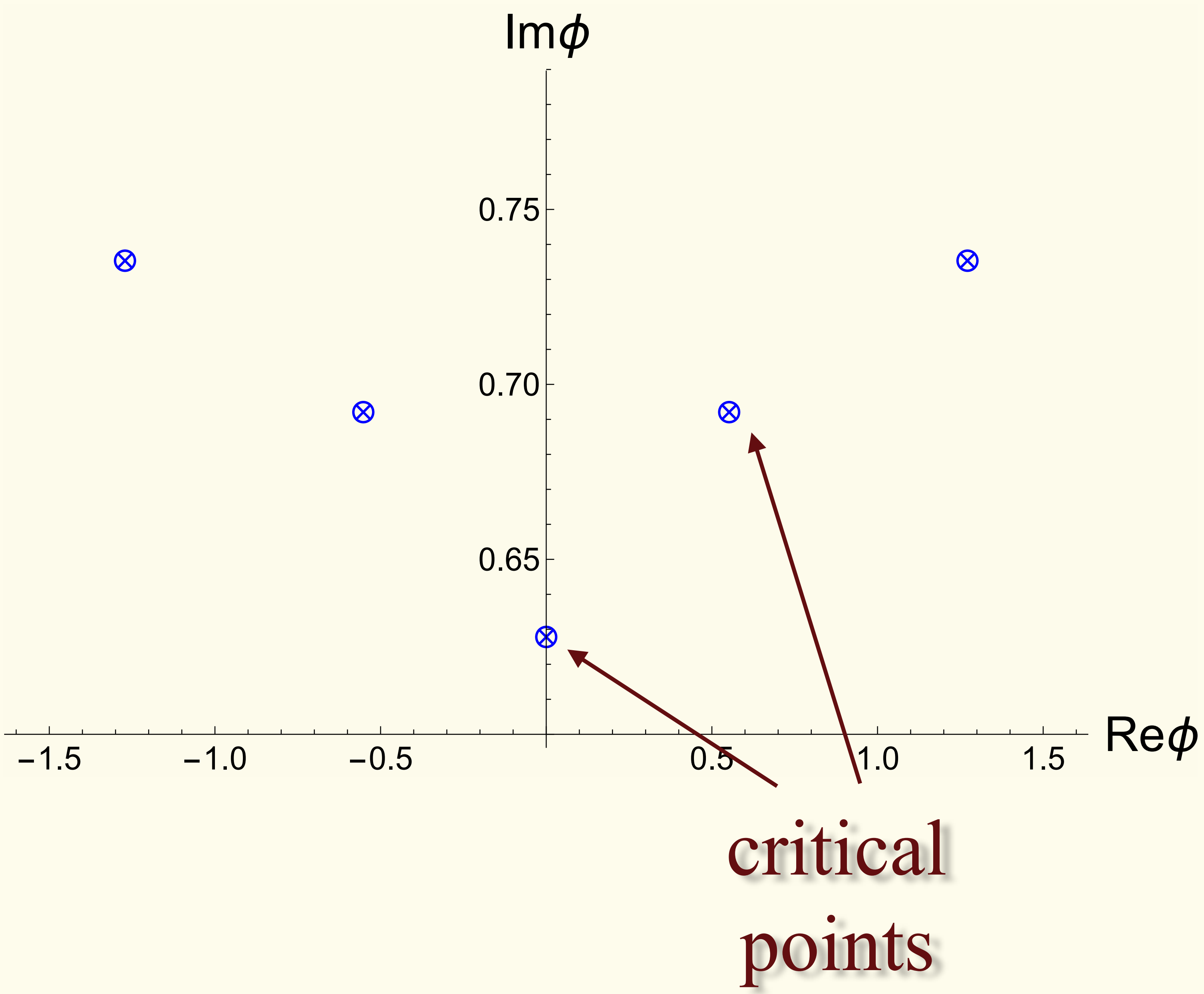


consistent with other thimbles contributions

Fujii,Kamata, Kikukawa, '15

Alexandru,Basar,Bedaque, '15

Behold (a projection of) the thimbles: $\phi = \frac{1}{N}\sum_{t=1}^{N}\phi_t$



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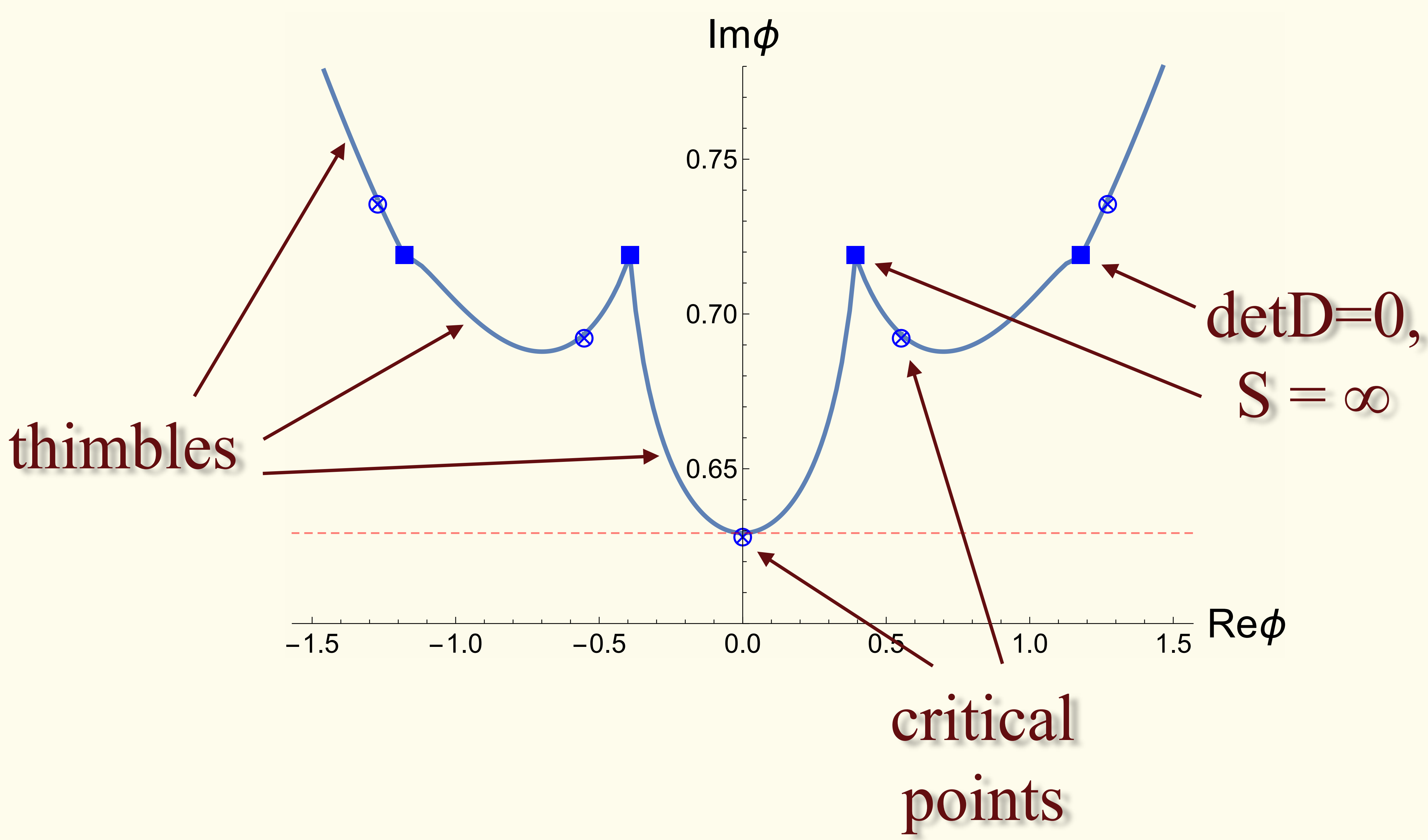

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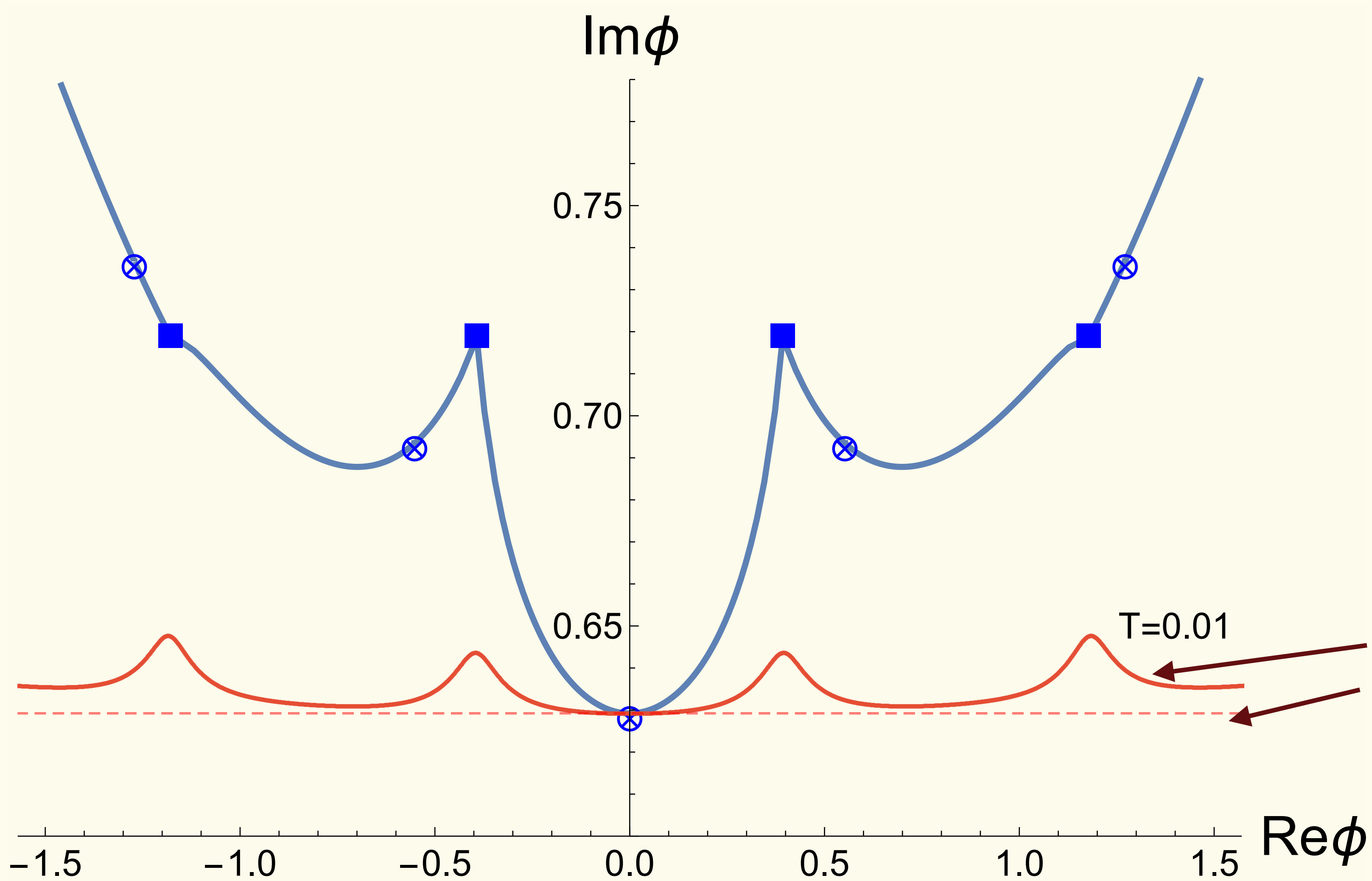
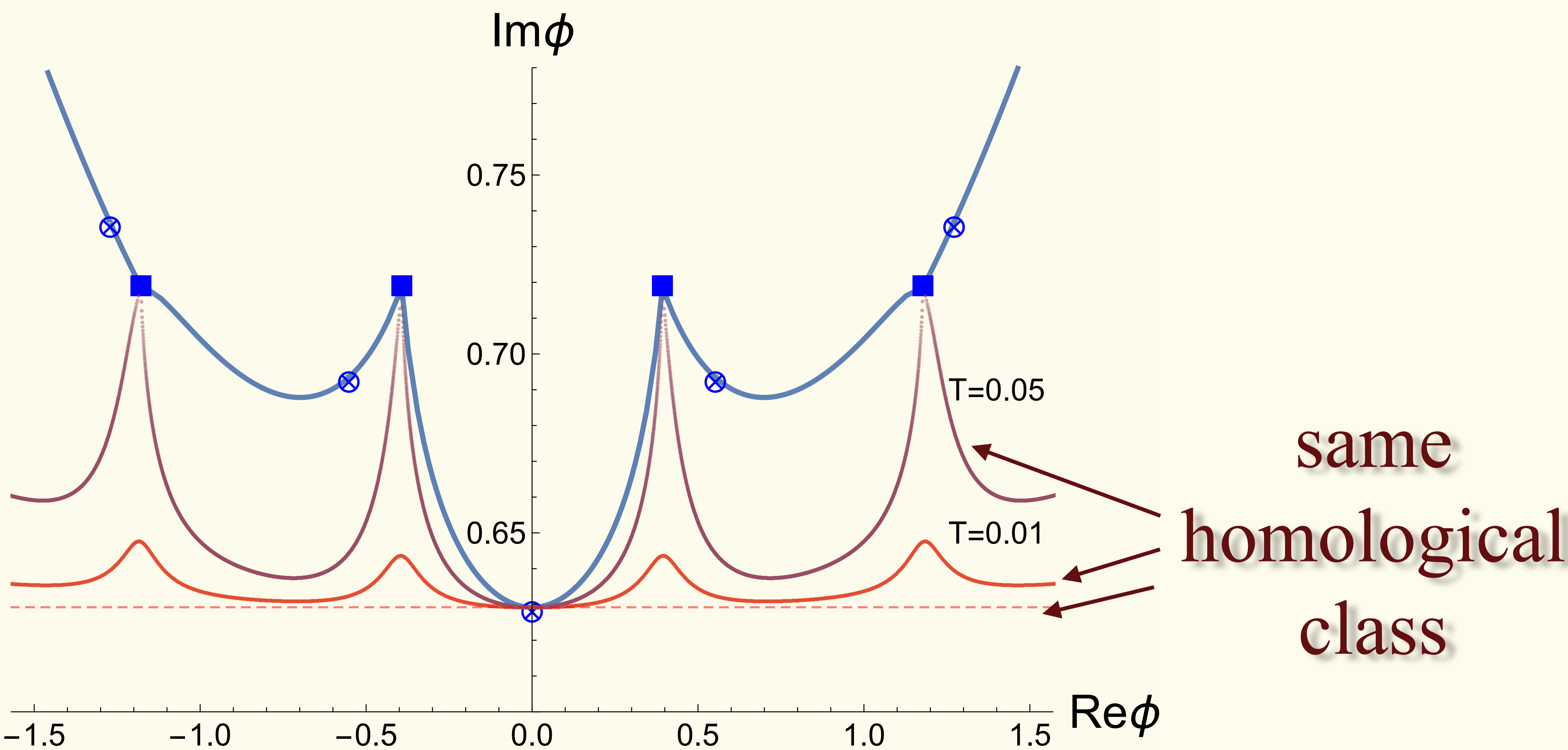


same homological class

Behold (a projection of) the thimbles: $\phi = \frac{1}{N}\sum_{t=1}^{N}\phi_t$



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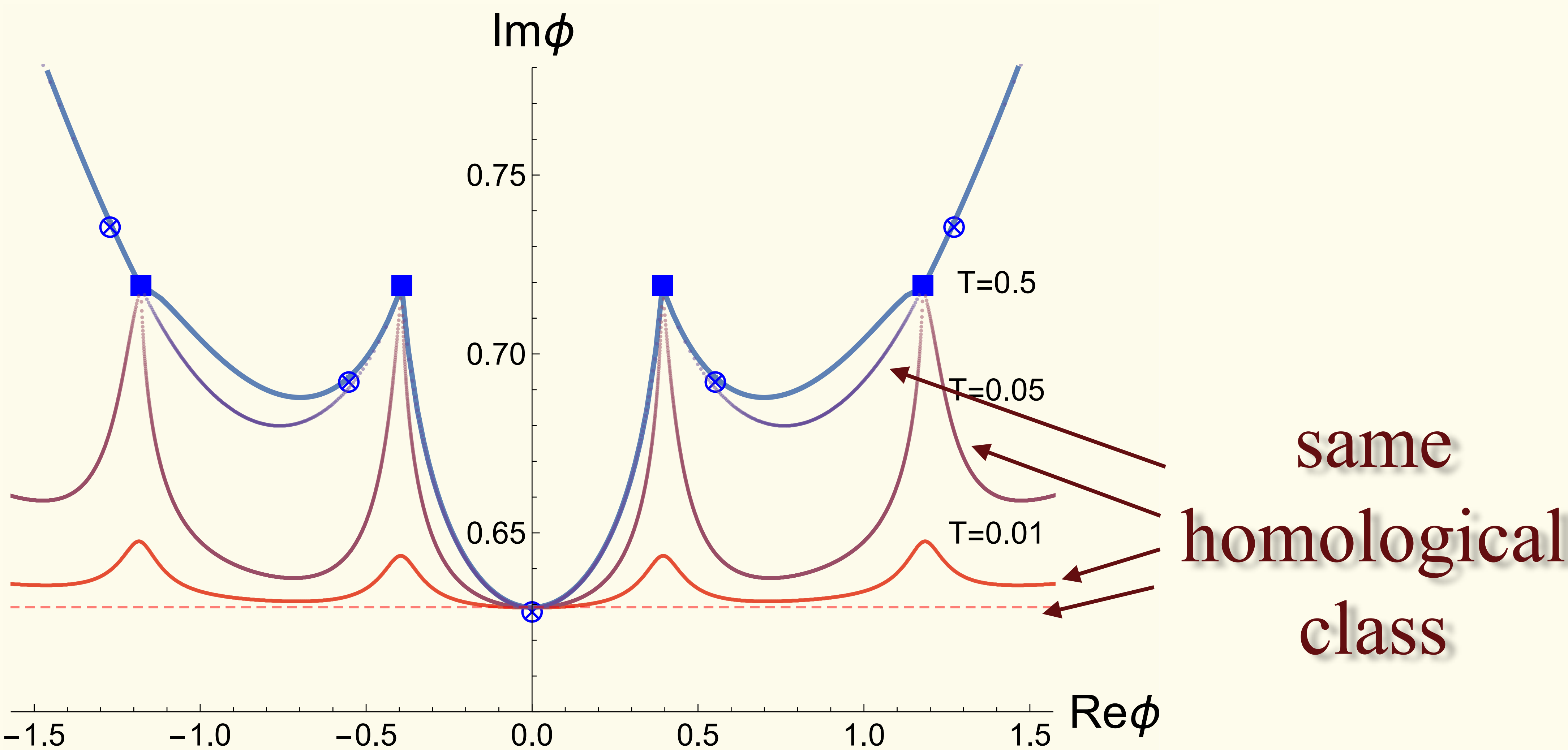

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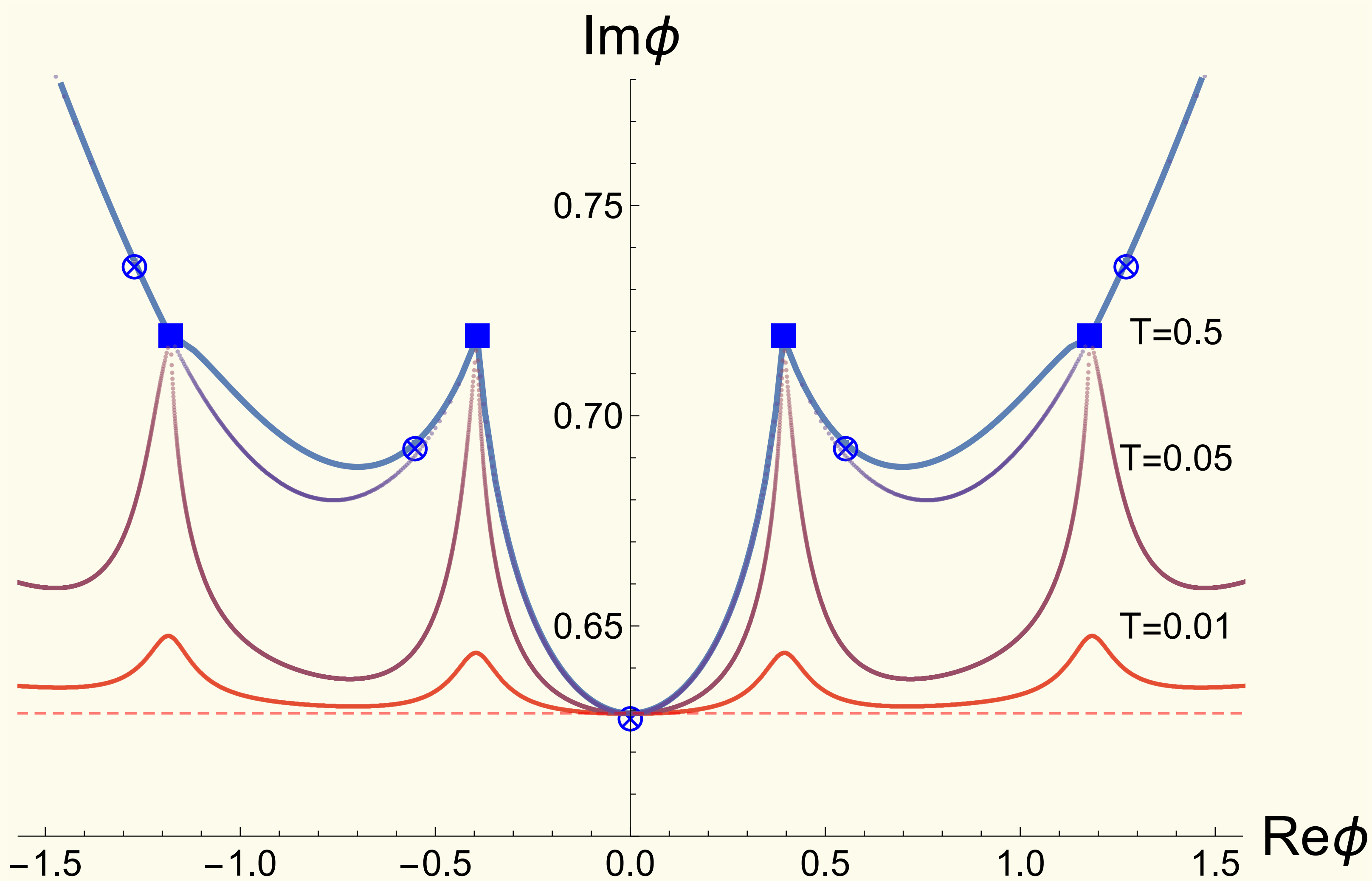
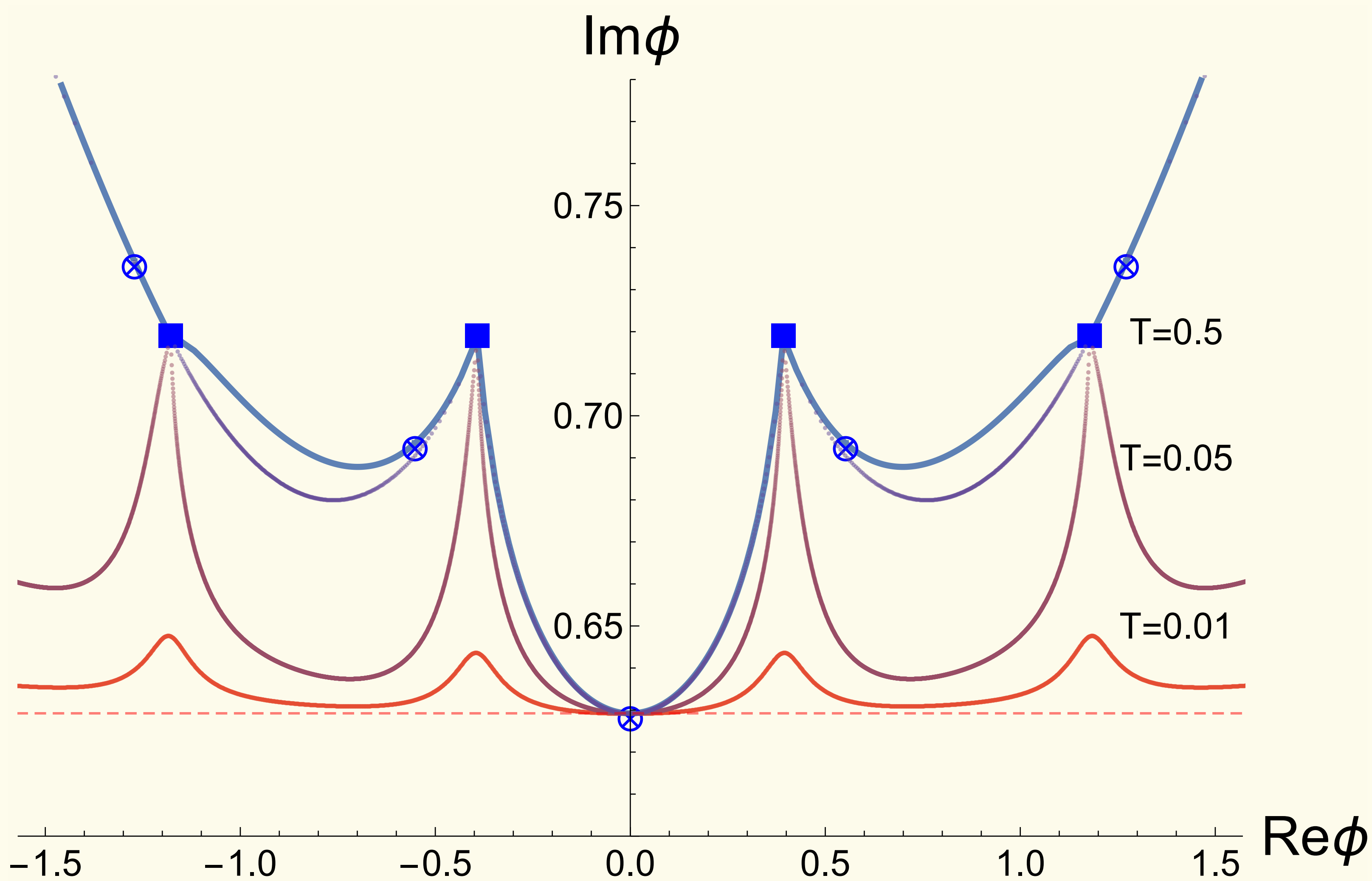


Thimbles that get hit by the flow are the ones contributing to the original integral

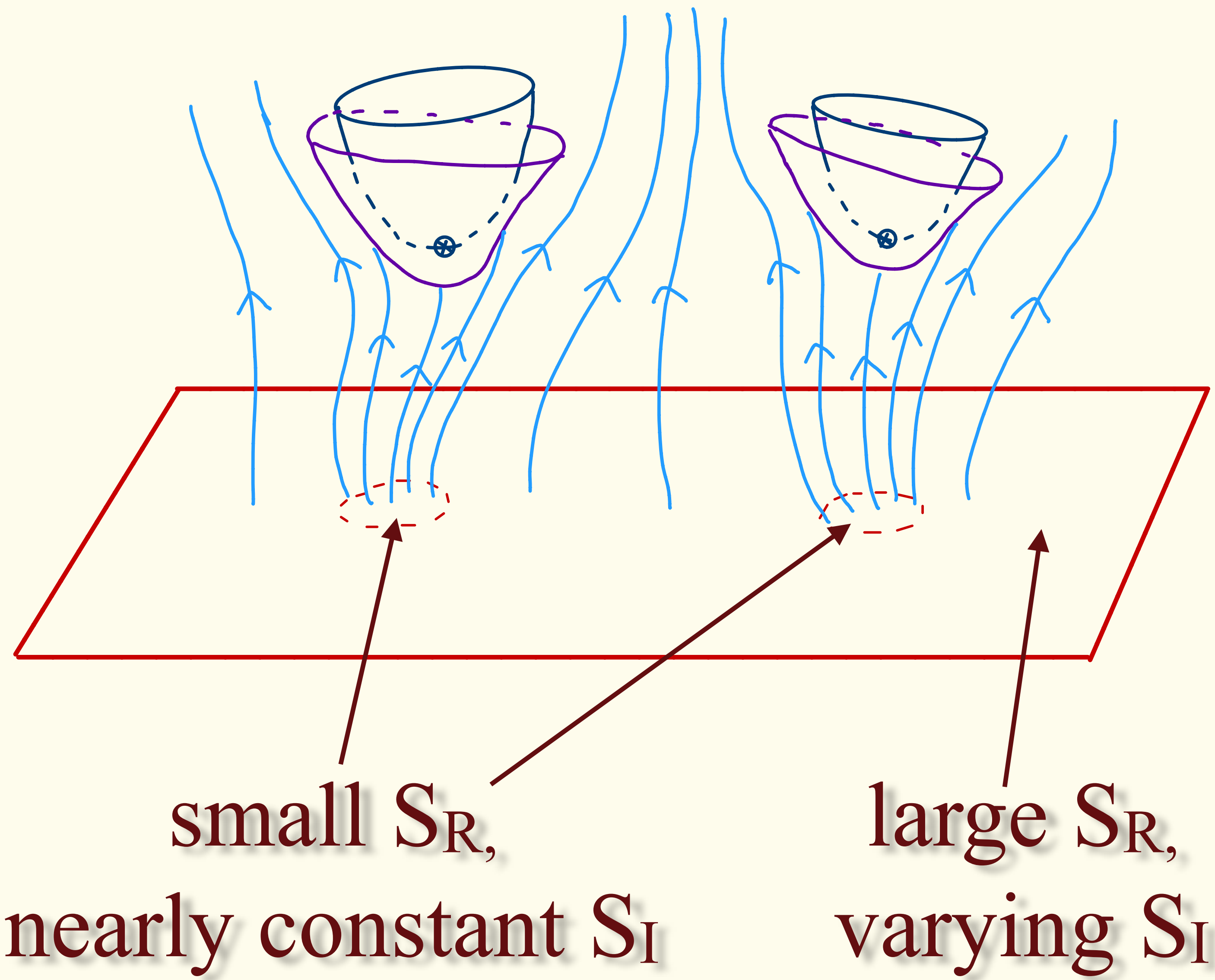
Behold (a projection of) the thimbles: $\phi = \frac{1}{N}\sum_{t=1}^{N}\phi_t$



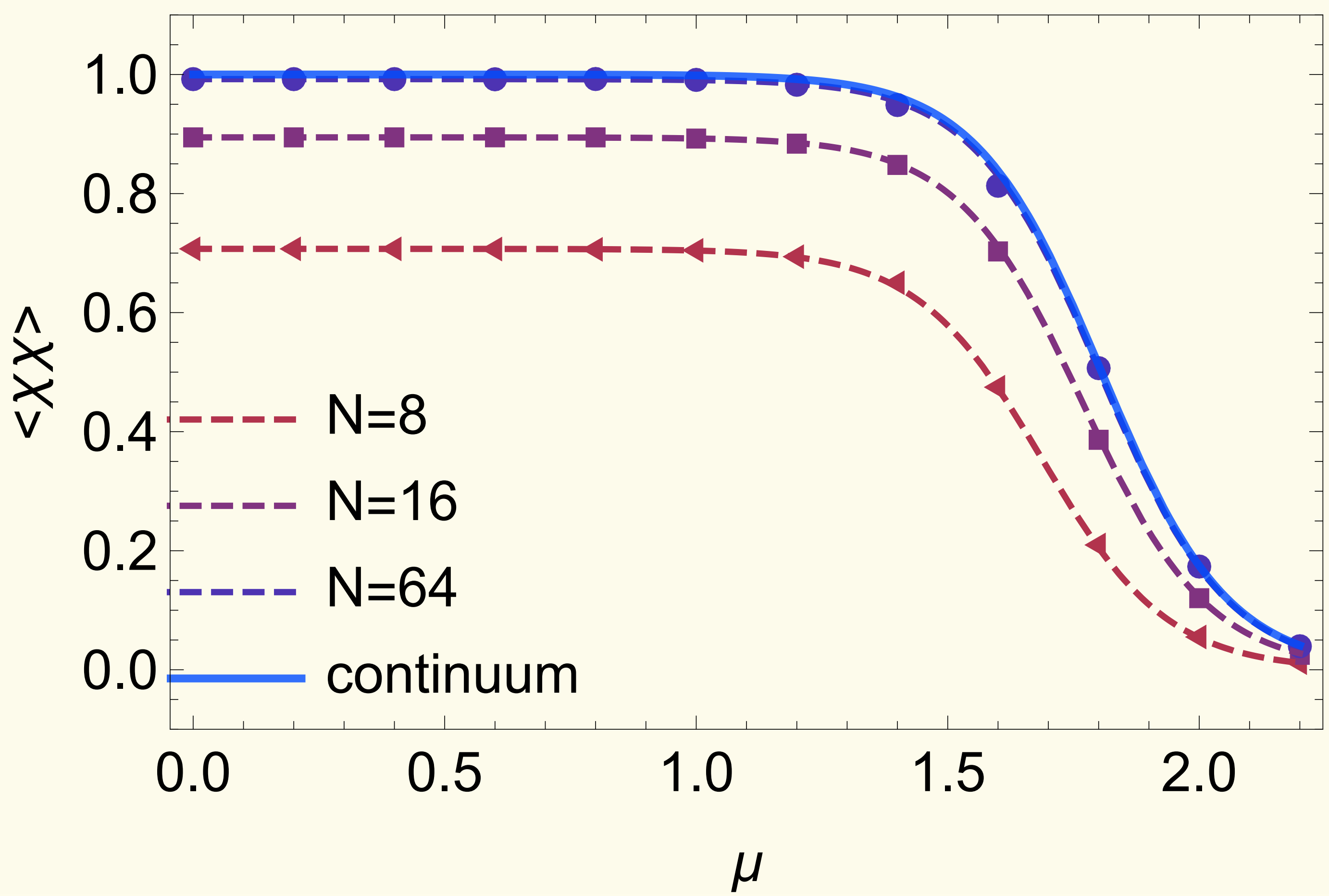
Choose any of these manifolds,
contraction algorithm correct for any T.

small T : worse sign problem, S_R smooth

large T : milder sign problem, deep pockets in S_R



The correct ("all thimbles") integral is captured by the T=0 calculation



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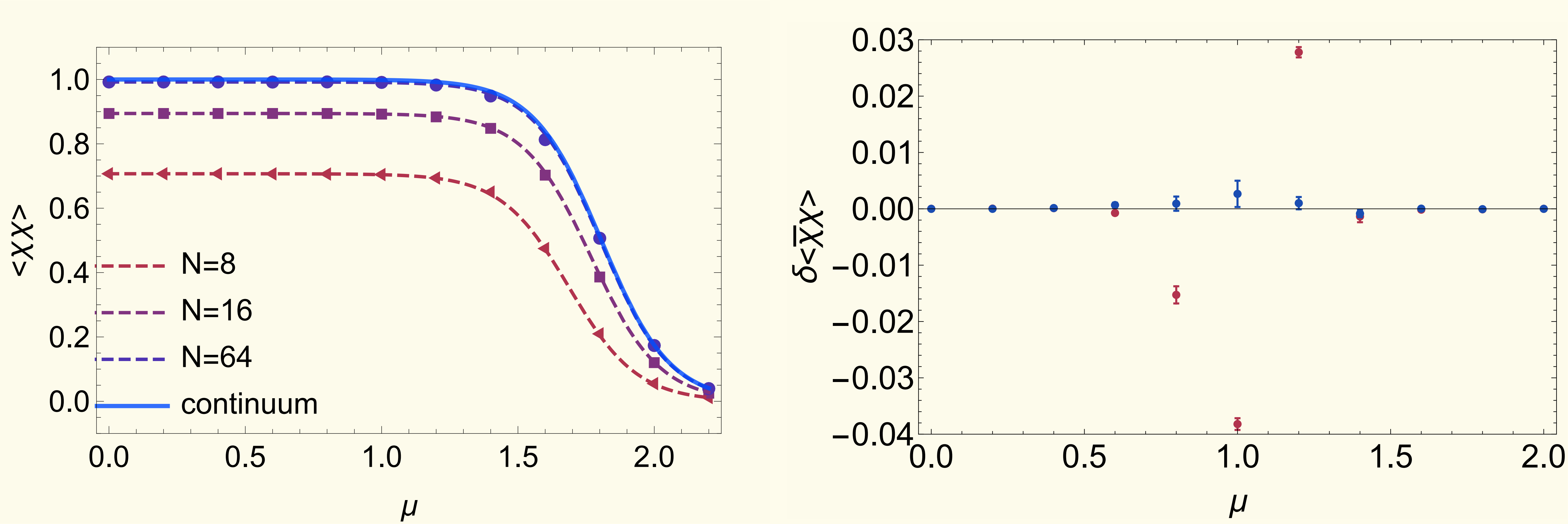

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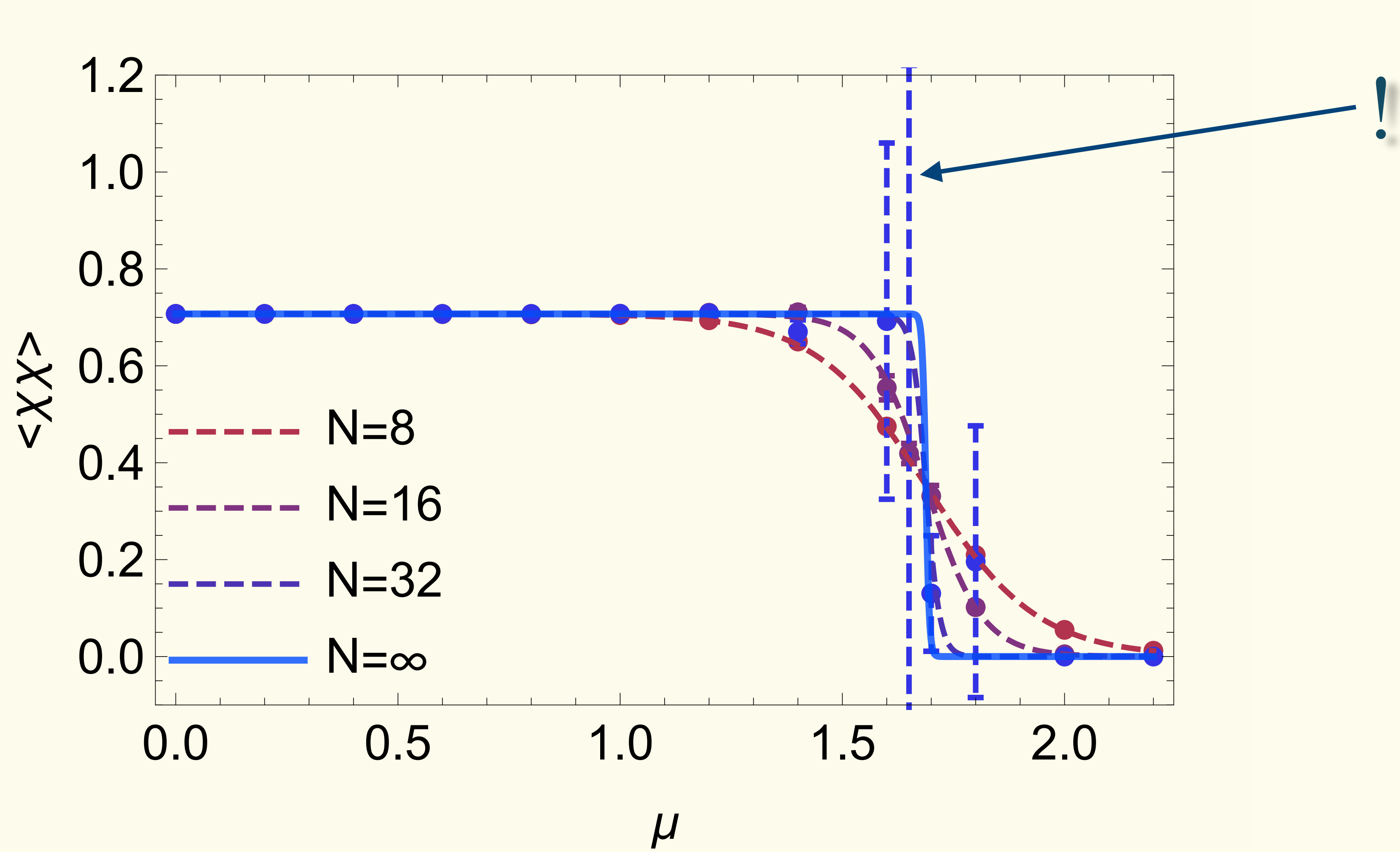
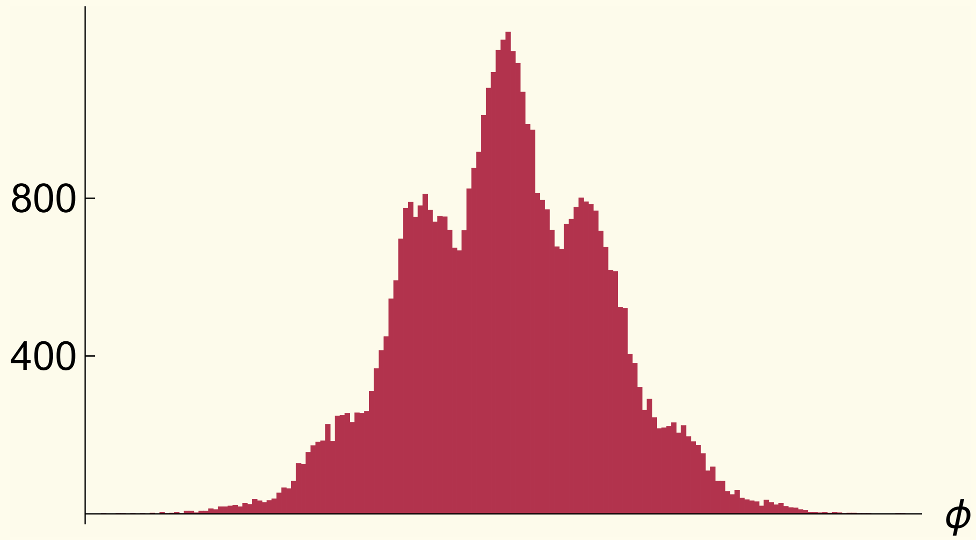


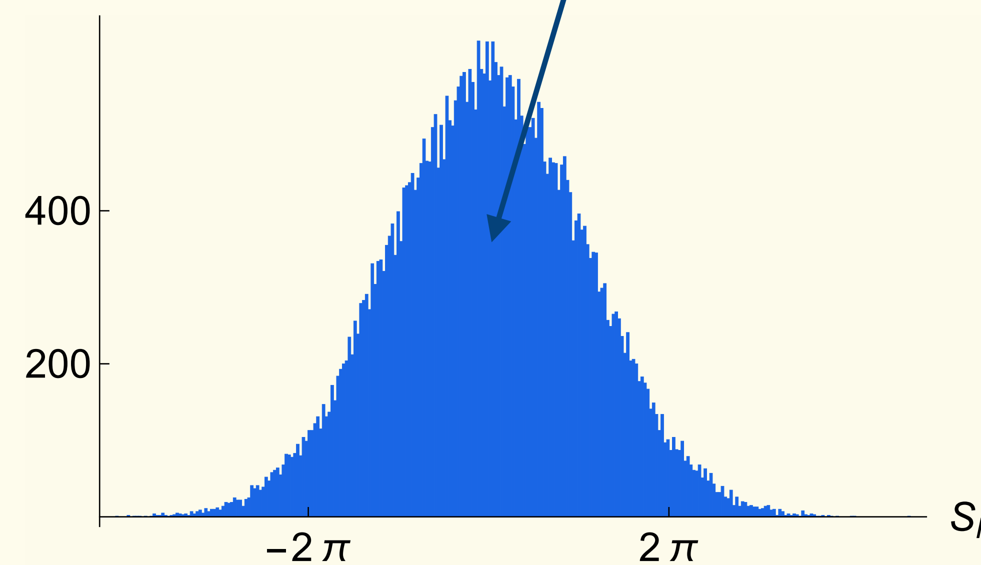
As expected, residual sign problem comes back at zero temperature. So, we flow.

$N=32, \mu=1.688$

bad sign problem

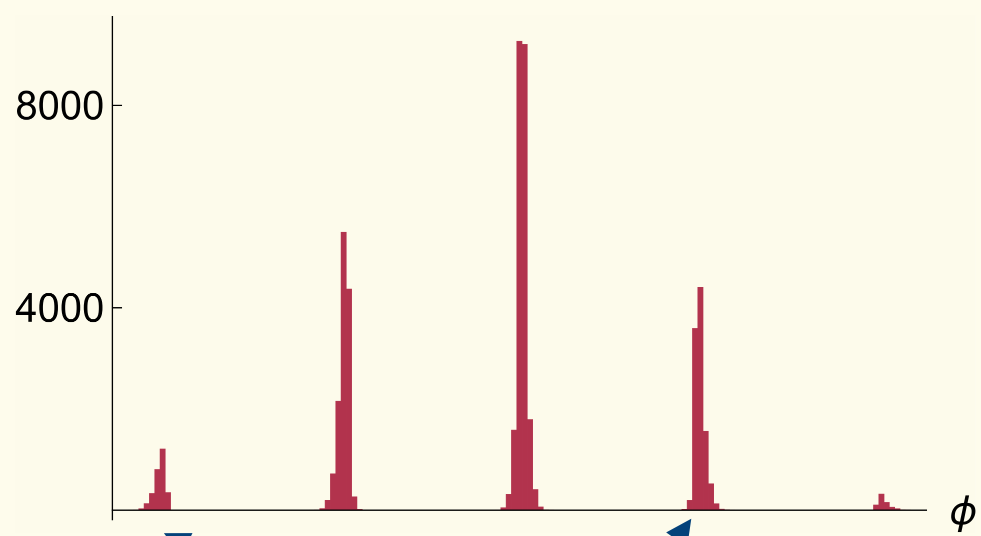
$T=0$

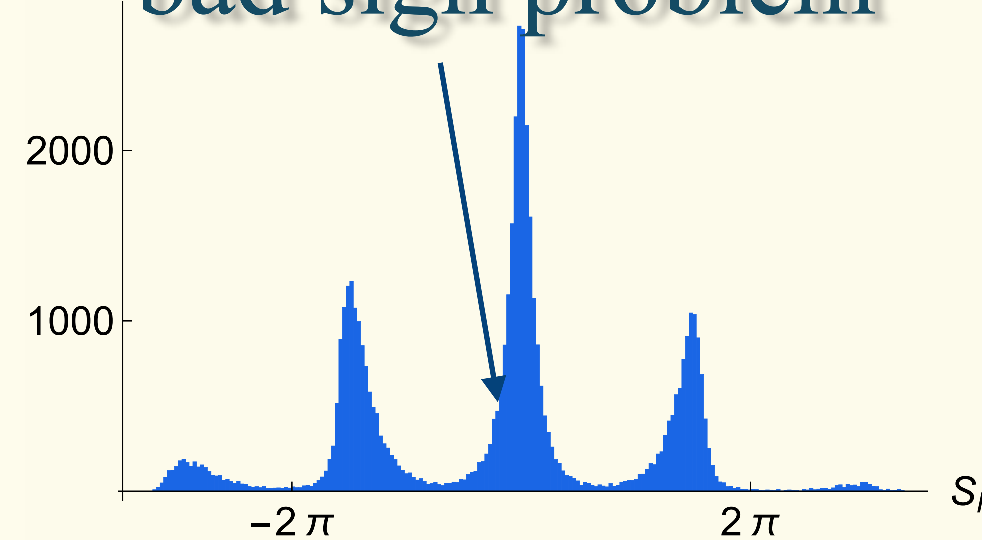




not nearly so
bad sign problem

$T=0.5$





"thimbles"

After 2000000 Metropolis steps (acceptance = 16%) …

$$\langle \bar{\chi}\chi \rangle = 0.345(46), \qquad \langle \bar{\chi}\chi \rangle_{exact} = 0.353$$

sign problem = multimodal distributions

Combining the contraction algorithm philosophy with a method to handle multimodal distributions (tempering ?) seems to be the way to go.

Alexandru, Basar, Bedaque, Ridgway, Warrington, '15

- Deforming the integration on complex space is a good thing

- Thimbles are optimal if only one dominates; other manifolds are better in other cases

- Improvements in method:

  estimator for J (see N. Warrington's talk),

  $\sim L^8$ phase space

- Models:

  φ^4 at finite μ, real time (Schwinger-Keldish),

  1+1 Thirring

One thimble computation:

$$\frac{dz_i}{dt} = \overline{\frac{\partial S}{\partial z_i}} \quad \Rightarrow \quad z_i(T)$$

$$z_i(0) = \tilde{z}$$

point near critical point

~

point on tangent plane

point on the thimble