Going with the flow: sign problem, thimbles and beyond

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

What if S is not real ?

That’s what happens in :

- 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
- …

But this is a QCD conference so …

- QCD at finite chemical potential (quark or nuclear matter) matter
- real time dynamics
- QCD with a θ term

Sign problem

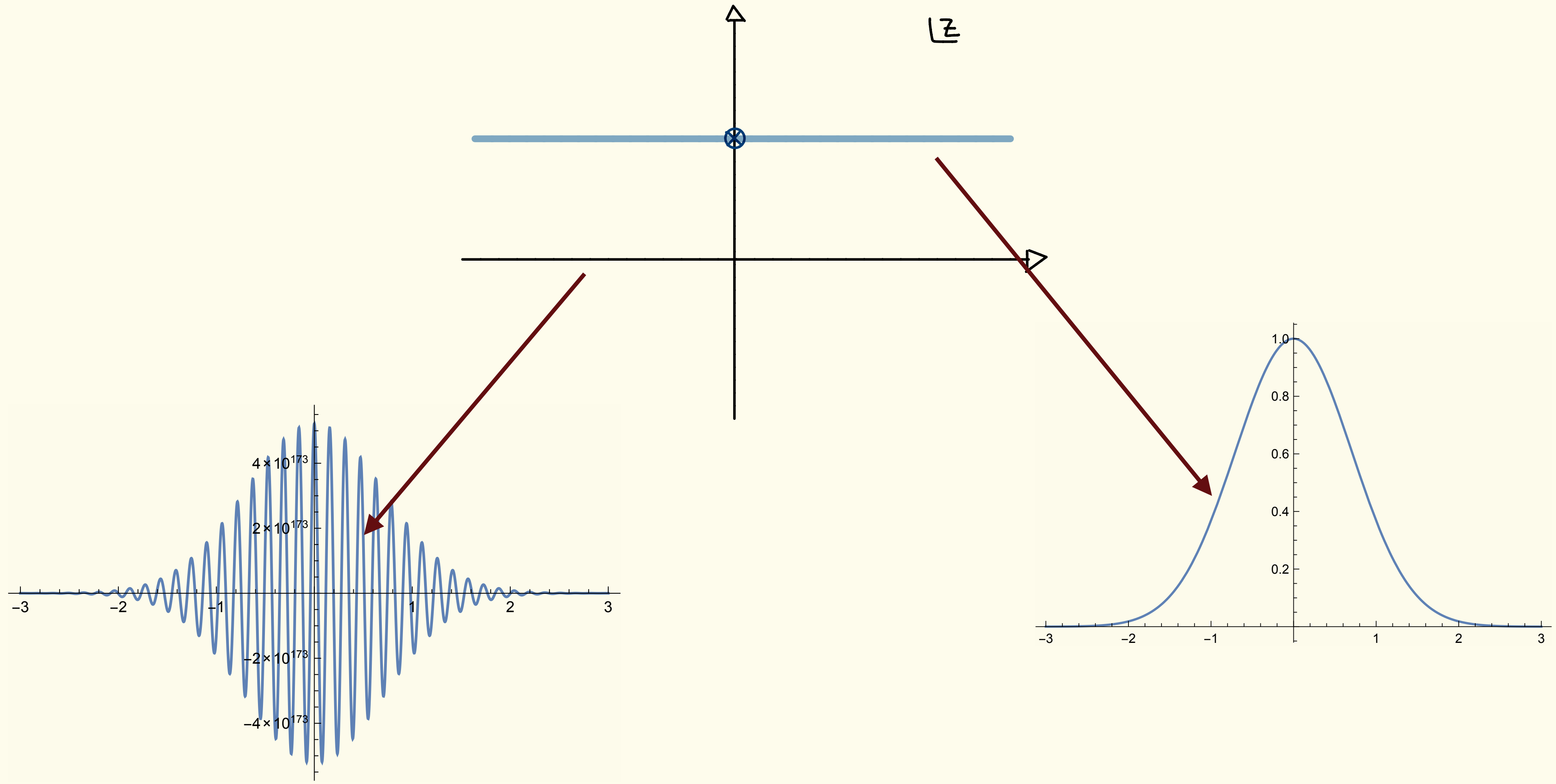
Reweighting:

$$\begin{aligned}\langle \mathcal{O} \rangle &= \frac{\int D\phi\ e^{-S_R[\phi]} e^{-iS_I[\phi]} \mathcal{O}}{\int D\phi\ e^{-S_R[\phi]} e^{-iS_I[\phi]}} \\ &= \frac{\int D\phi\ e^{-S_R[\phi]} e^{-iS_I[\phi]} \mathcal{O}}{\int D\phi\ e^{-S_R[\phi]}} \frac{\int D\phi\ e^{-S_R[\phi]}}{\int D\phi\ e^{-S_R[\phi]} e^{-iS_I[\phi]}} \\ &= \frac{\langle e^{-iS_I[\phi]} \mathcal{O} \rangle_{S_R}}{\langle e^{-iS_I[\phi]} \rangle_{S_R}}\end{aligned}$$

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

Central idea: deform the contour into the complex plane:

$$\int dx\ e^{-(z-i20)^2} = \sqrt{\pi}$$



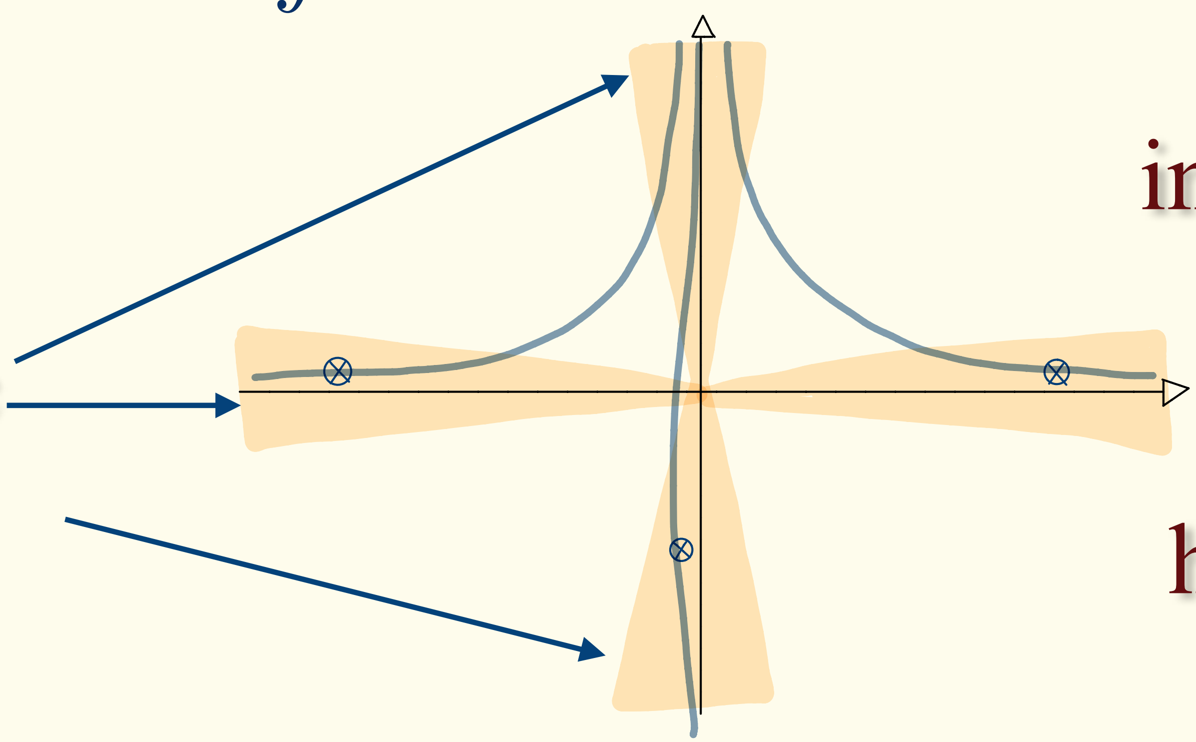
Cristoforetti, DiRenzo, Scorzato, '12

How to find good deformations ?

- Integrands have no pole except at *infinity*
- Outside the “good” asymptotic directions the integral diverges

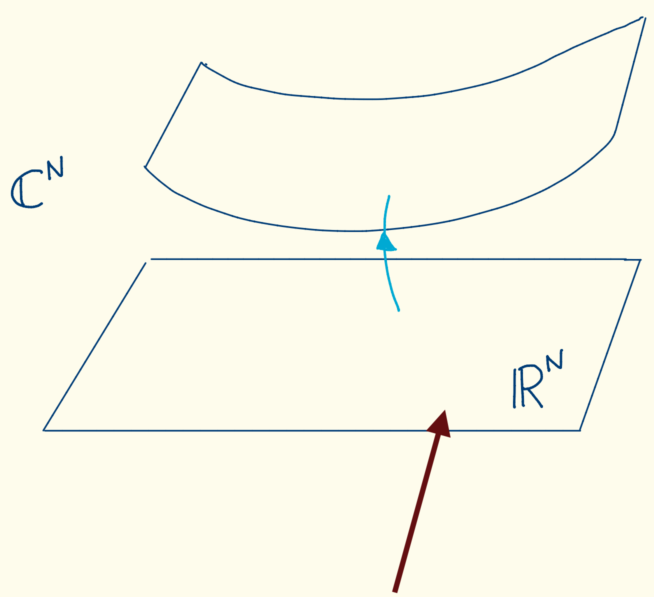
$$\int dz\ e^{-(hz+z^2+z^4)}$$

good asymptotic directions



integral depends only on initial and final directions: homological classes

How to find good deformations ?



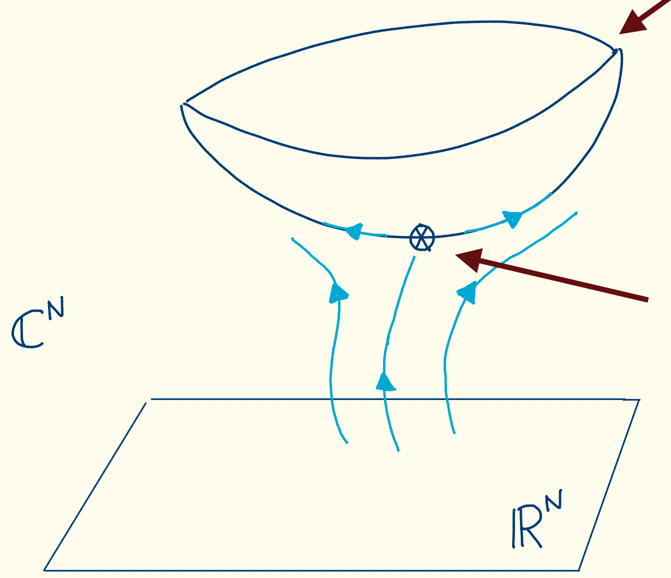
(real) field space

$$\frac{d\phi_i}{dt} = \overline{\frac{\partial S}{\partial \phi_i}} \Rightarrow \begin{array}{l} \dfrac{d\phi_i^R}{dt} = \dfrac{\partial S^R}{\partial \phi_i^R} = \dfrac{\partial S^I}{\partial \phi_i^I} \\[2ex] \dfrac{d\phi_i^I}{dt} = \dfrac{\partial S^R}{\partial \phi_i^I} = -\dfrac{\partial S^I}{\partial \phi_i^R} \end{array}$$

gradient flow of S^R, keeps integral well defined

hamiltonian flow of S^I, keeps phase fixed

How to find good deformations ?

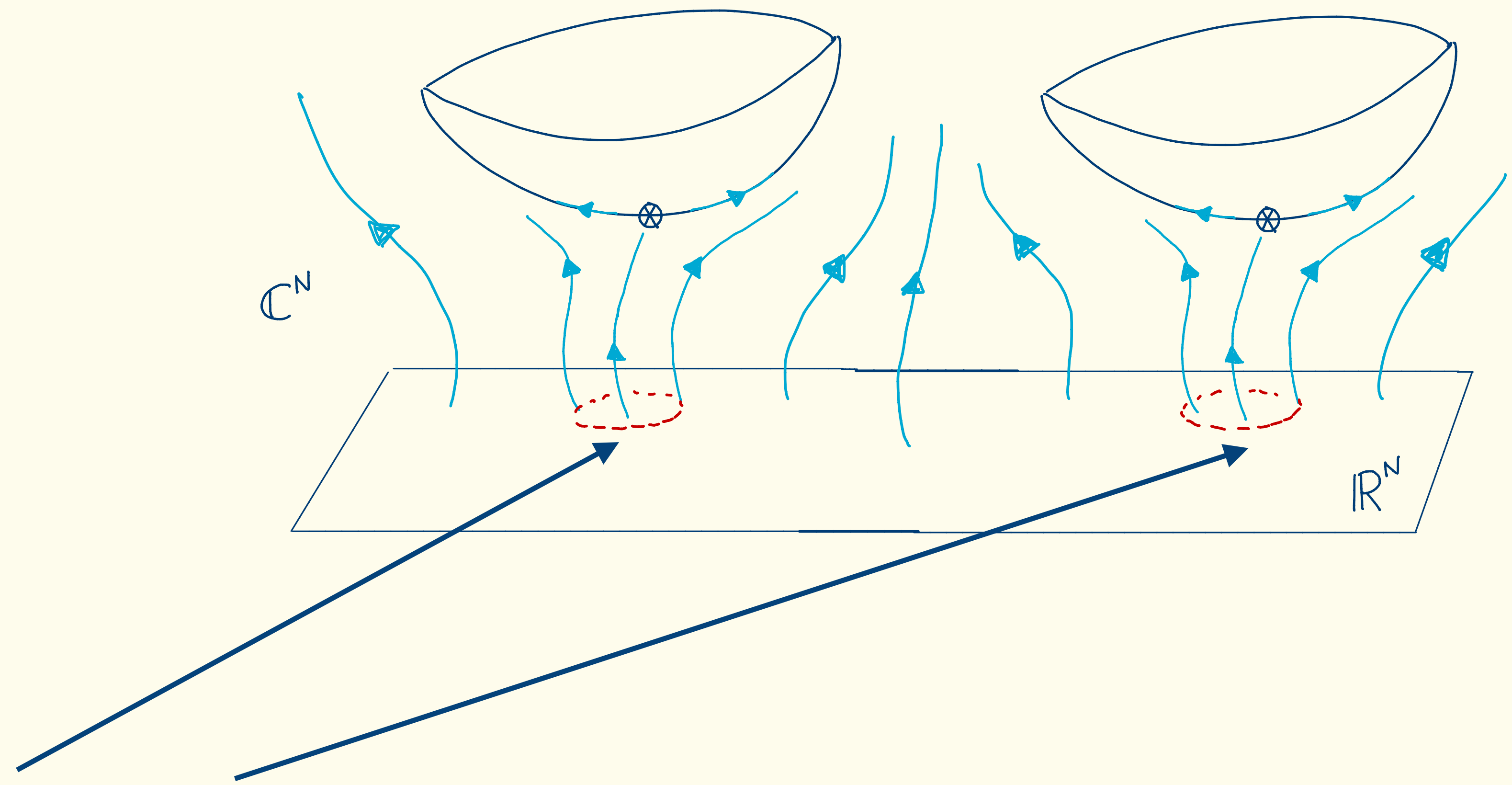


N-dimensional
"thimble" (multidimensional steepest descent/constant phase path)

flow gets stuck at critical point: $\frac{\partial S}{\partial \phi_i} = 0$

R^N flows towards the equivalent combination of thimbles

How to find good deformations ?



Small regions are mapped (close) to thimbles and contribute significantly to the integral, S_I varies little.

The other regions flow towards $S=\infty$ and contribute little to the integral.

Previous attempts concentrated on using thimbles. Issues:

- Monte Carlo chain to stay on the thimble
- solution of classical e.o.m.=critical point: many thimbles
- which thimble contribute?
- maybe only one thimble matters in the i) thermodynamic limit and/or ii) continuum limit

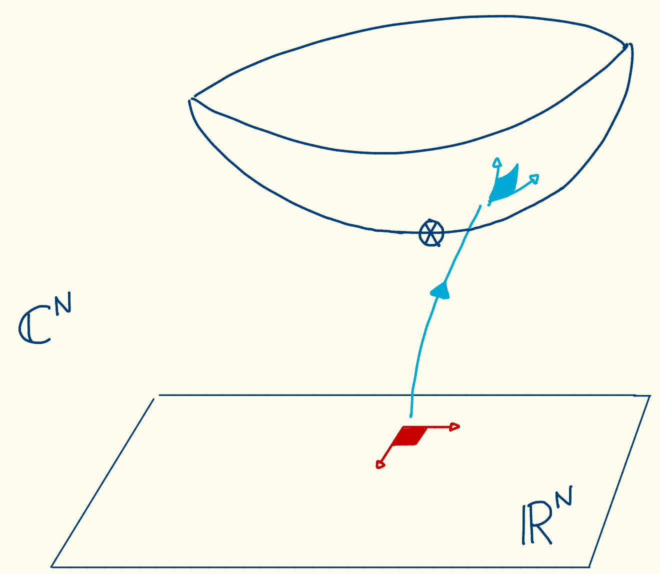
We'll take a different route:

- too little flow=sign problem not ameliorated enough
- too much flow=Monte Carlo gets stuck into one region in field space

The algorithm

$$\langle \mathcal{O} \rangle = \frac{\int d\phi_i \; \mathcal{O} e^{-S_R - iS_I}}{\int d\phi_i \; e^{-S_R - iS_I}} = \frac{\int d\tilde{\phi}_i \; \overbrace{\det\left(\frac{\partial \phi_i}{\partial \tilde{\phi}_i}\right)}^{J} \mathcal{O} e^{-S_R - iS_I}}{\int d\tilde{\phi}_i \; \det\left(\frac{\partial \phi_i}{\partial \tilde{\phi}_i}\right) e^{-S_R - iS_I}}$$

$$= \frac{\int d\tilde{\phi}_i \; \mathcal{O} e^{-iS_I + i\mathrm{Im}J} e^{-\overbrace{(S_R - \mathrm{Re}J)}^{S_{eff}}}}{\int d\tilde{\phi}_i \; e^{-iS_I + i\mathrm{Im}J} e^{-(S_R - \mathrm{Re}J)}} = \frac{\langle \mathcal{O} e^{-iS_I + i\mathrm{Im}J} \rangle_{S_{eff}}}{\langle e^{-iS_I + i\mathrm{Im}J} \rangle_{S_{eff}}}$$



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

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

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

this is the expensive part

The algorithm

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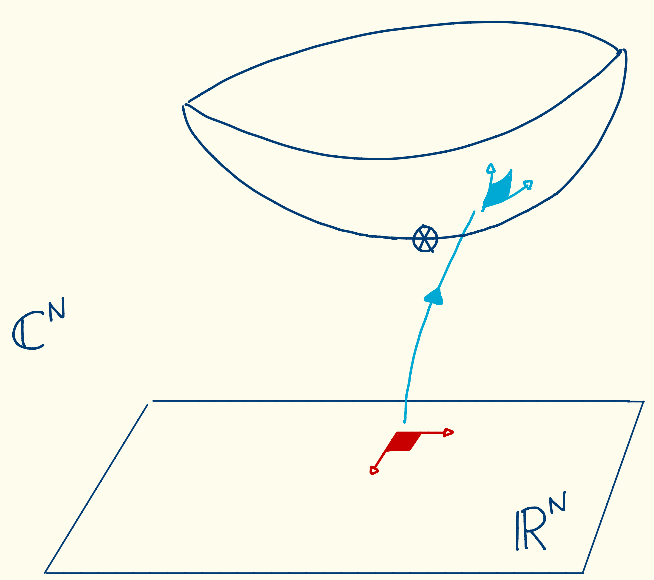

our algorithm

=

Metropolis in the real space,

action S_{eff} and

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

The algorithm

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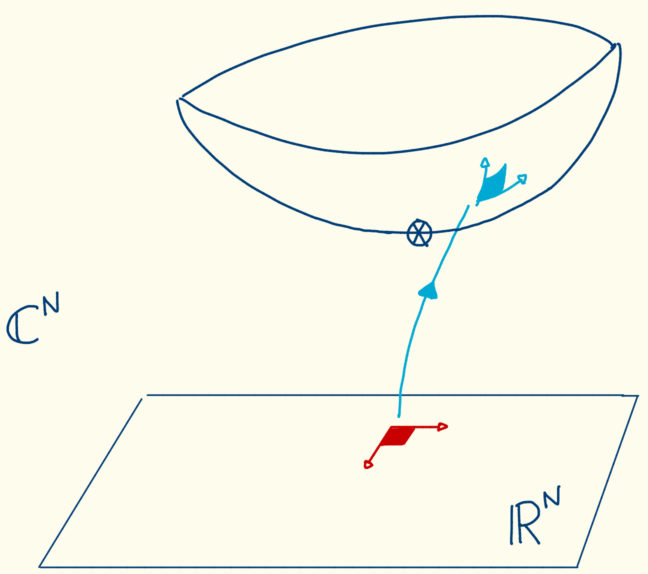

our algorithm

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Metropolis in the real space,

action S_{eff} and

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

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

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

↑

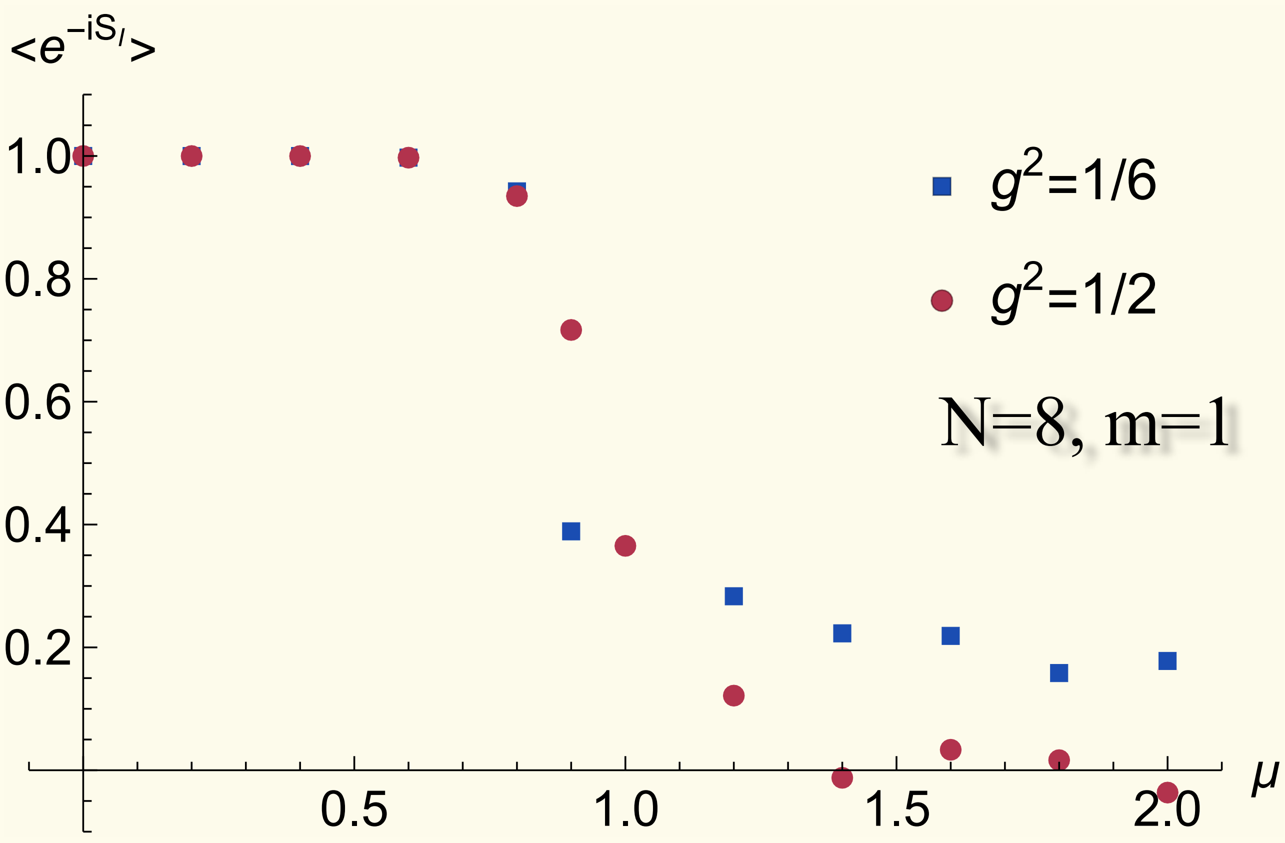
just a 4-level system

↓

discretize (staggered),
Hubbard-Stratanovich,
integrate over χ

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

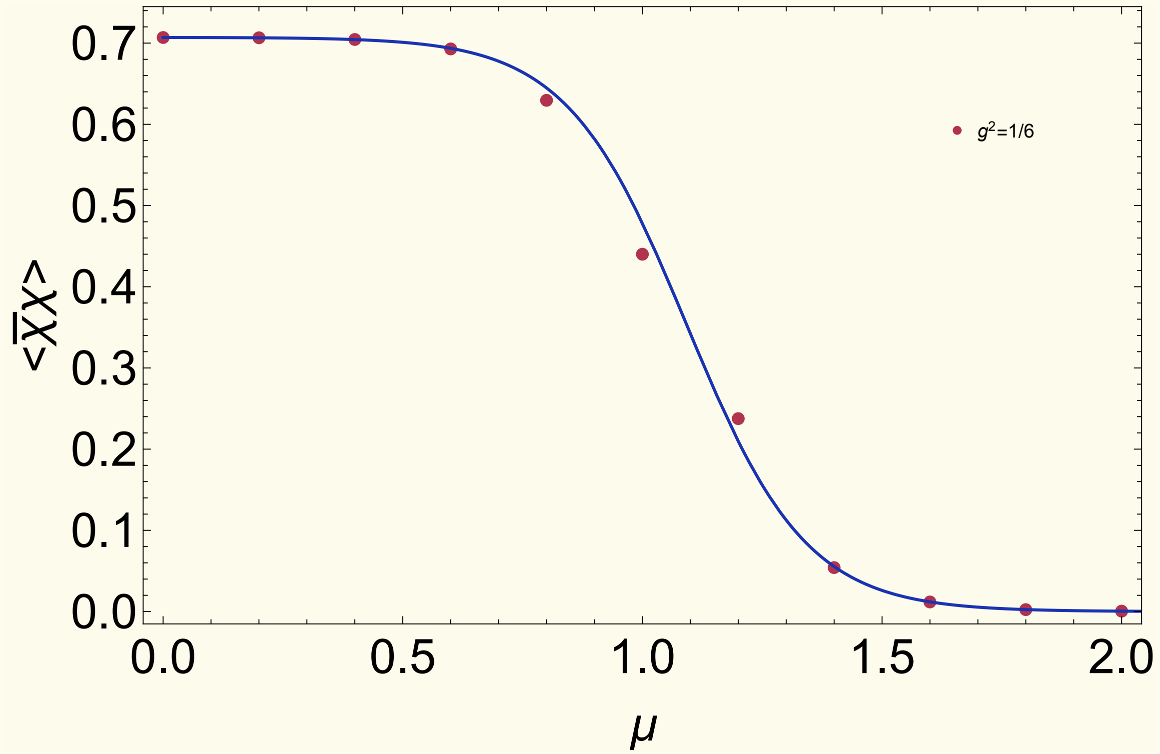
Is there a sign problem ?



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

Finally, the results:

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



Fujii,Kamata, Kikukawa, '15

Alexandru,Basar,Bedaque, '15

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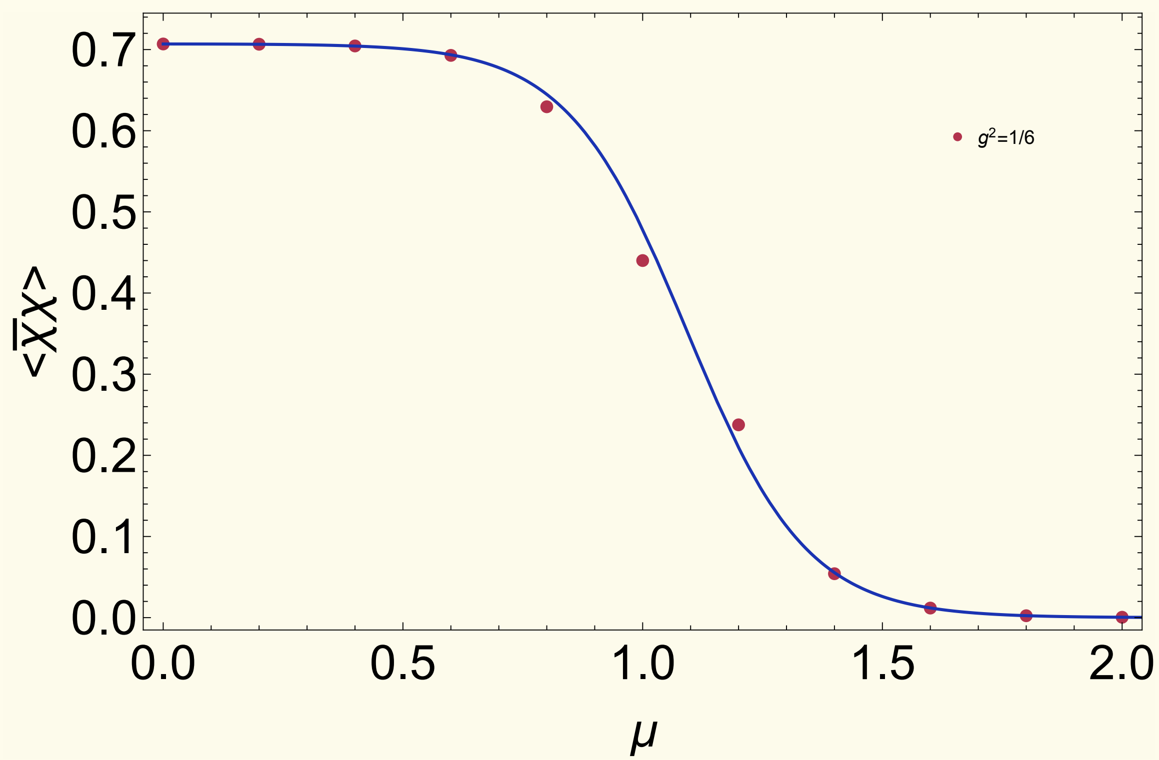
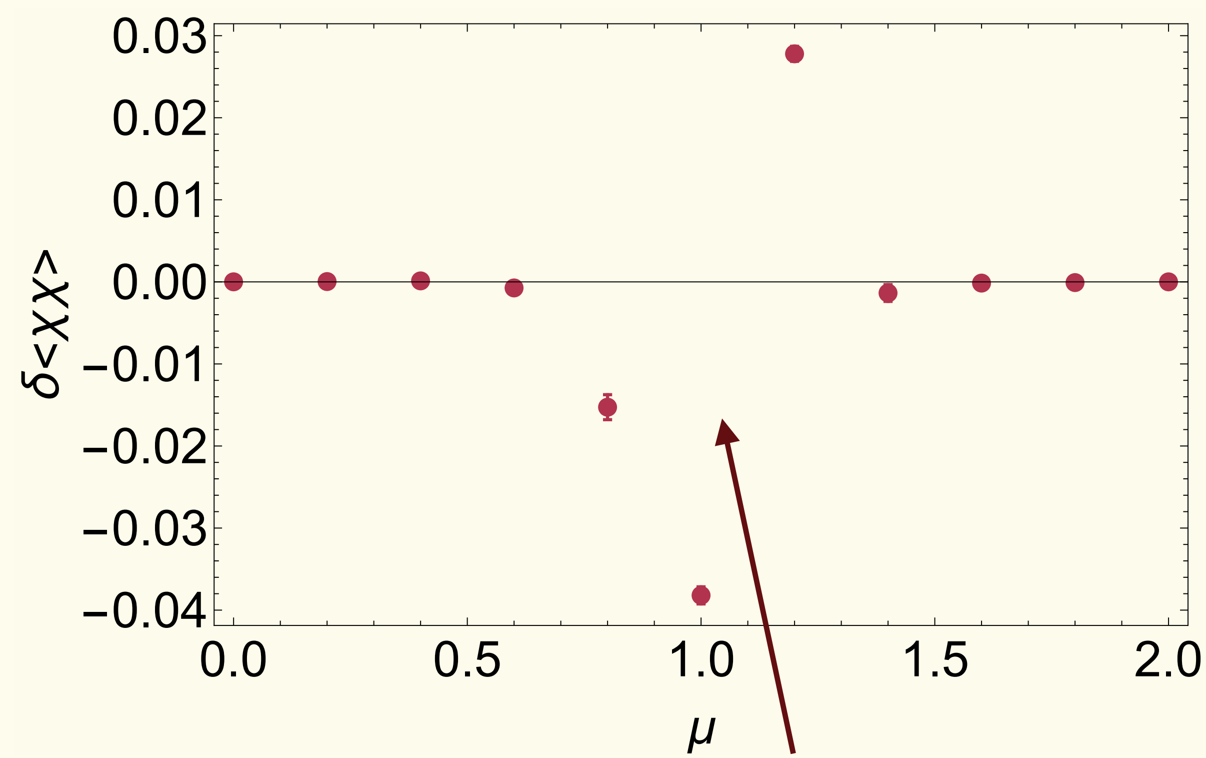




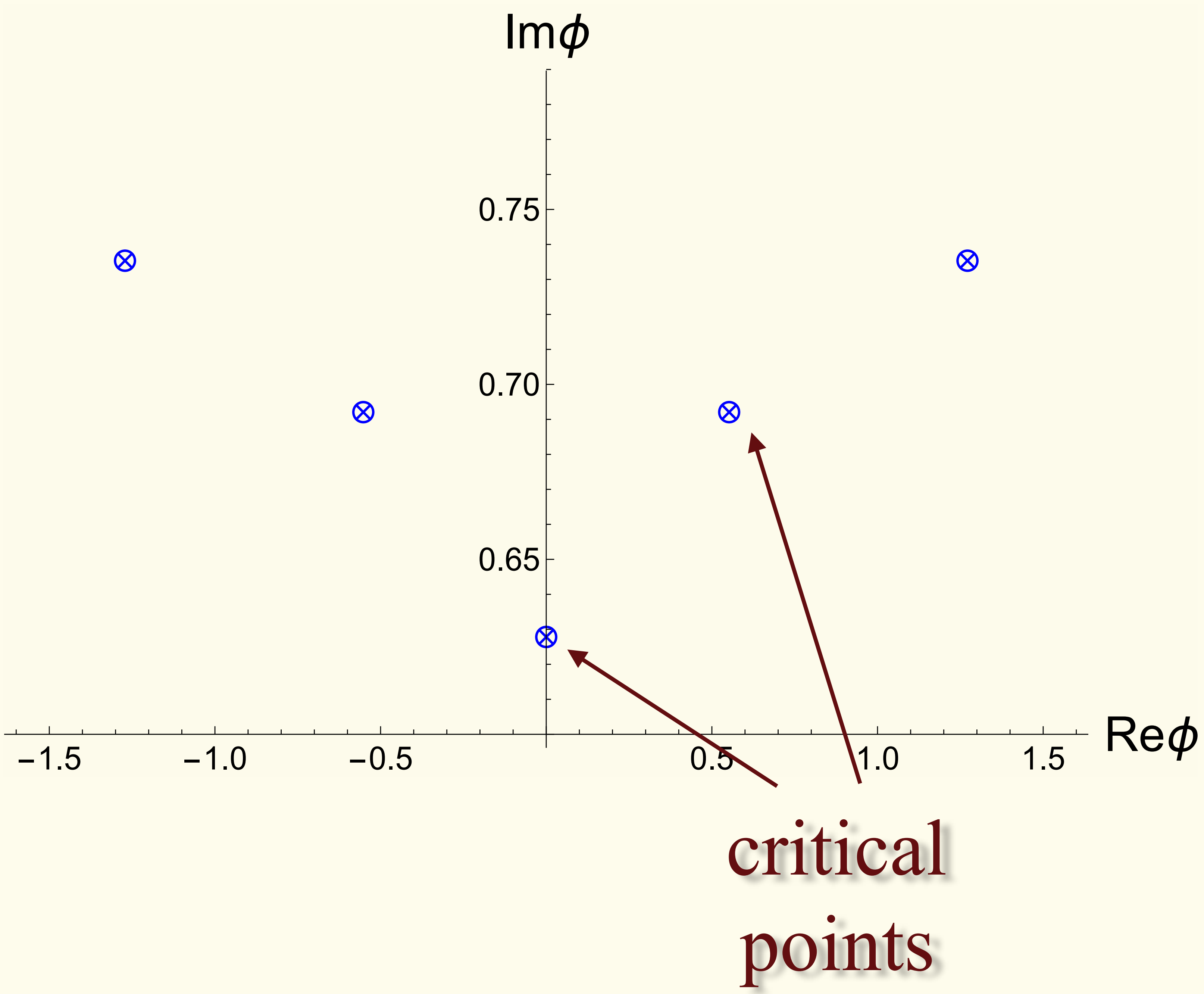
consistent with other thimbles contributions

Fujii,Kamata, Kikukawa, '15

Alexandru,Basar,Bedaque, '15

A projection of the thimbles:

$$\phi = \frac{1}{N}\sum_{t=1}^{N}\phi_t$$



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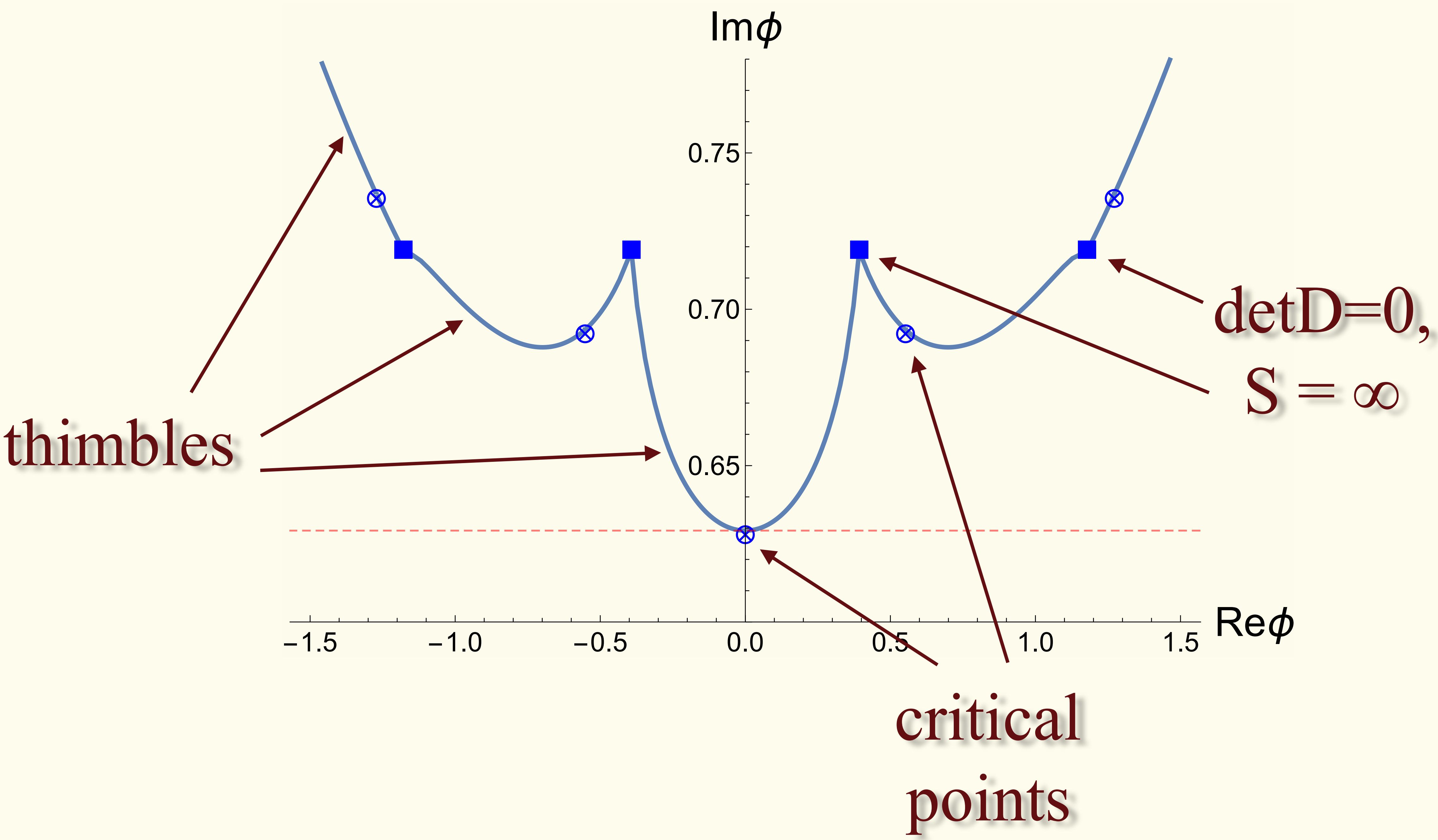

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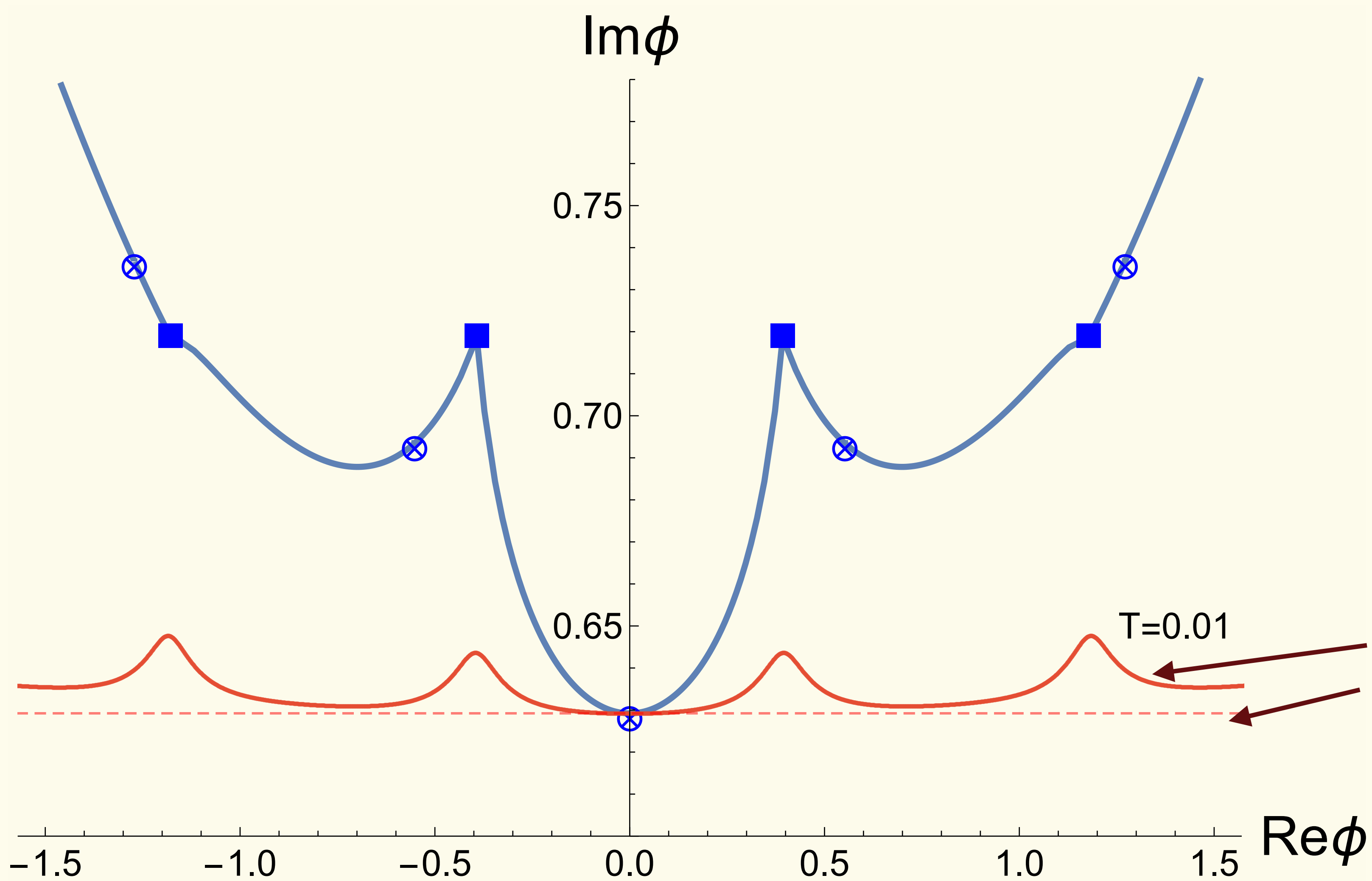

same homological class

A projection of the thimbles:

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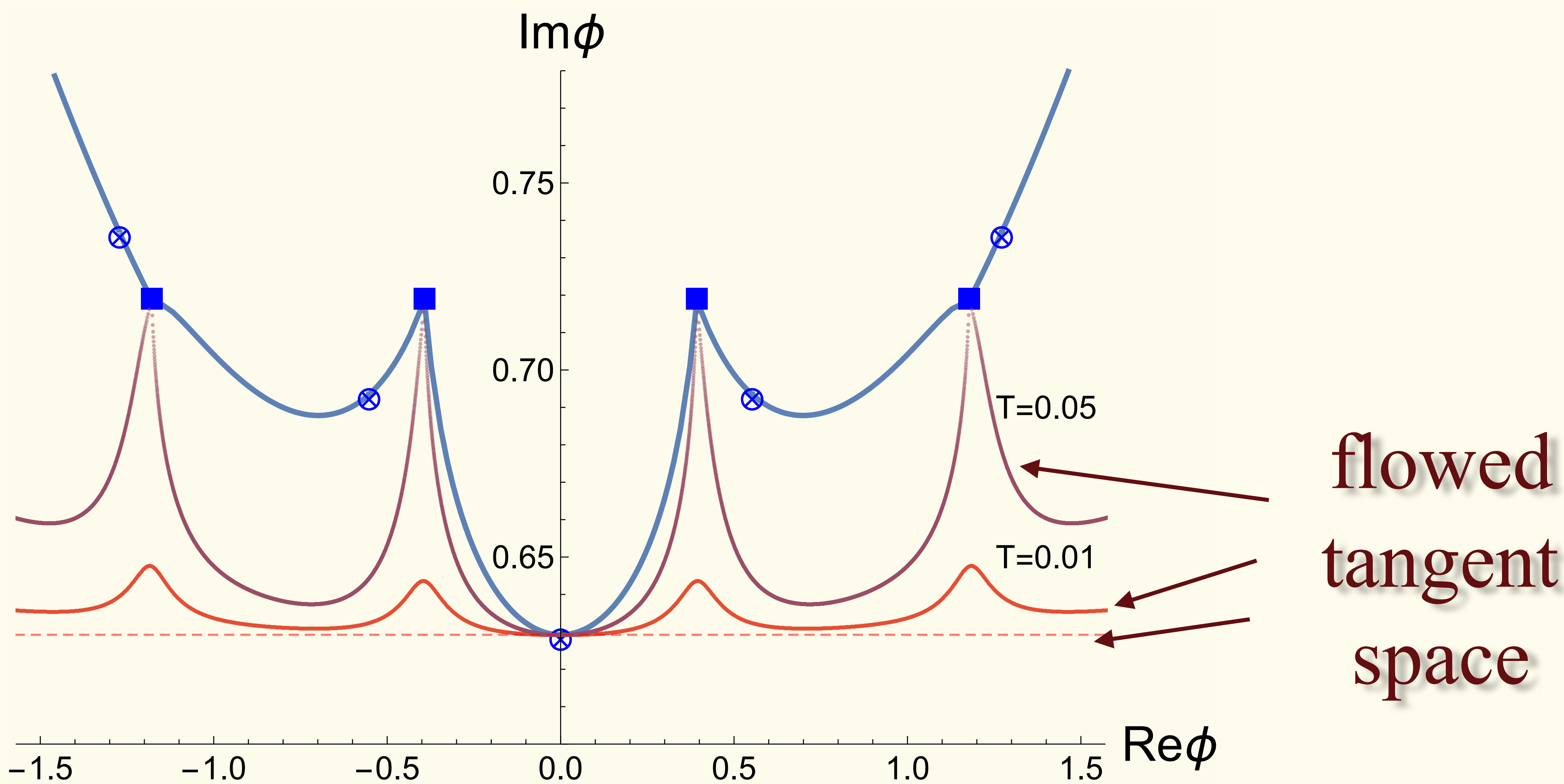

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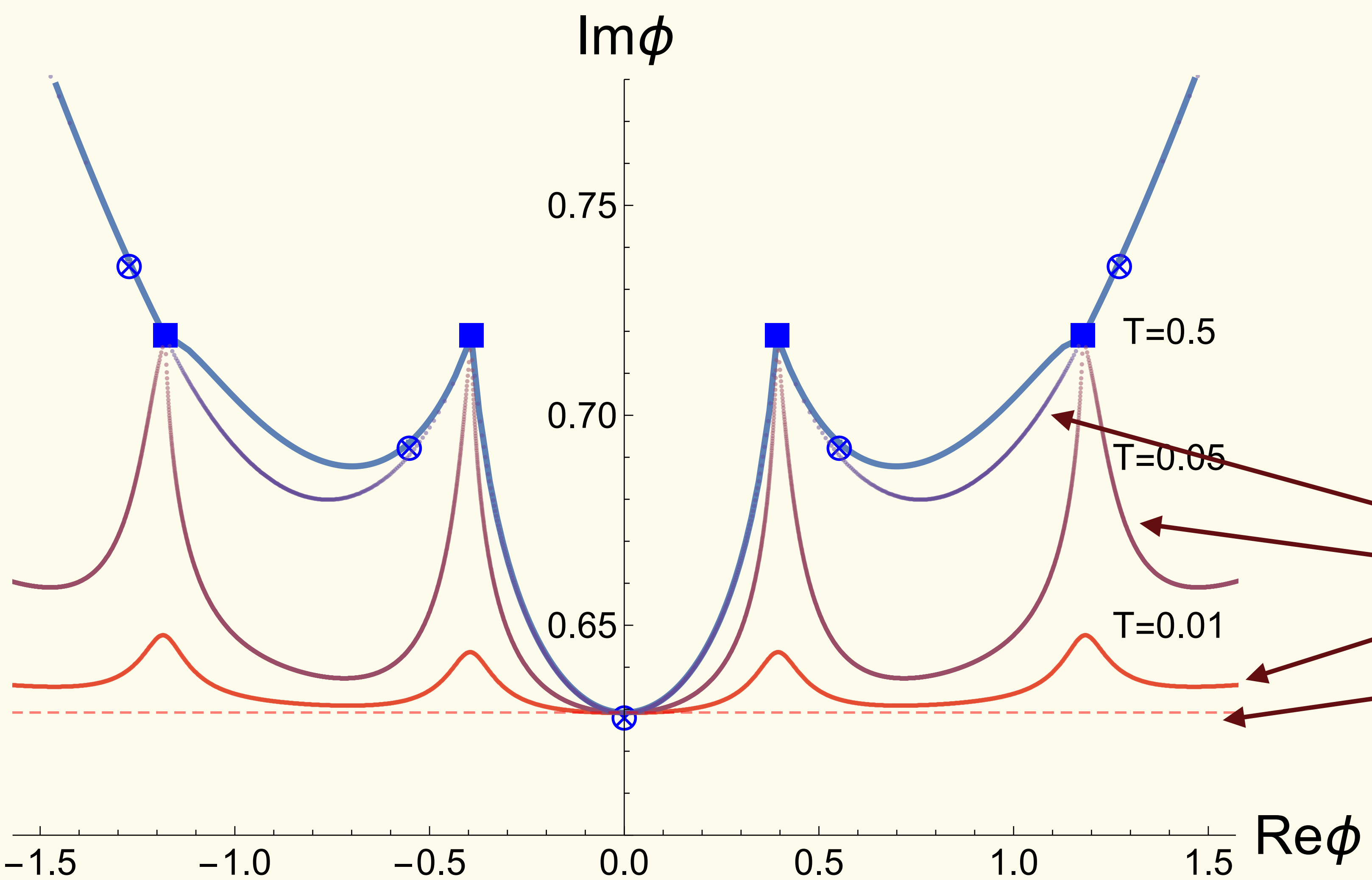
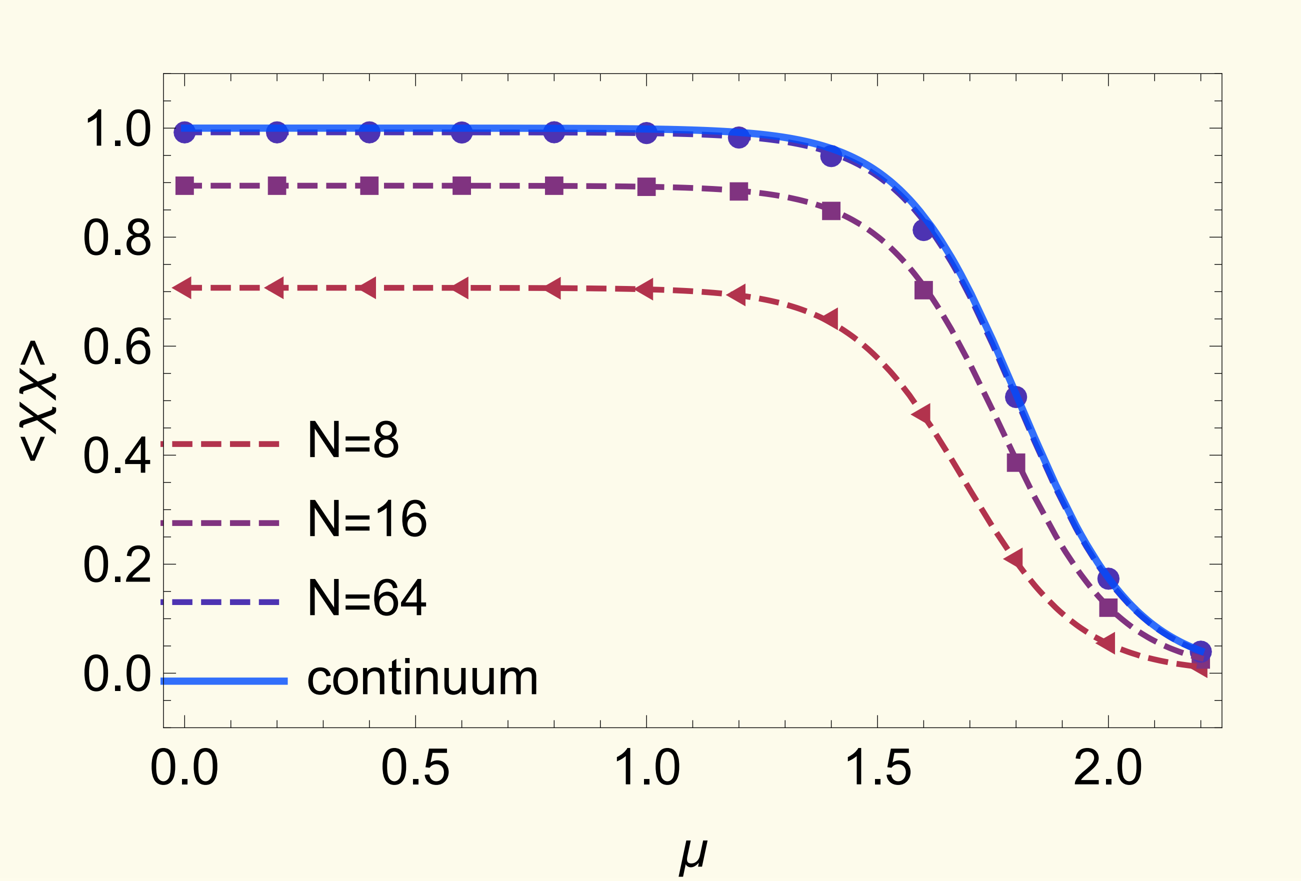
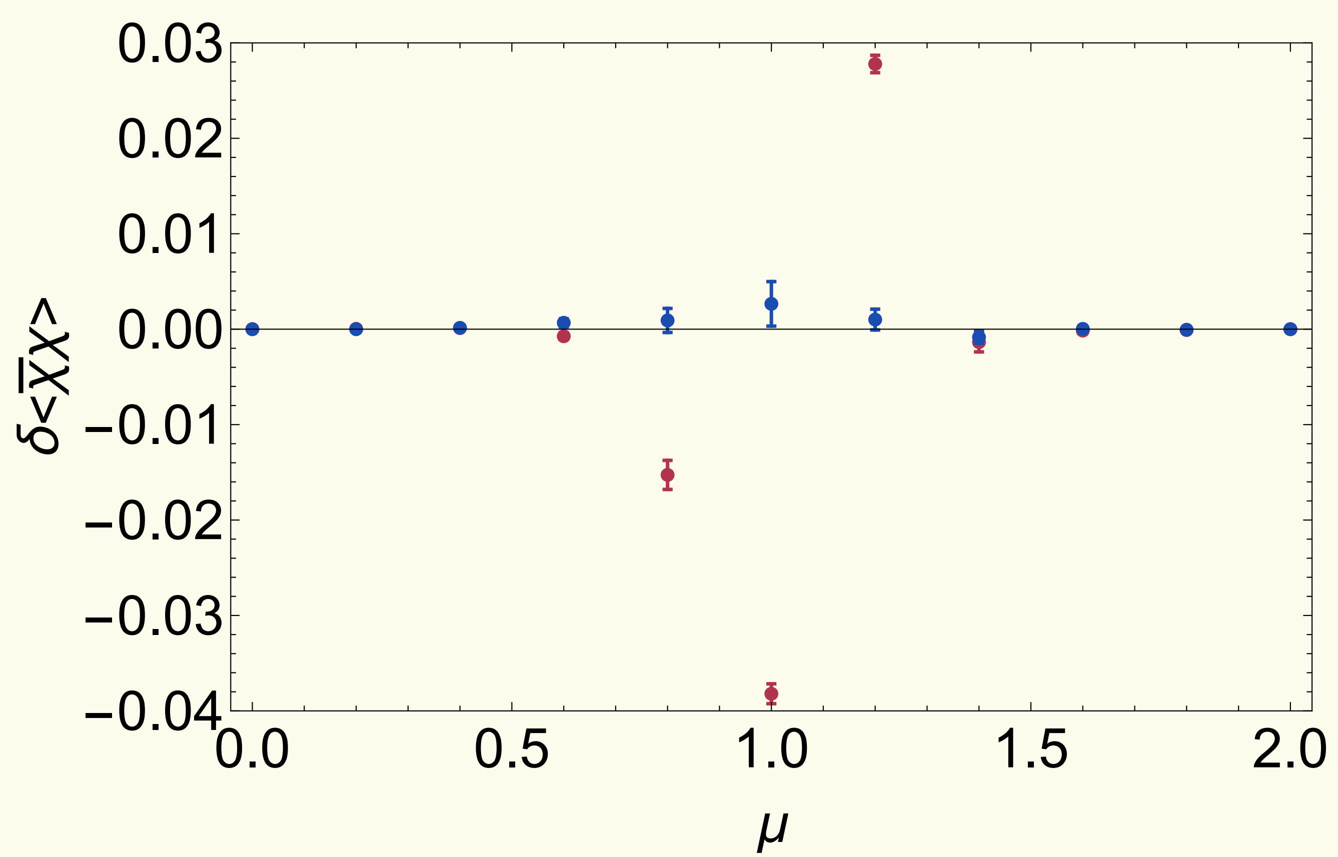


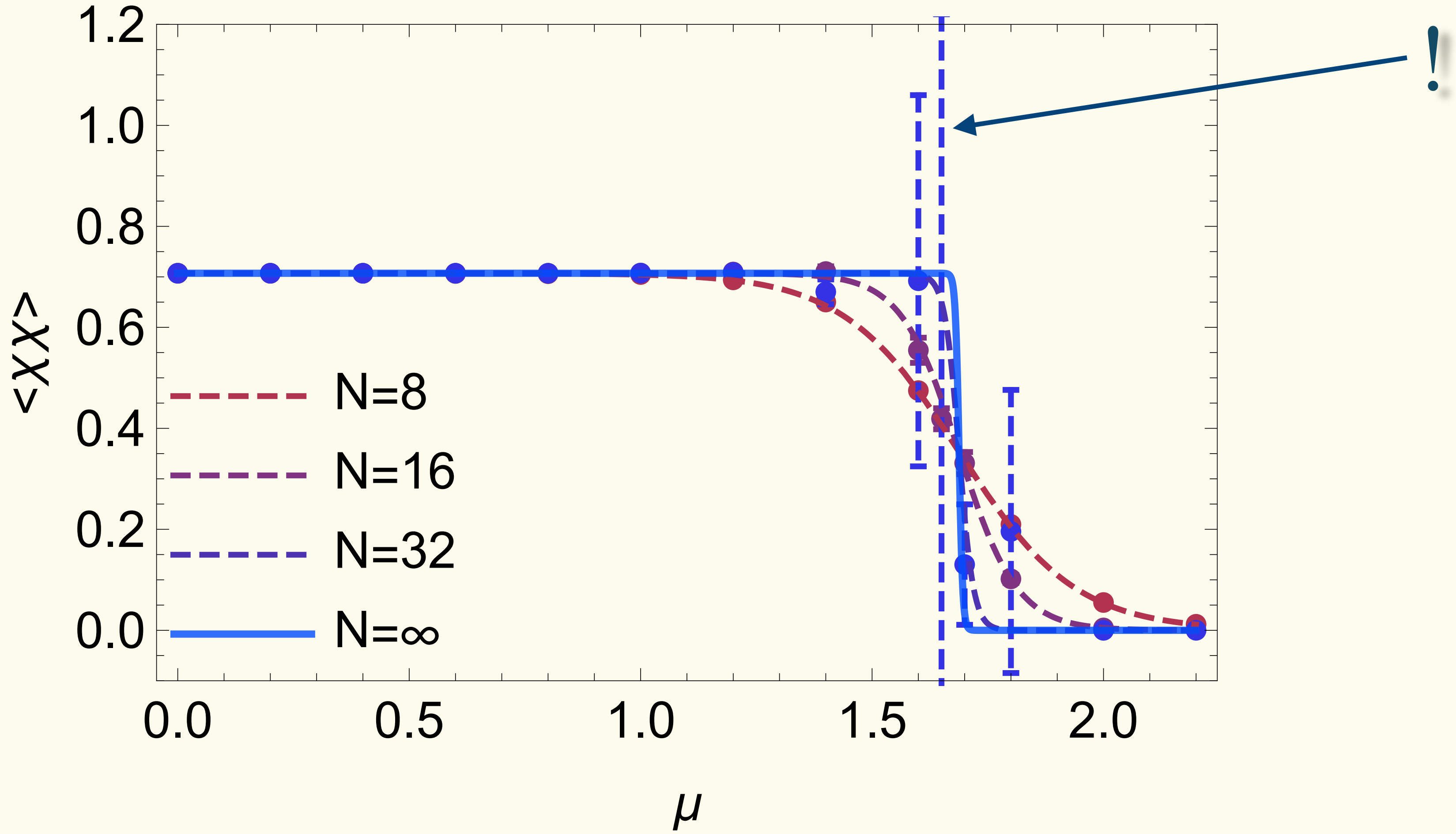
flowed tangent space

The correct ("all thimbles") integral is captured by the integral over the tangent space





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

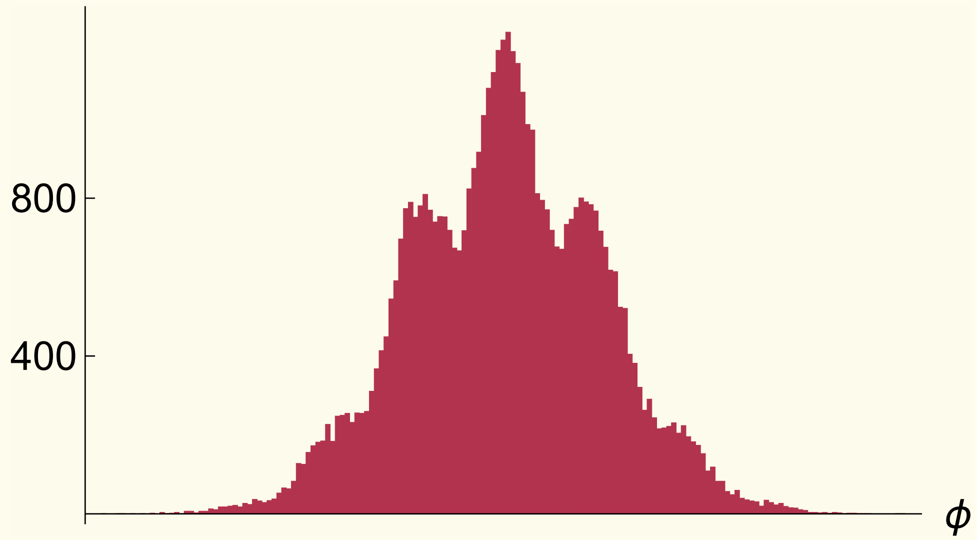


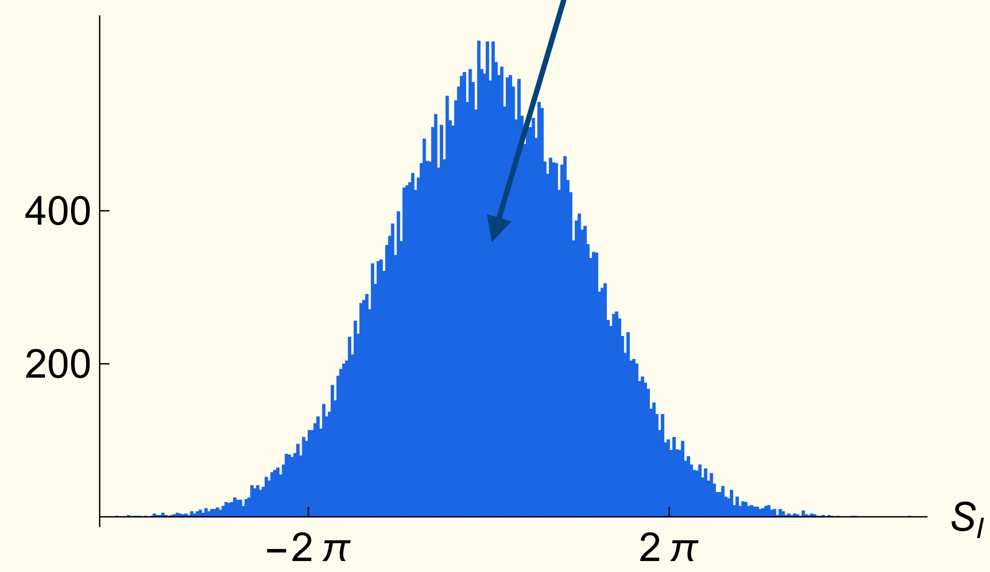
As expected, residual sign problem comes back at zero temperature. So, we flow.

N=32, μ=1.688

bad sign problem

T=0





So we flow …

N=32, μ=1.688

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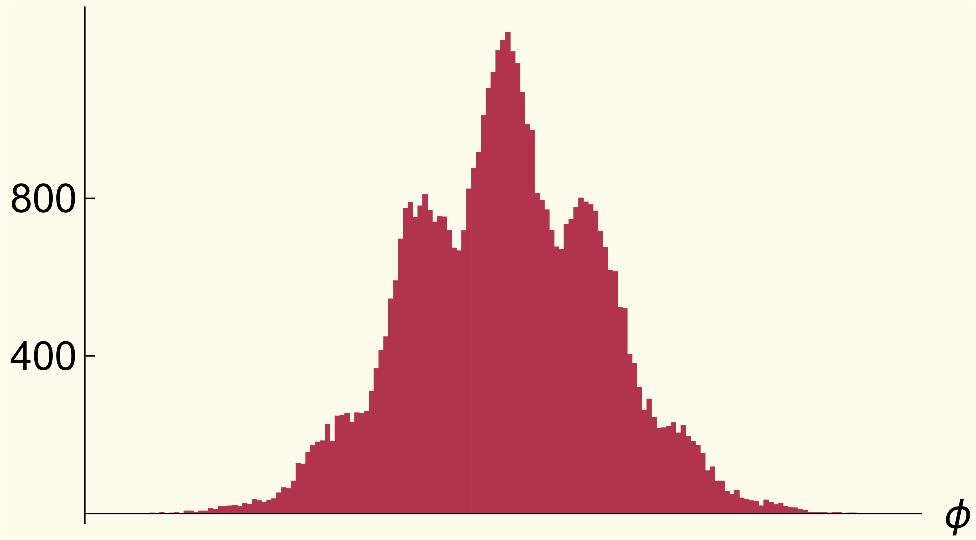
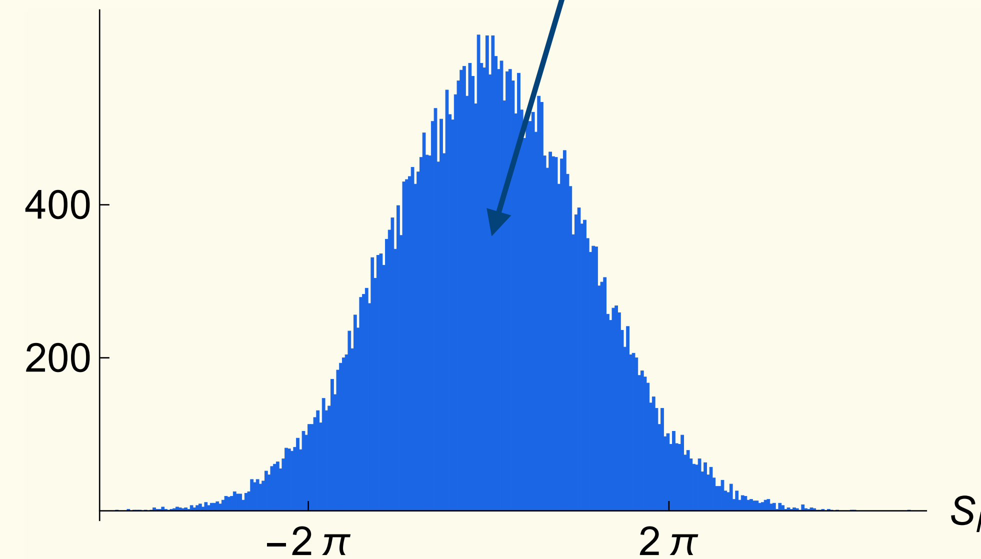
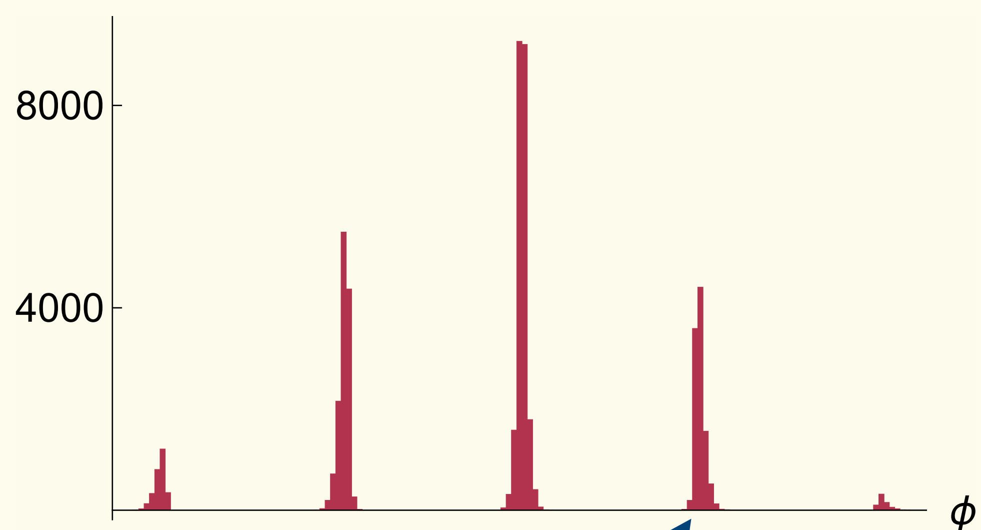
T=0

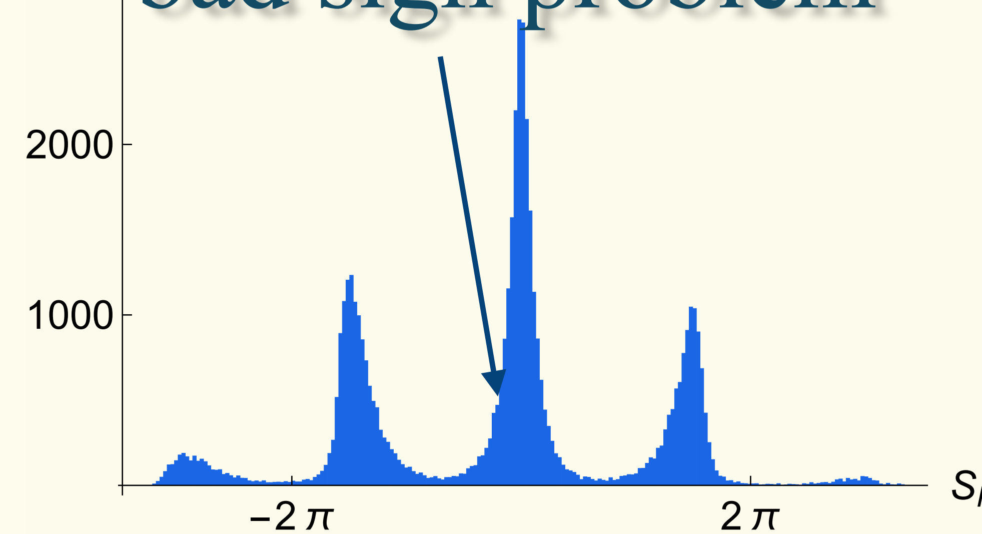




not nearly so
bad sign problem

T=0.5



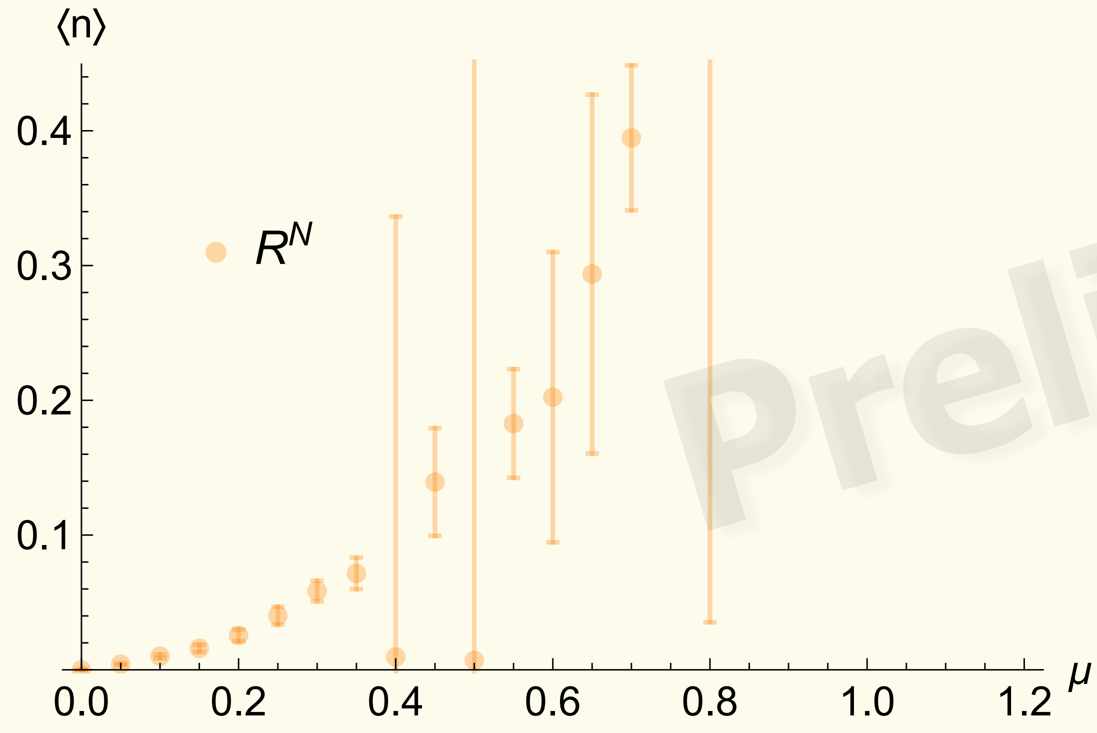


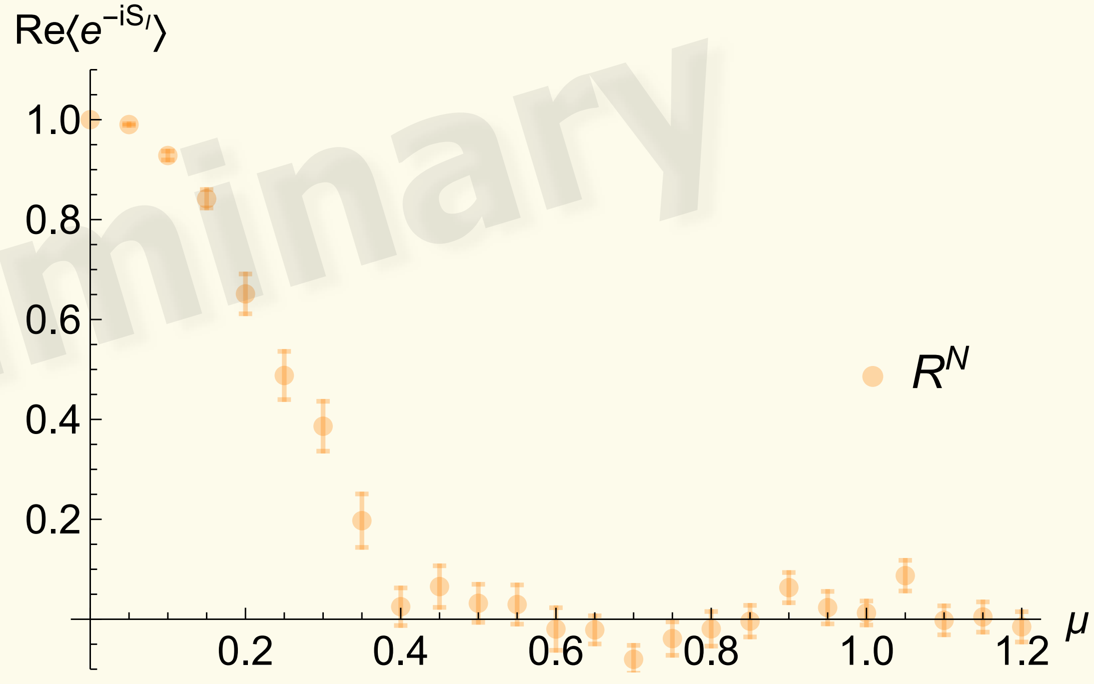
“thimbles”

1+1 dimensional Thirring model

$$\mathcal{L} = \bar{\psi}^a(\gamma_\mu \partial_\mu + m + \mu\gamma_0)\psi^a + \frac{g^2}{2N_F}\bar{\psi}^a\gamma_\mu\psi^a\bar{\psi}^b\gamma_\mu\psi^b$$

Wilson, 10 x10 lattice, N_F=2, am_f=0.3





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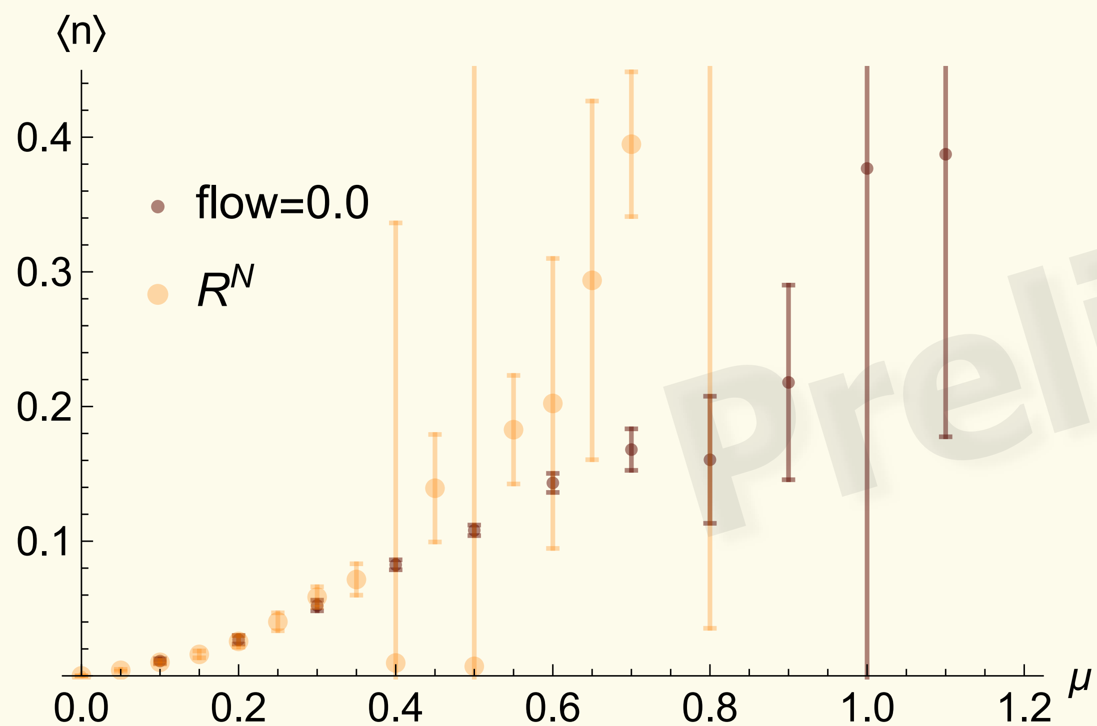

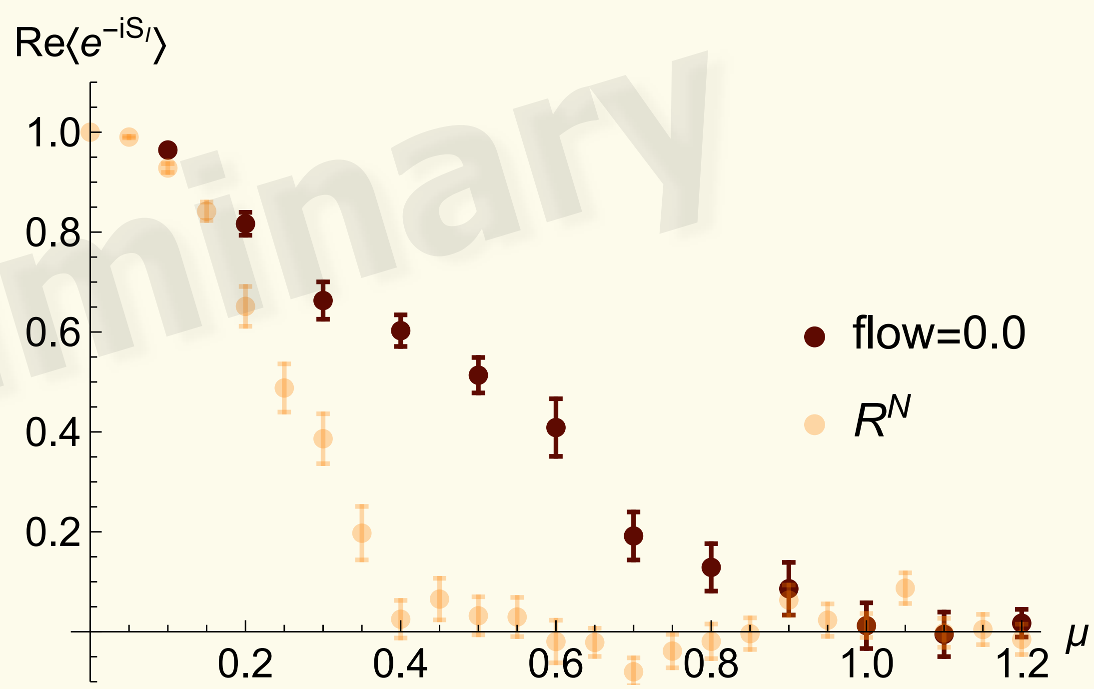

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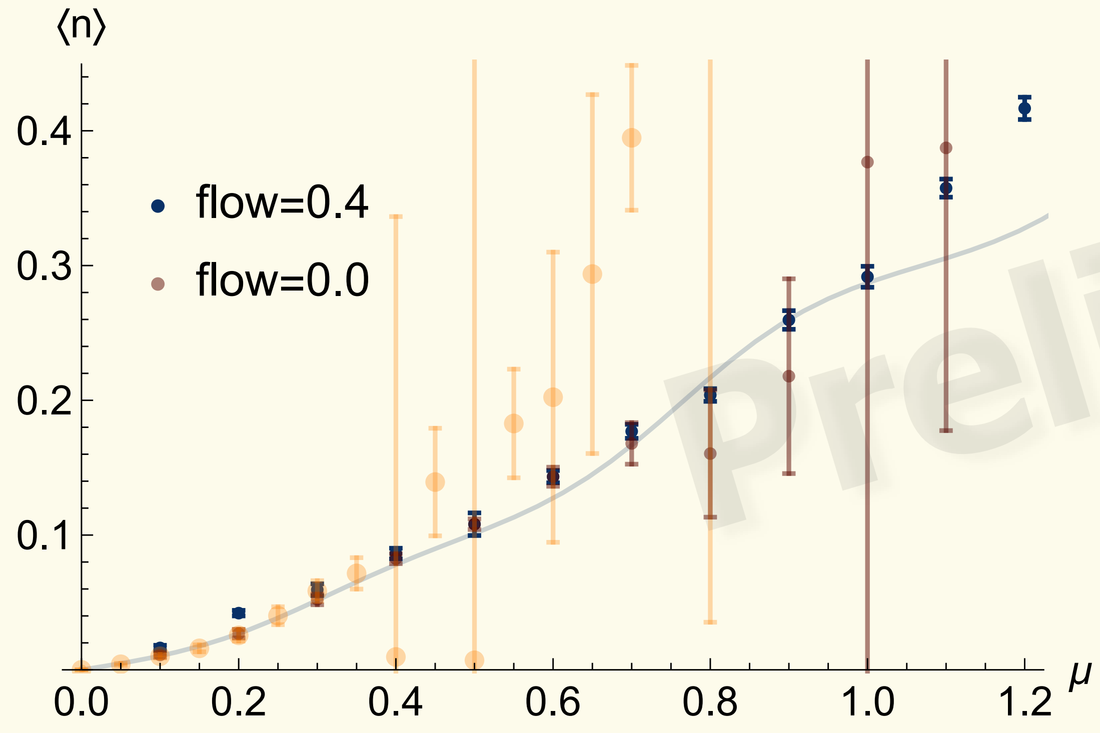
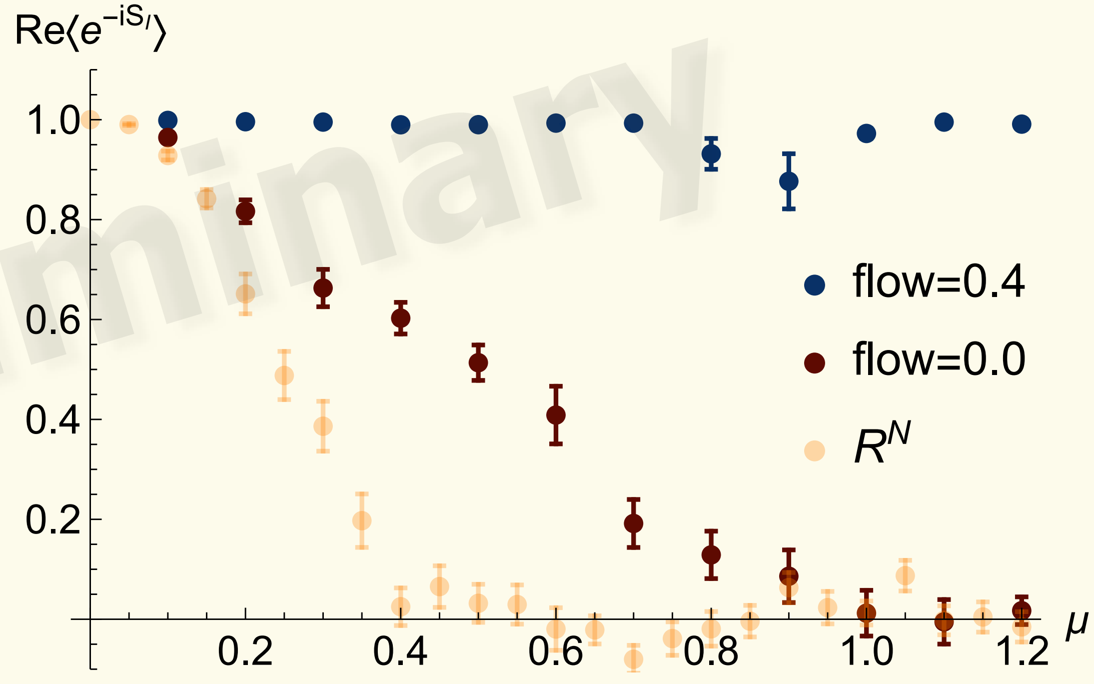
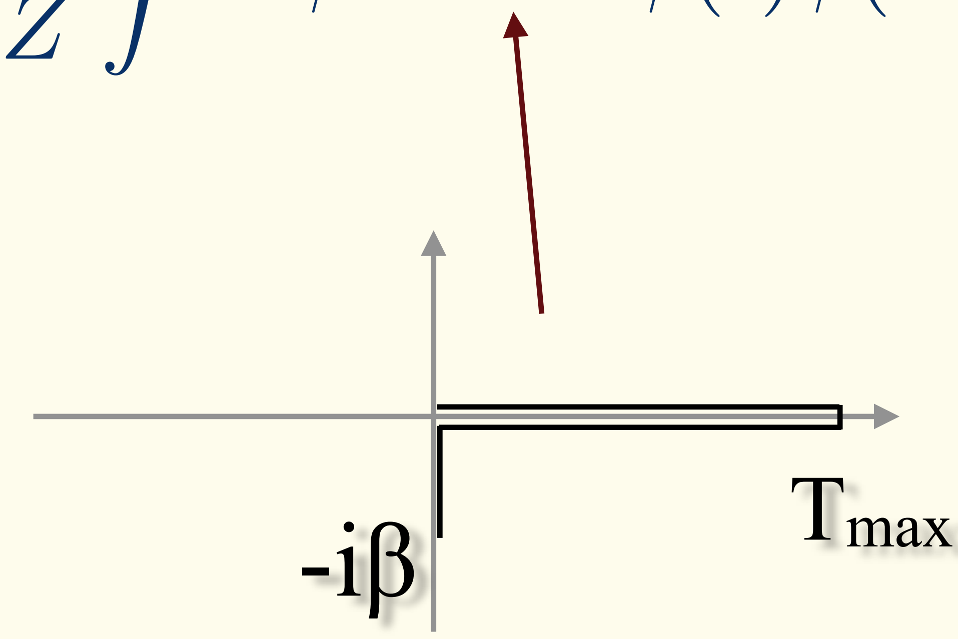




Real Time Dynamics

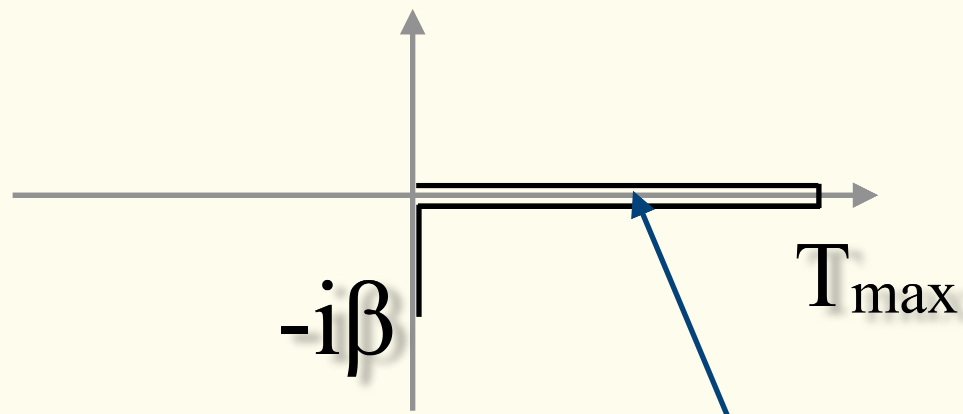
Viscosities, conductivities, …. require:

$$\langle \phi(t)\phi(t')\rangle_\beta = \frac{1}{Z}\mathrm{Tr}(e^{-\beta H}\phi(t)\phi(t')) = \frac{1}{Z}\int D\phi\ e^{iS_c[\phi]}\phi(t)\phi(t')$$



Schwinger-Keldish contour

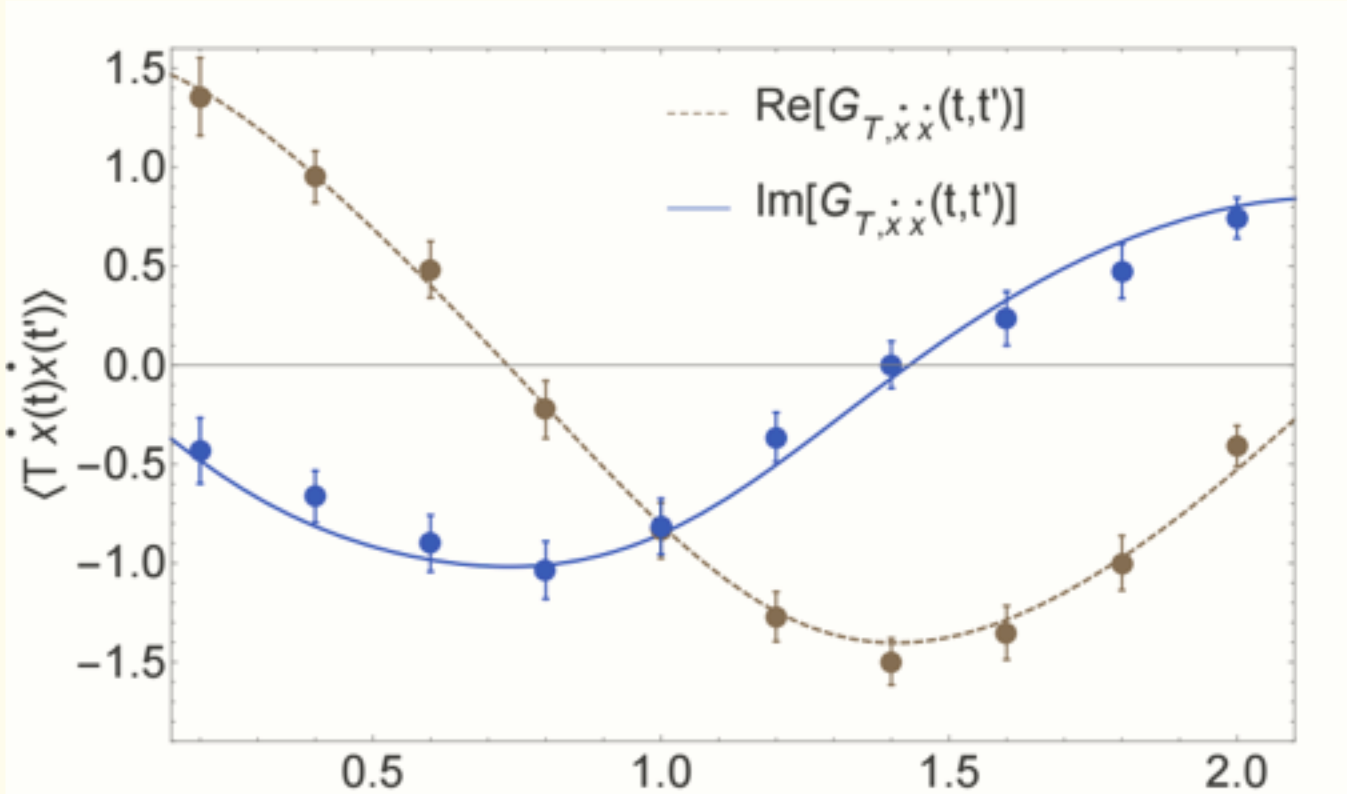
The Mother of All Sign Problems:

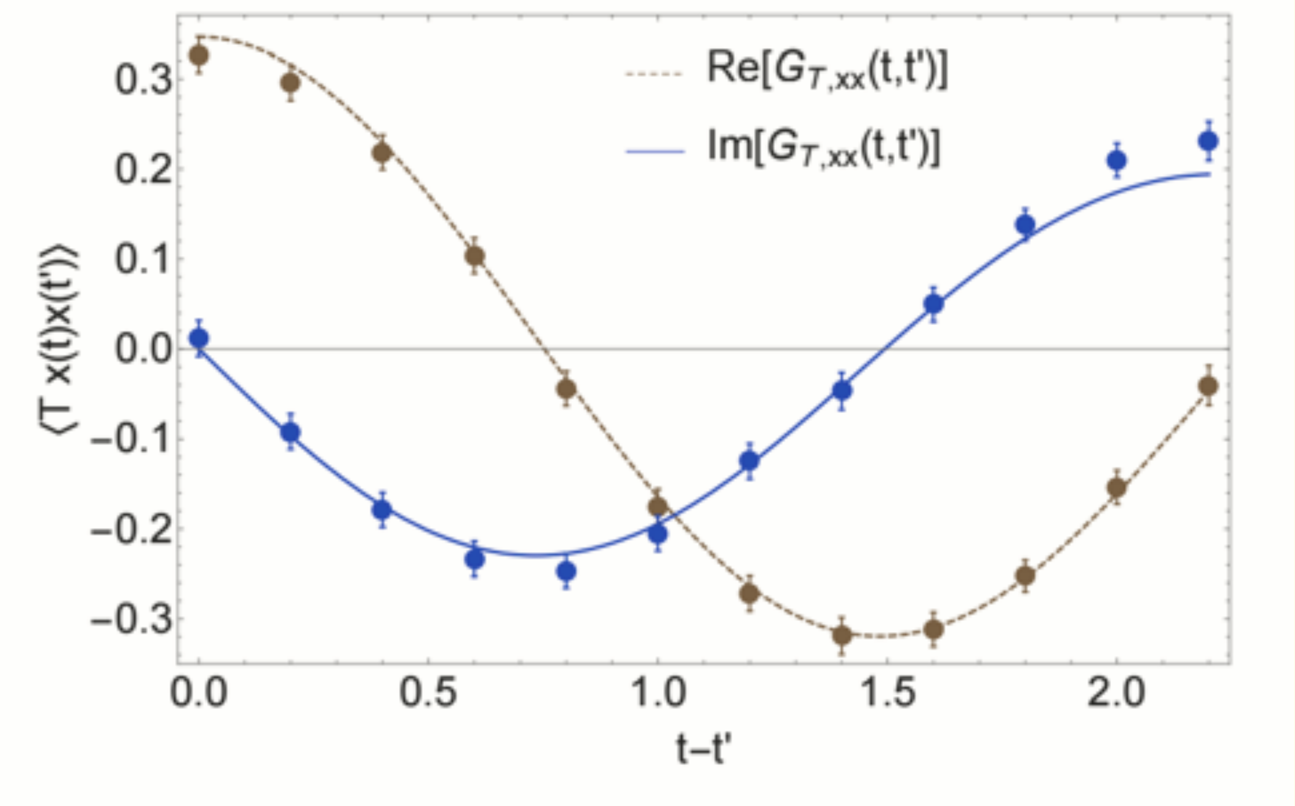


field at a point in the real axis does not contribute to the damping factor in e^{iSc}

$$\langle e^{i\mathrm{Im}(iS_c)} \rangle = 0$$

Test: anharmonic oscillator





Very slow convergence

- Deforming the integration on complex space is a good thing
- Thimbles are optimal if only one dominates; other manifold
  are better in other cases
- Improvements in method:

  estimator for J (arXiv:1604.00956)

  ~L^8 tangent space

  pseudo-fermions

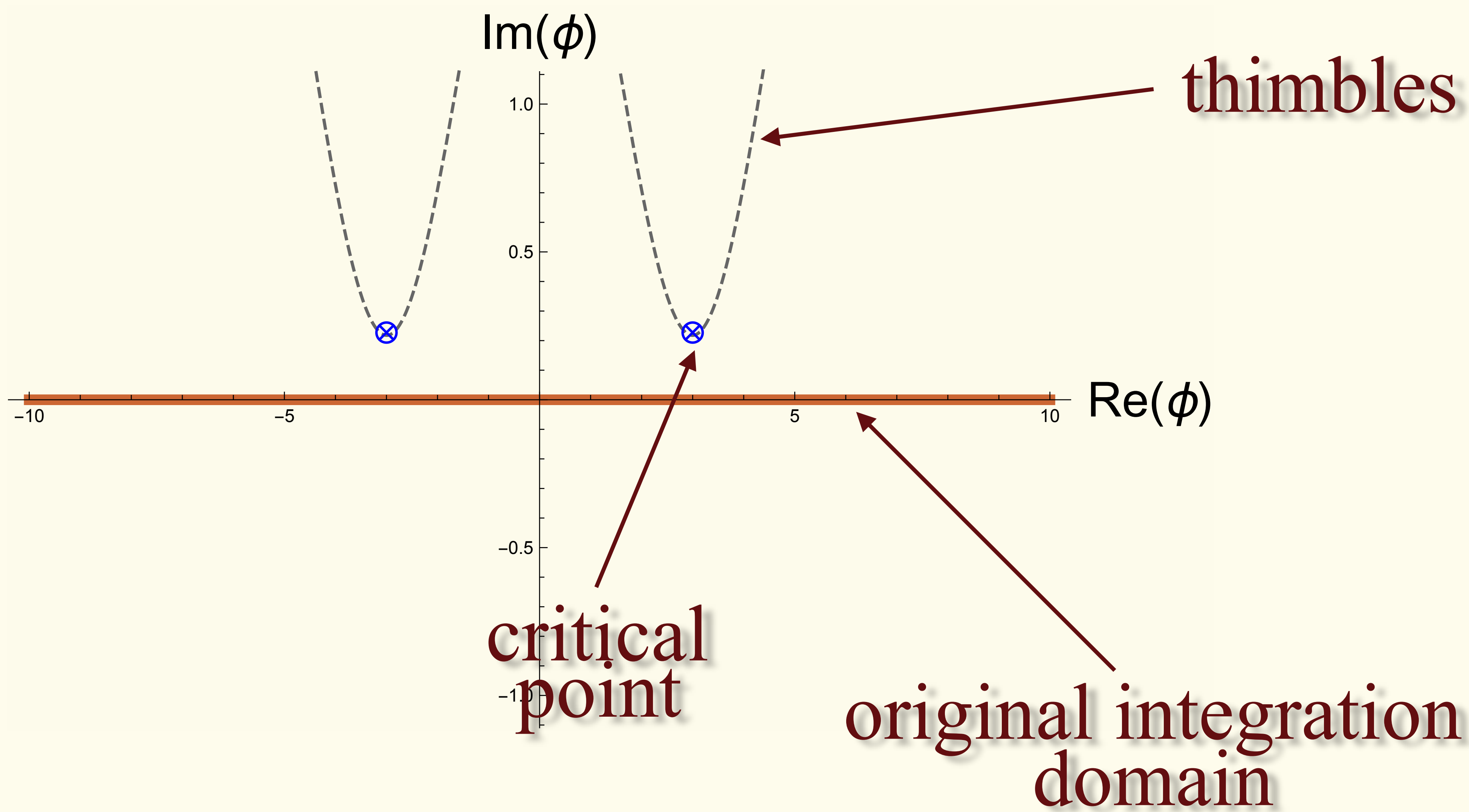
- Models:

  4D φ^4 at finite μ (small lattice)

  1+1 real time (Schwinger-Keldish),

  1+1 Thirring

From real plane to thumbs (and everything in between): flow preserves the integral



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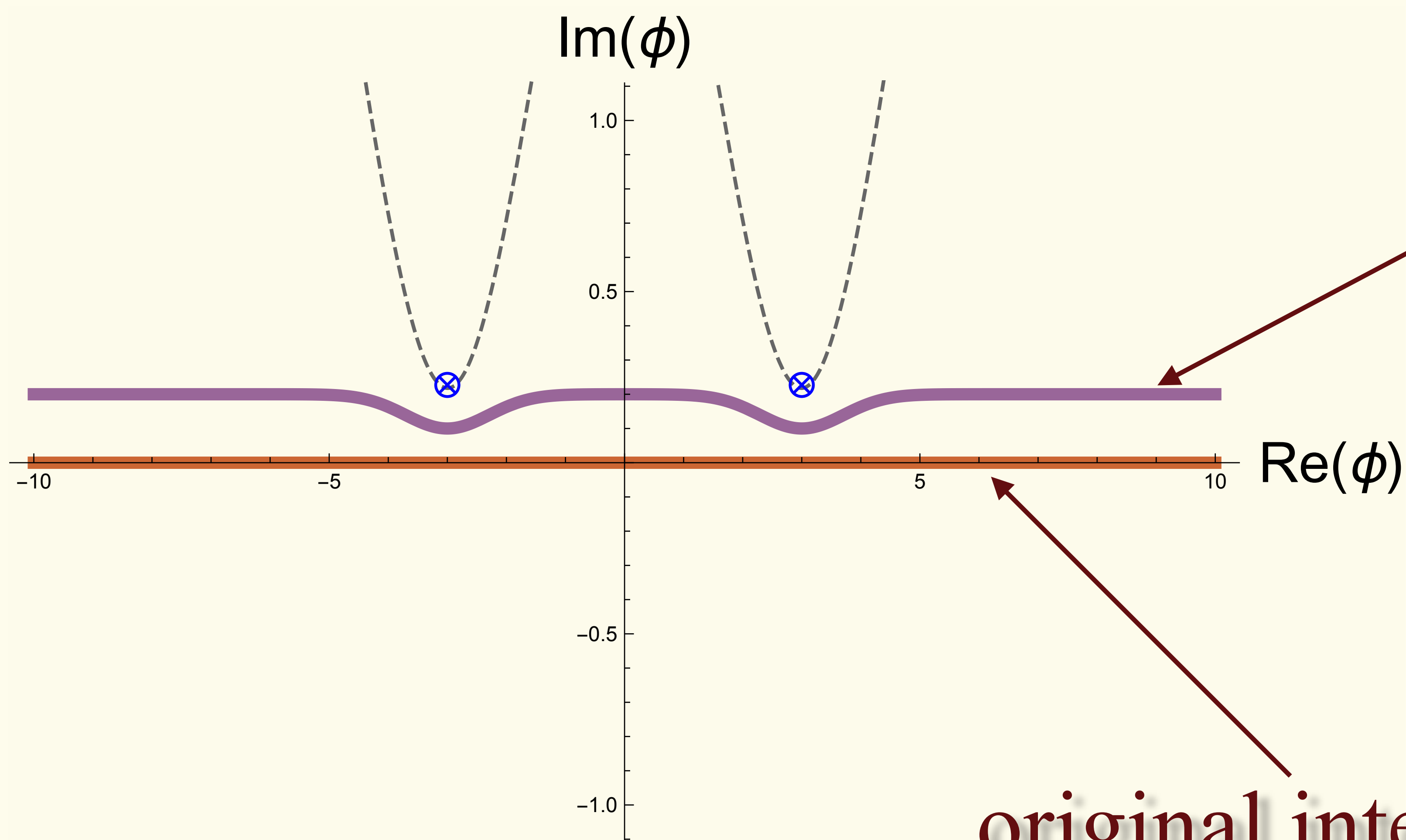
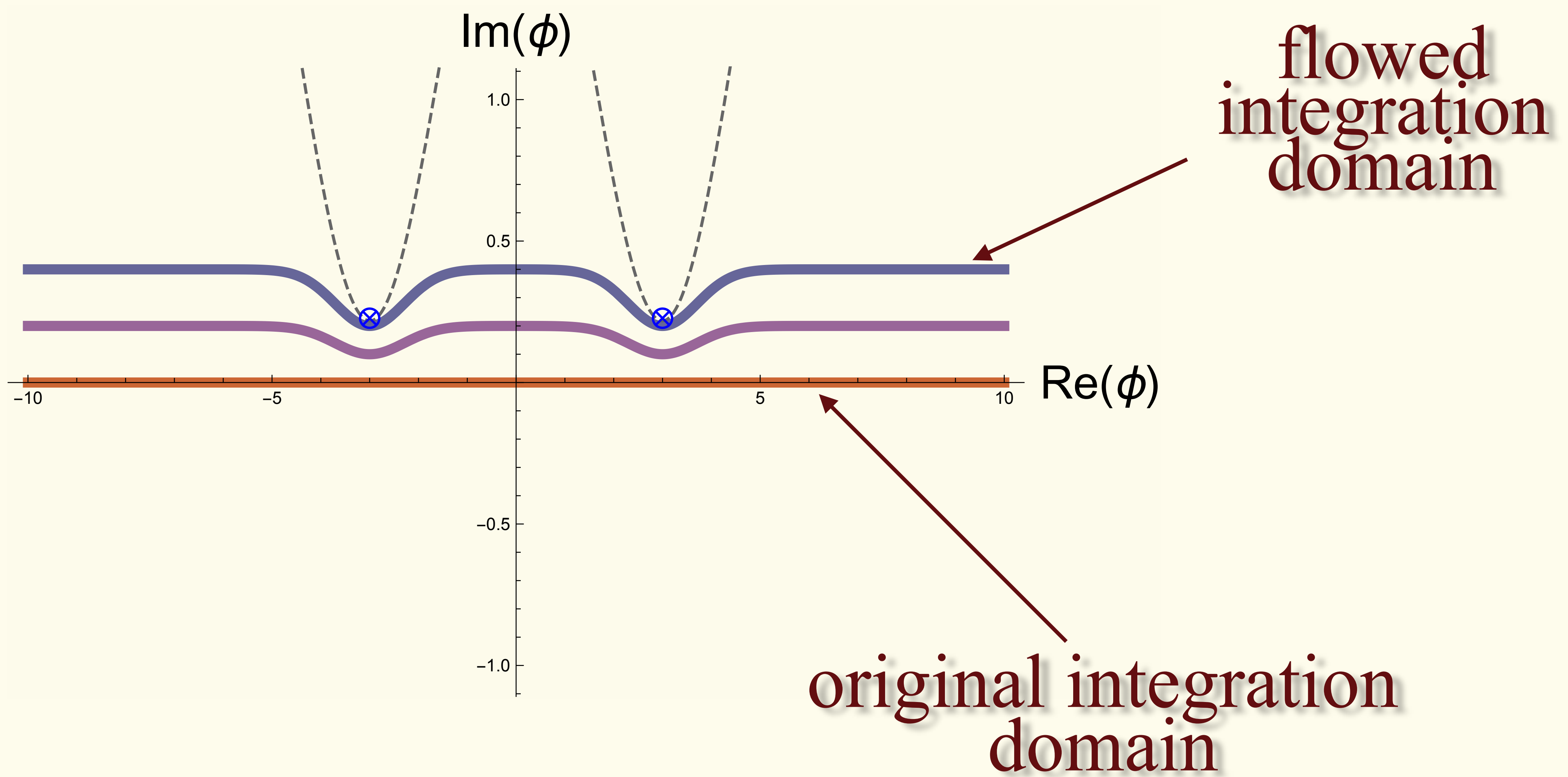


flowed integration domain

original integration domain

From real plane to thumbs (and everything in between): flow preserves the integral



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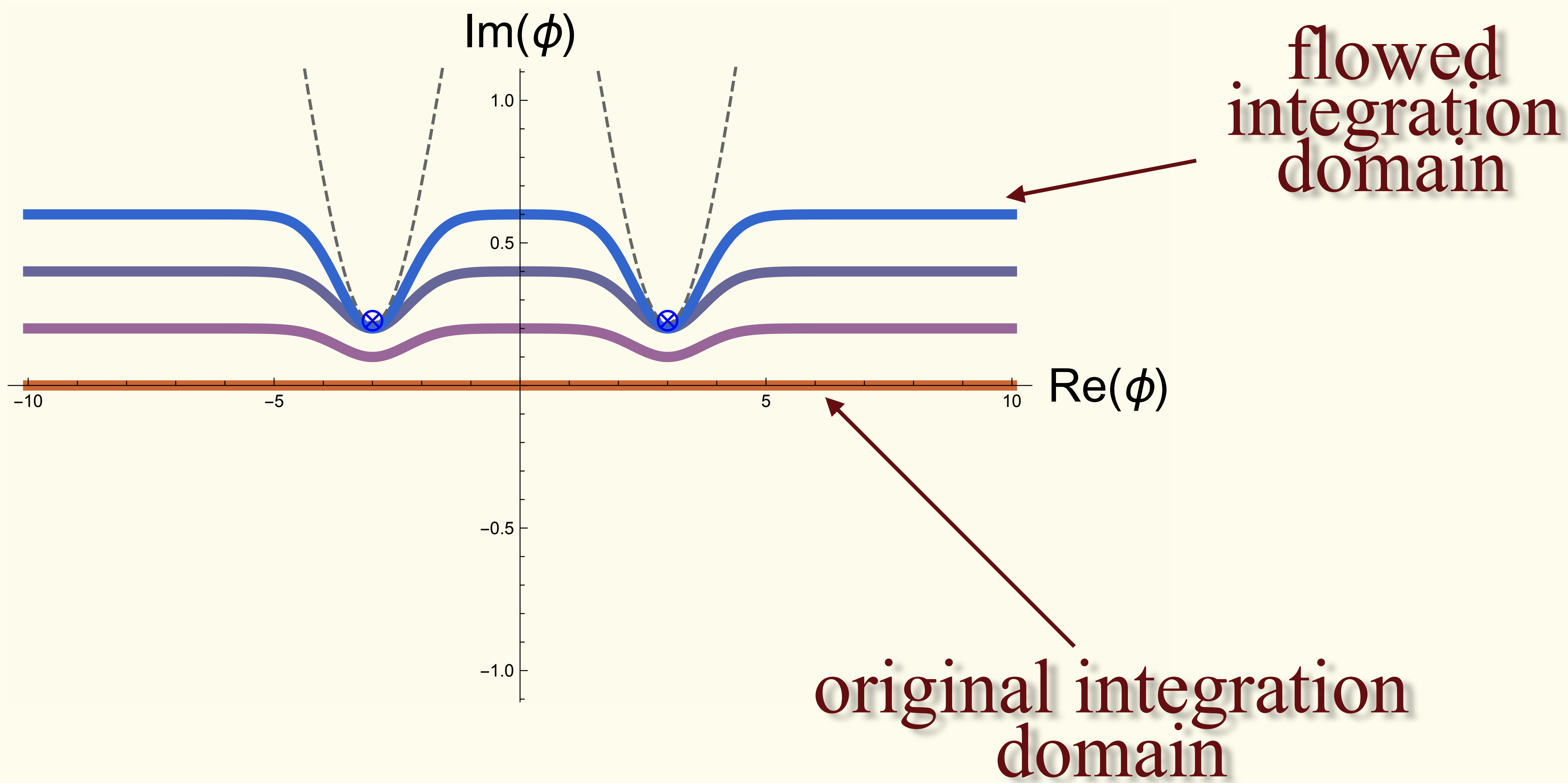

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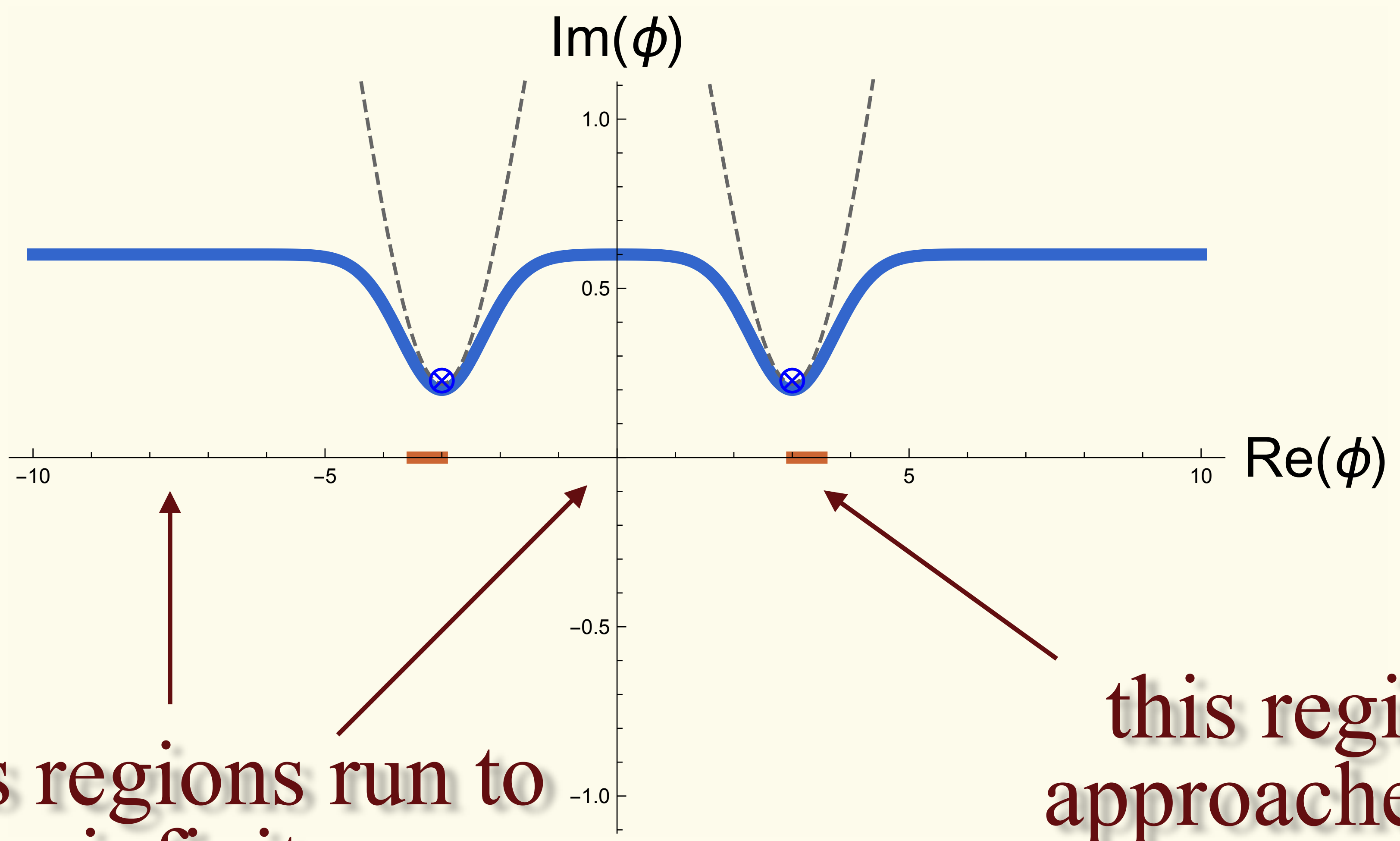
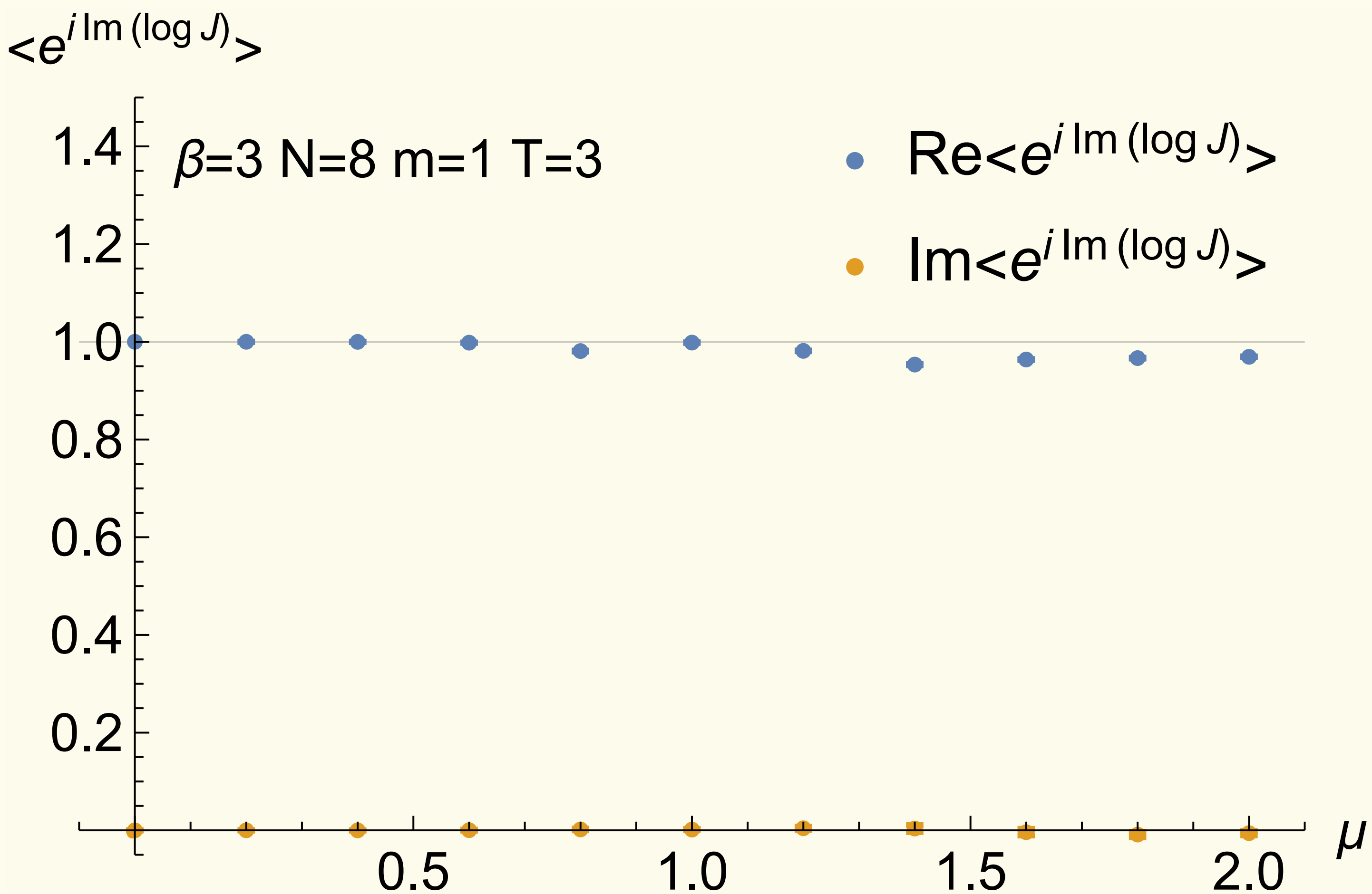


this regions run to infinity

this regions approaches the thimbles (nearly fixed S_I)

Is there a remaining sign problem with the contraction algorithm ?



Nope, not on this model with these parameters.