Going with the (holomorphic) flow: thimbles and the sign problem

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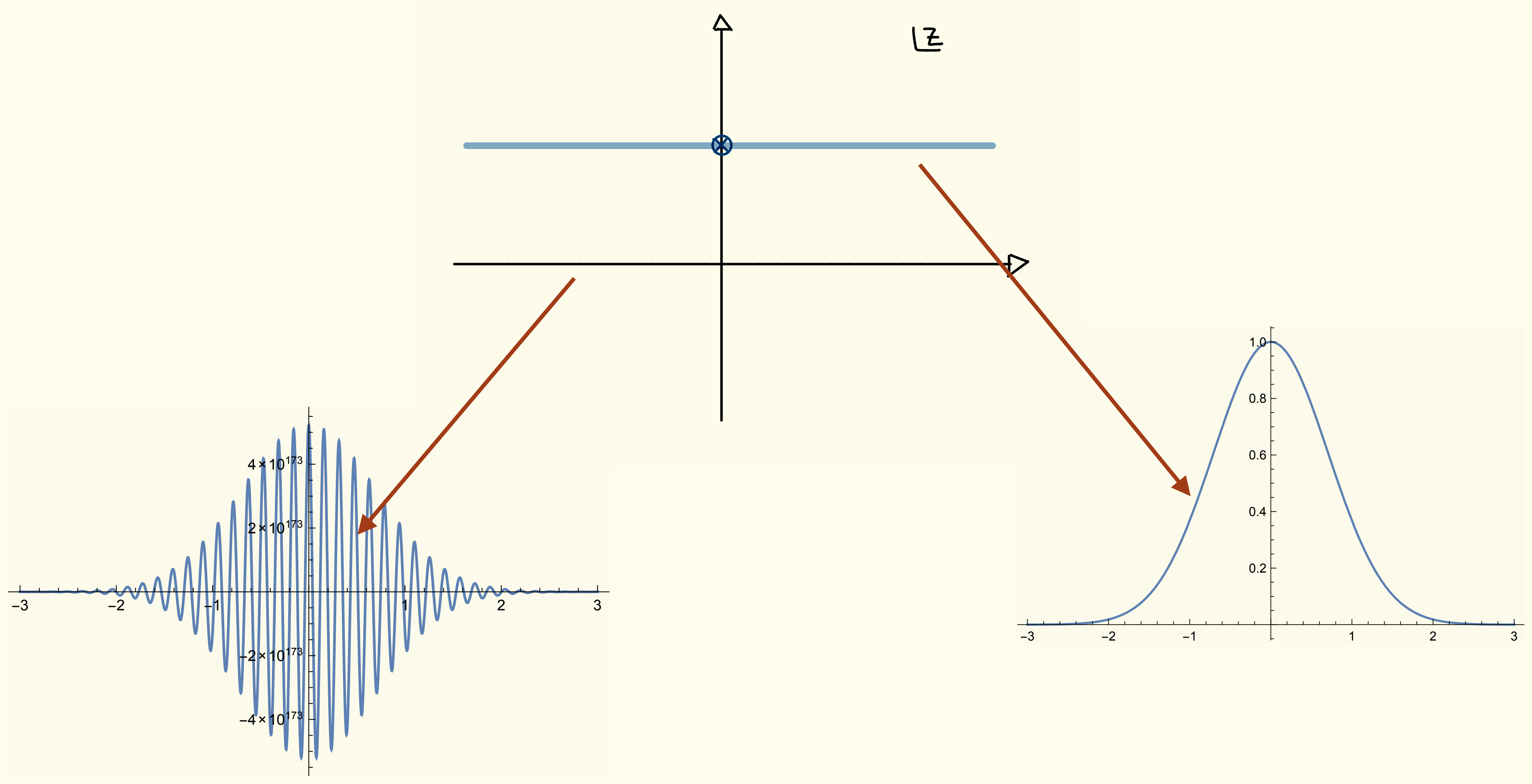
Central idea: deform the contour into the complex plane:

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



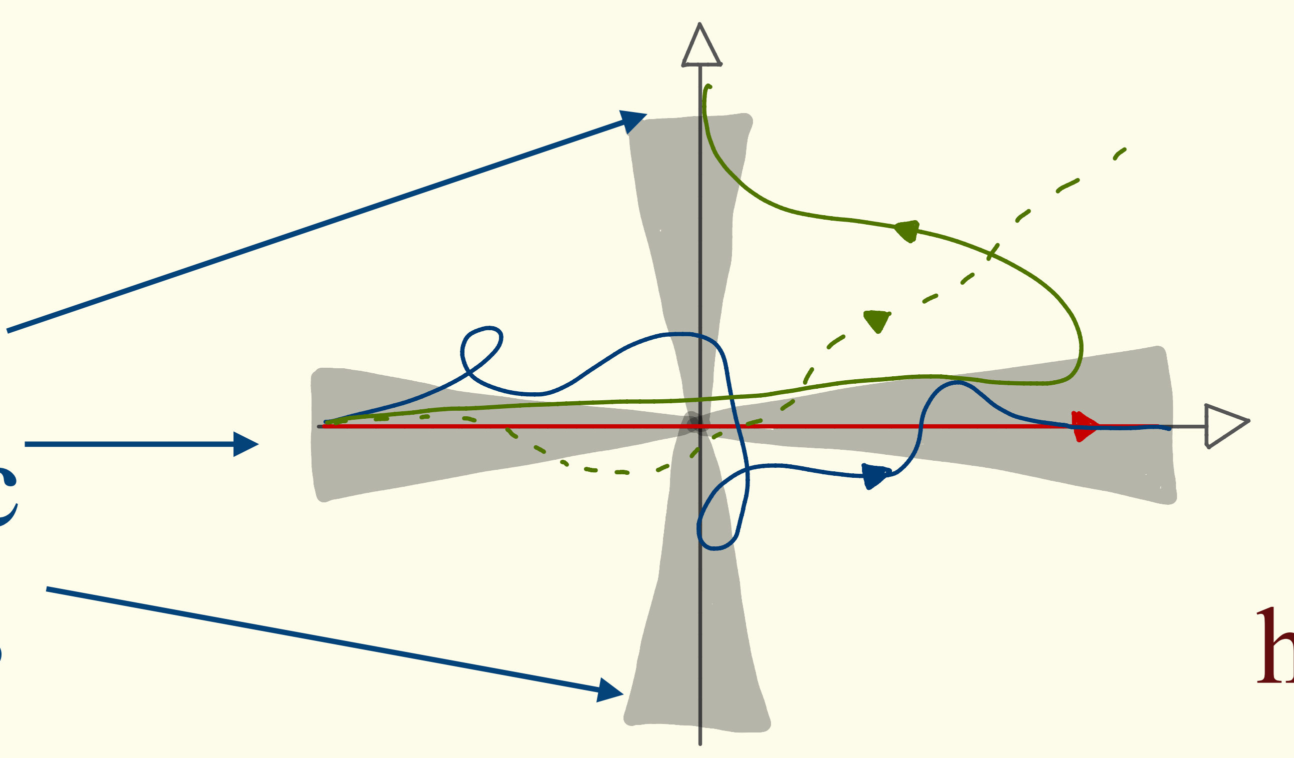
Cristoforetti, DiRenzo, Scorzato, '12

How to find good contour deformations ?

- integrands have no pole except at *infinity*
- outside the "good" asymptotic directions the integral diverges

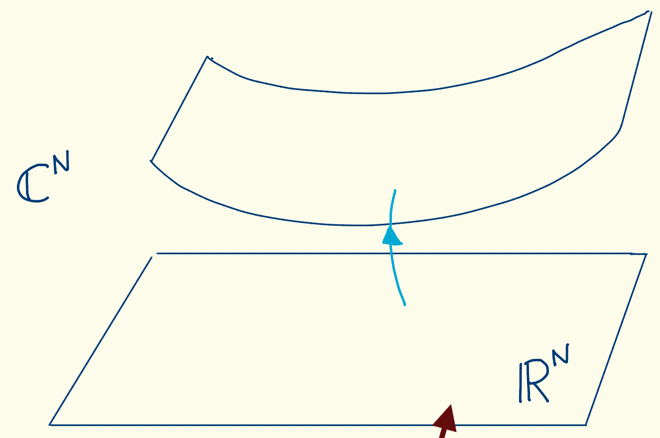
$$\int dz\ e^{-(hz+z^2+z^4)}$$

good asymptotic directions



integral depends only on initial and final directions: homological classes

How to find good deformations ?



(real) field space

$$\frac{d\phi_i}{dt} = \overline{\frac{\partial S}{\partial \phi_i}} \Rightarrow$$

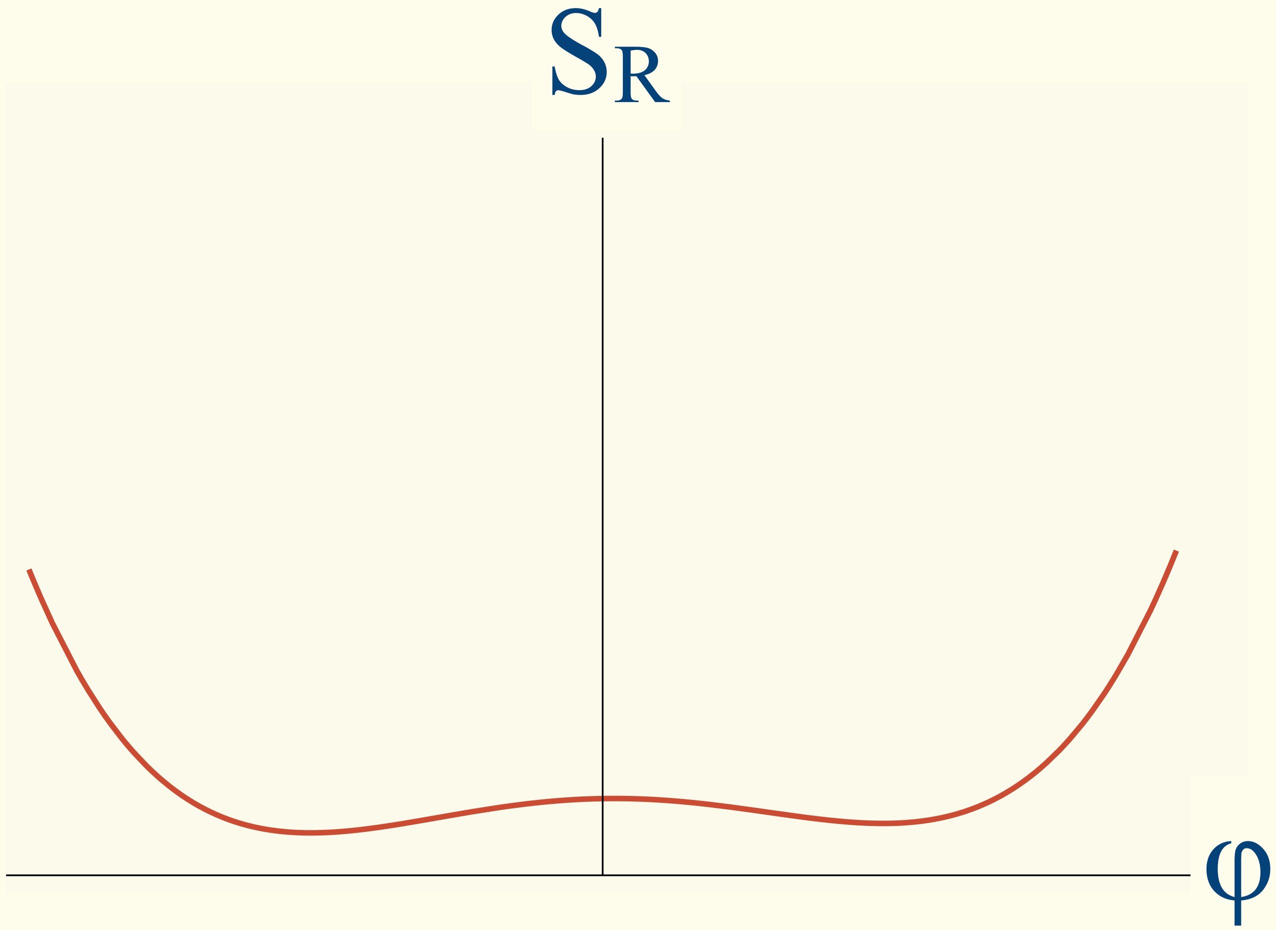
$$\frac{d\phi_i^R}{dt} = \frac{\partial S^R}{\partial \phi_i^R} = \frac{\partial S^I}{\partial \phi_i^I}$$

$$\frac{d\phi_i^I}{dt} = \frac{\partial S^R}{\partial \phi_i^I} = -\frac{\partial S^I}{\partial \phi_i^R}$$

gradient flow of S^R, keeps integral well defined

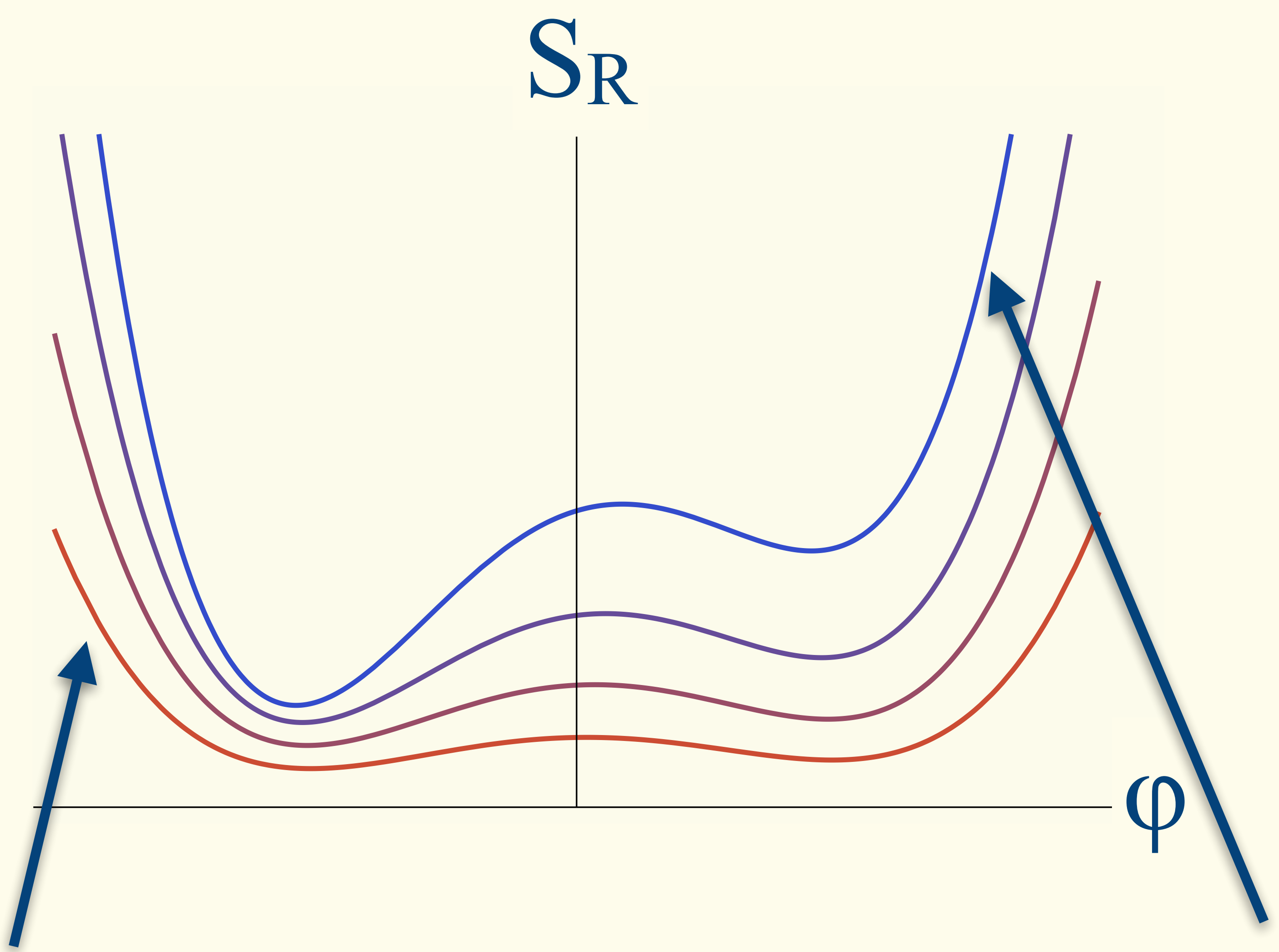
hamiltonian flow of S^I, keeps phase fixed

How to find good deformations ?



S_R under the flow

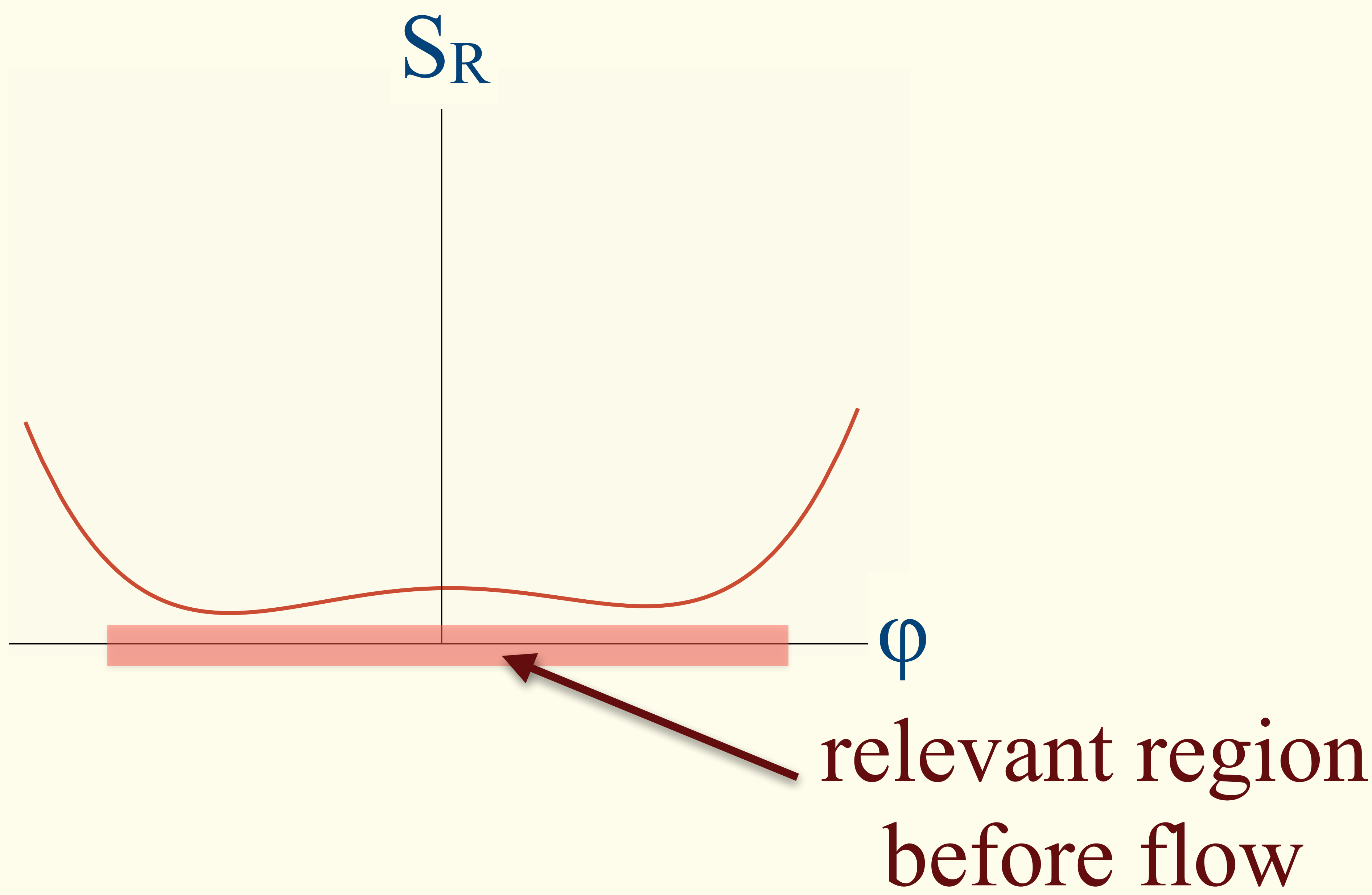
How to find good deformations ?



if this integral exists, so does that

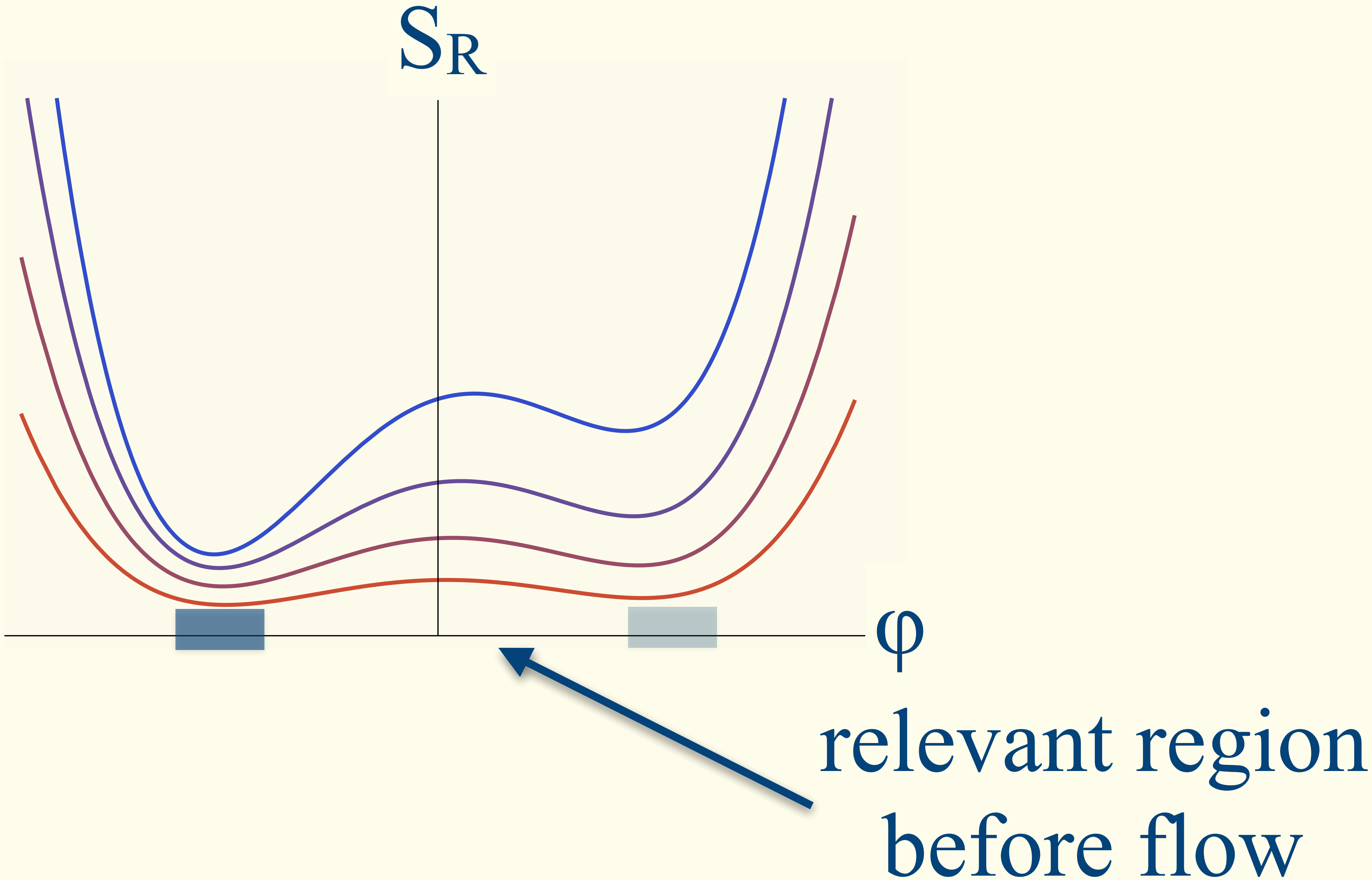
homology class preserved by the flow

How to find good deformations ?



S_R grows under the flow

How to find good deformations ?

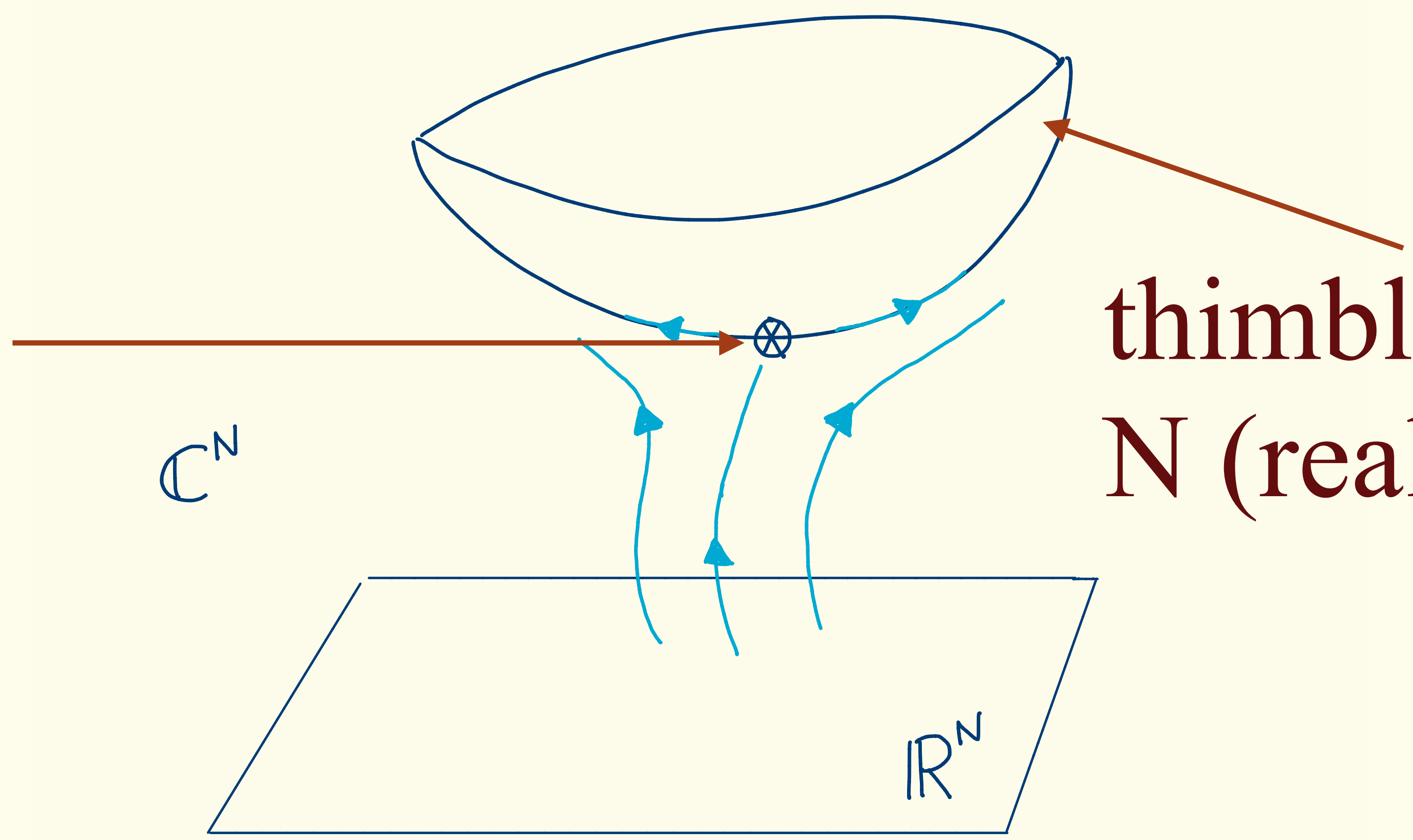


S_R grows under the flow
S_I stays constant

How to find good deformations ?

critical point:

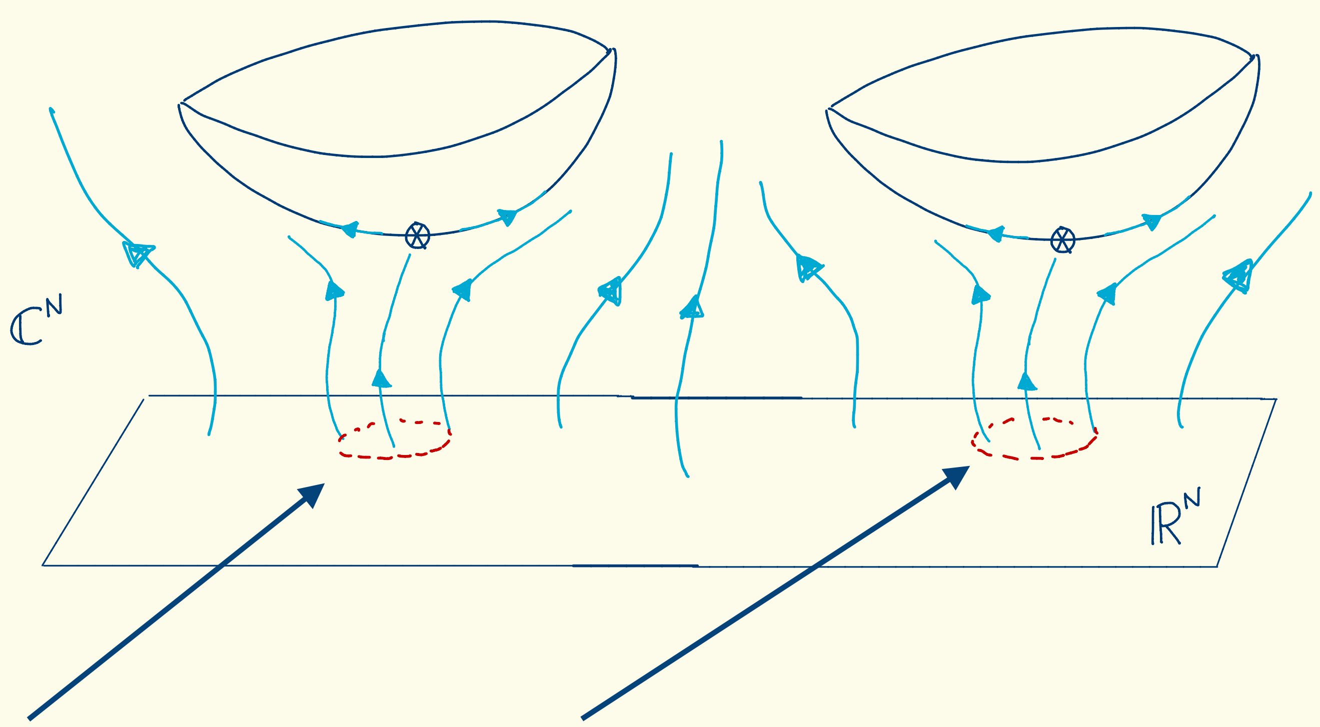
$$\frac{\partial \bar{S}}{\partial \phi_i} = 0$$



thimble: S^I=const.
N (real) dimensions

flow ends on the right 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:

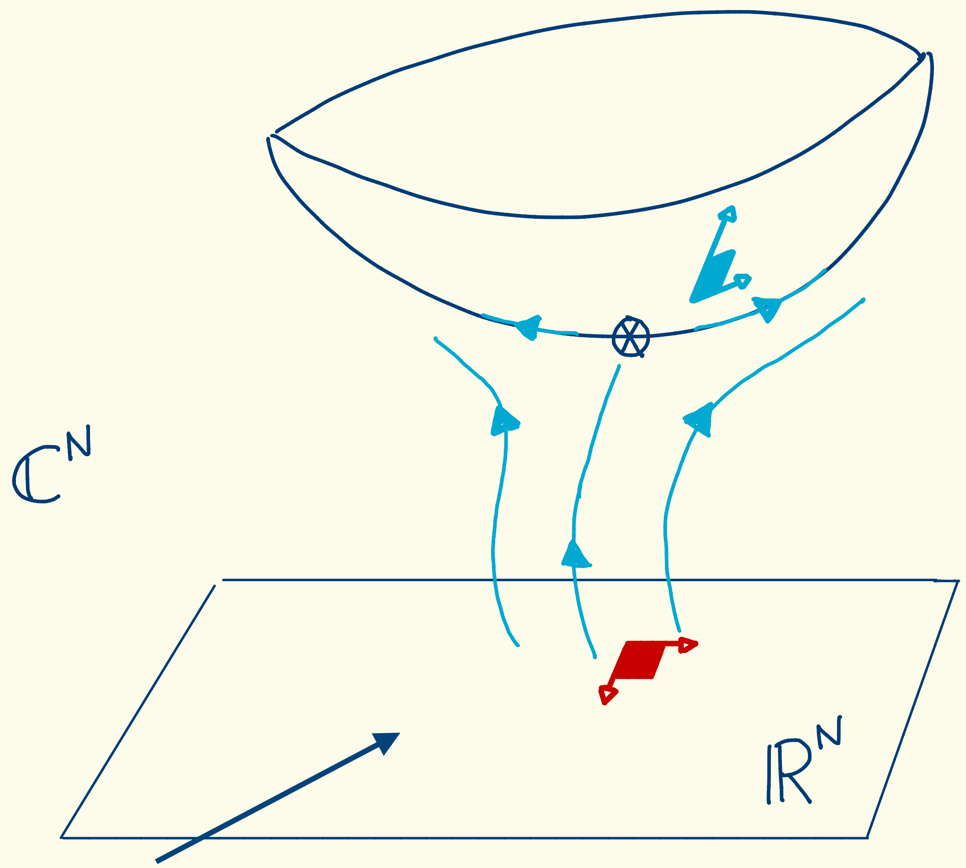
- Monte Carlo chain to stay on the thimble (Langevin *Cristoforetti et al. `12,* HMC *Fuji et al. `13*)

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

We'll take a different route:

- forget thimbles, use R^N flowed a "little"
- too little flow=sign problem not ameliorated enough
- too much flow=Monte Carlo gets stuck into one region in field space

How to find good deformations ?



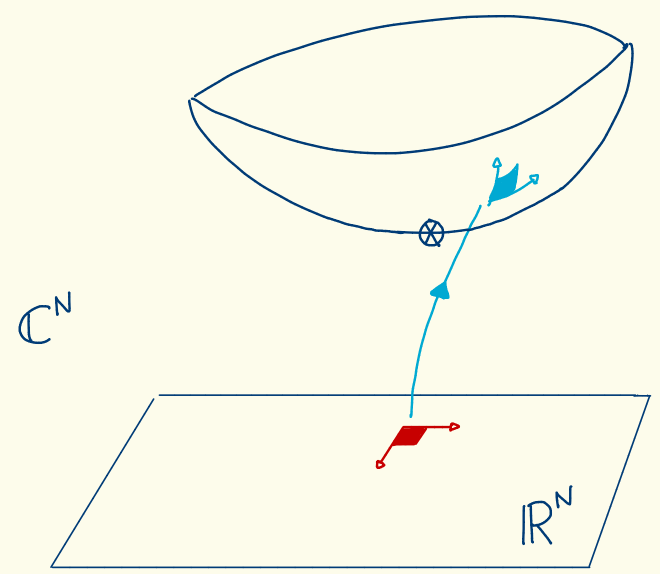
real fields $\tilde{\phi}$ parametrize the flowed R^N:

$$S_{eff}[\tilde{\phi}] = S[\phi(\tilde{\phi})] - \log J[\tilde{\phi}]$$

The algorithm

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

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



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

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

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

this is the expensive part

The algorithm

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

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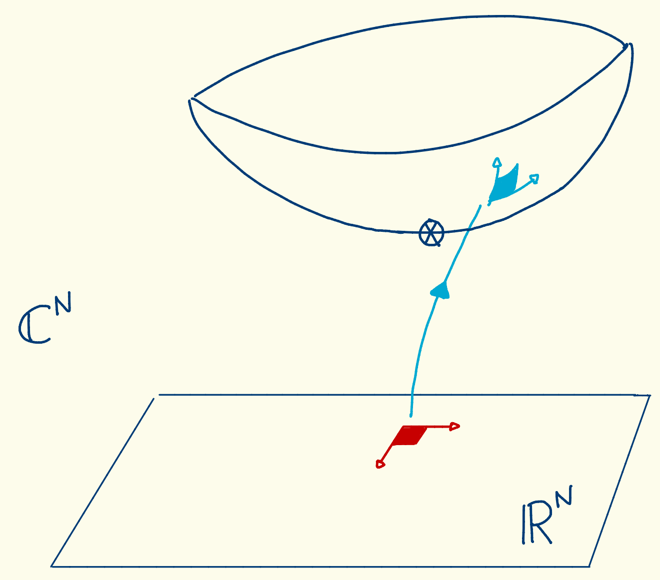


our algorithm

=

Metropolis in the real space,

action S_{eff} and

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

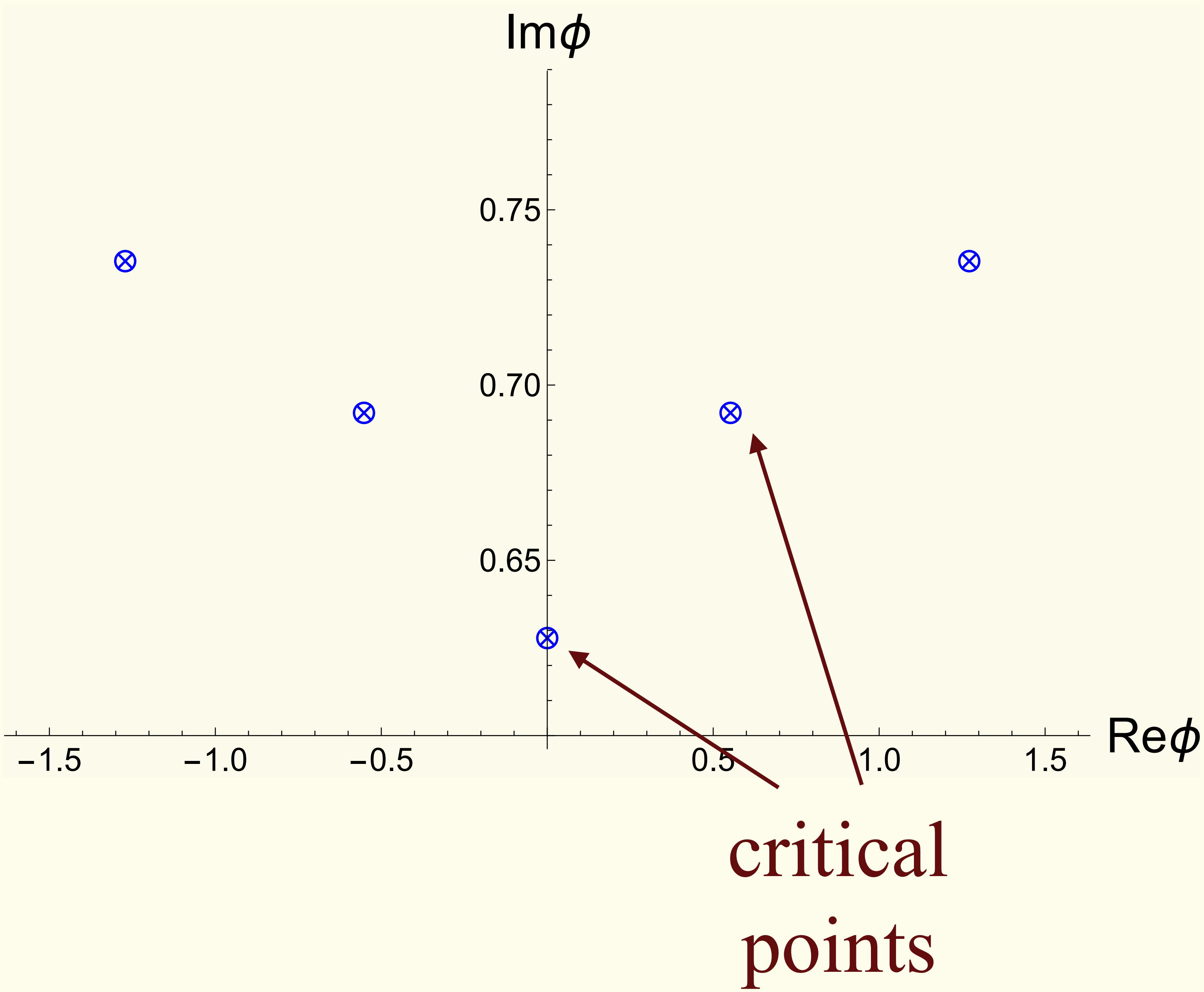
Case study 1: massive Thirring model at finite density (and temperature)

Relativistic fermions with $\bar{\psi}\gamma_\mu\psi\bar{\psi}\gamma_\mu\psi$ interaction

discretization:

Wilson and staggered
auxiliary field A_μ periodic
$e^{iA\mu}$ in links

A projection of the thimbles: $\phi = \frac{1}{L^2} \sum_x A_0(x)$



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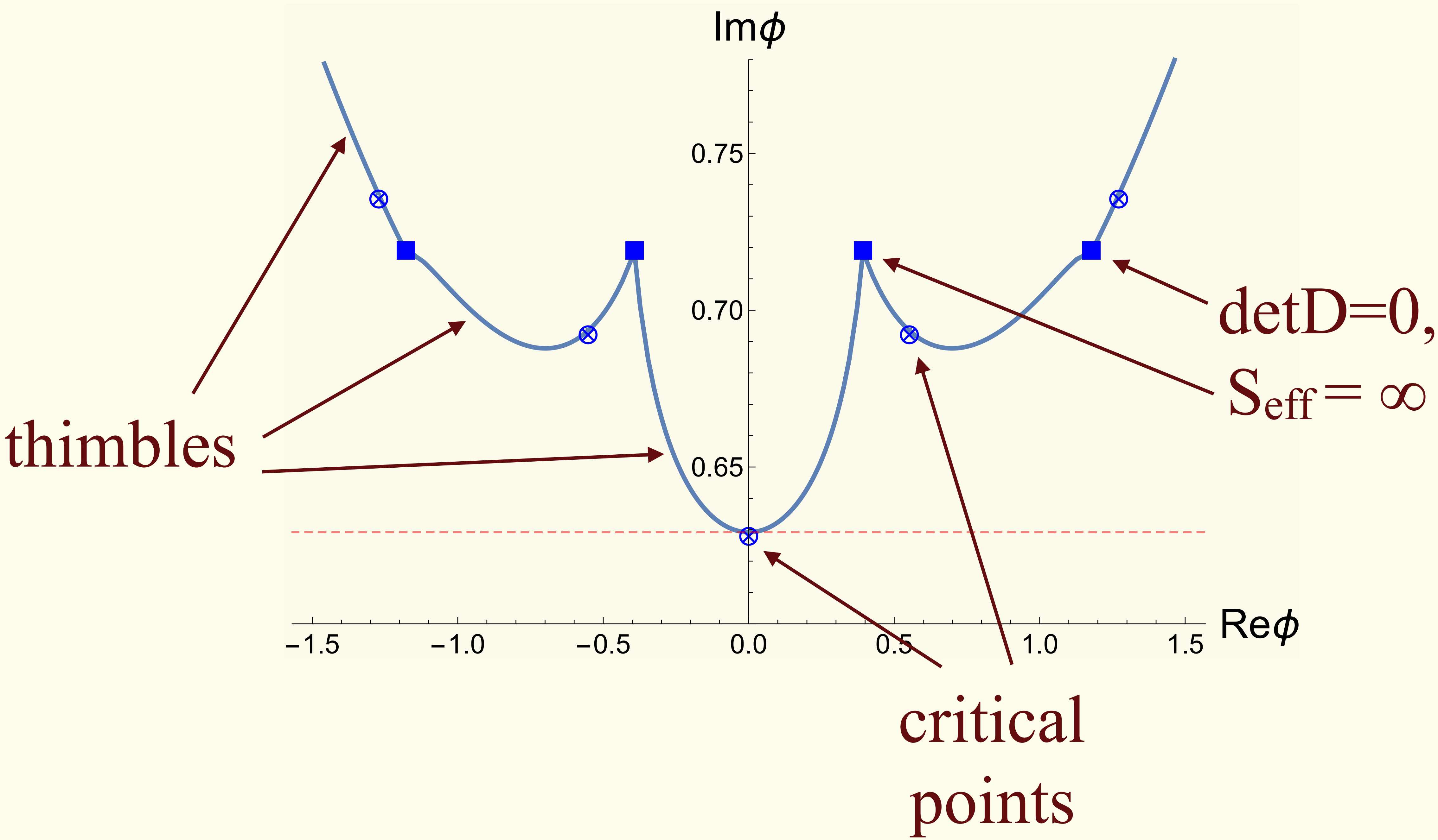
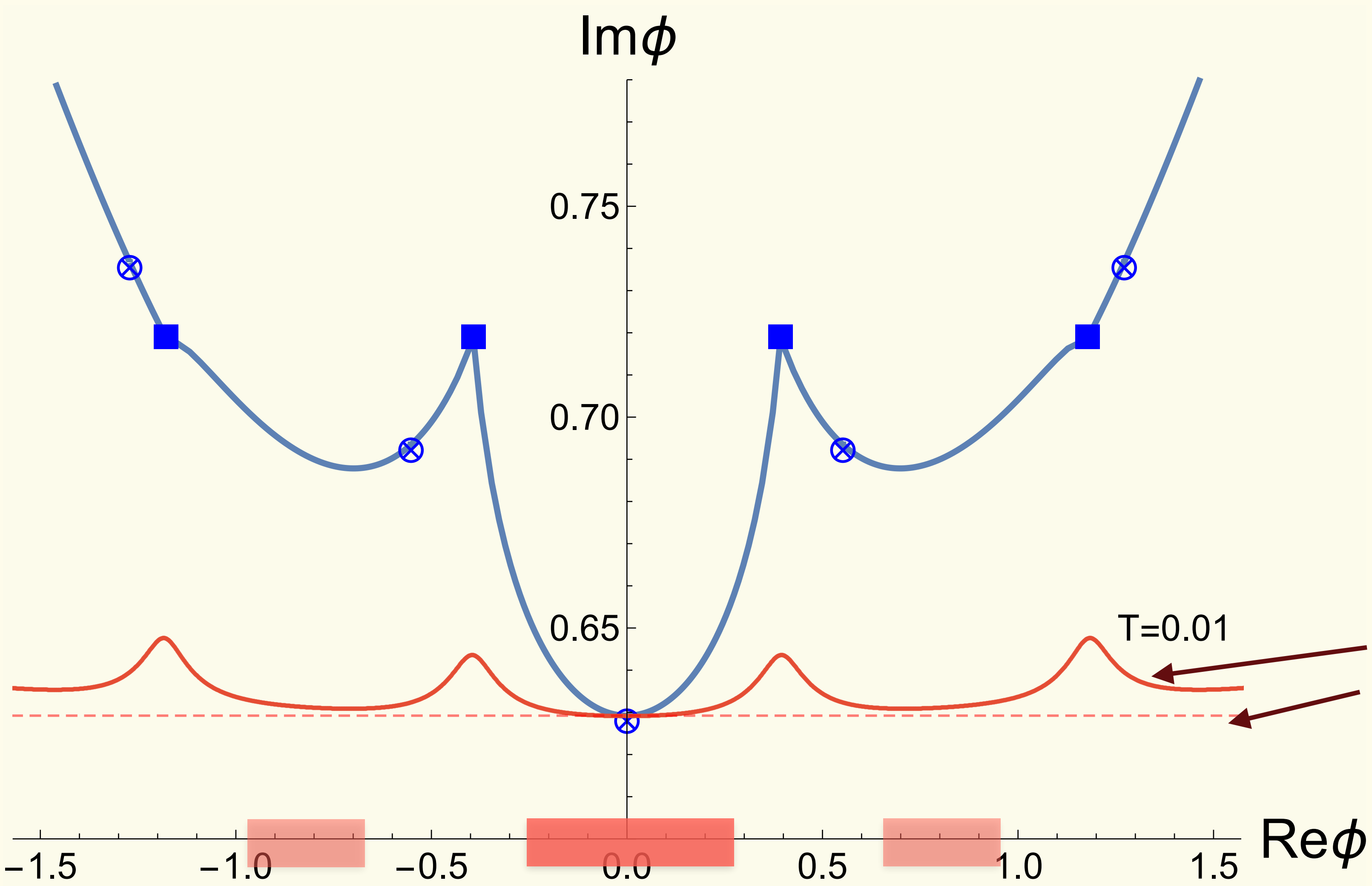
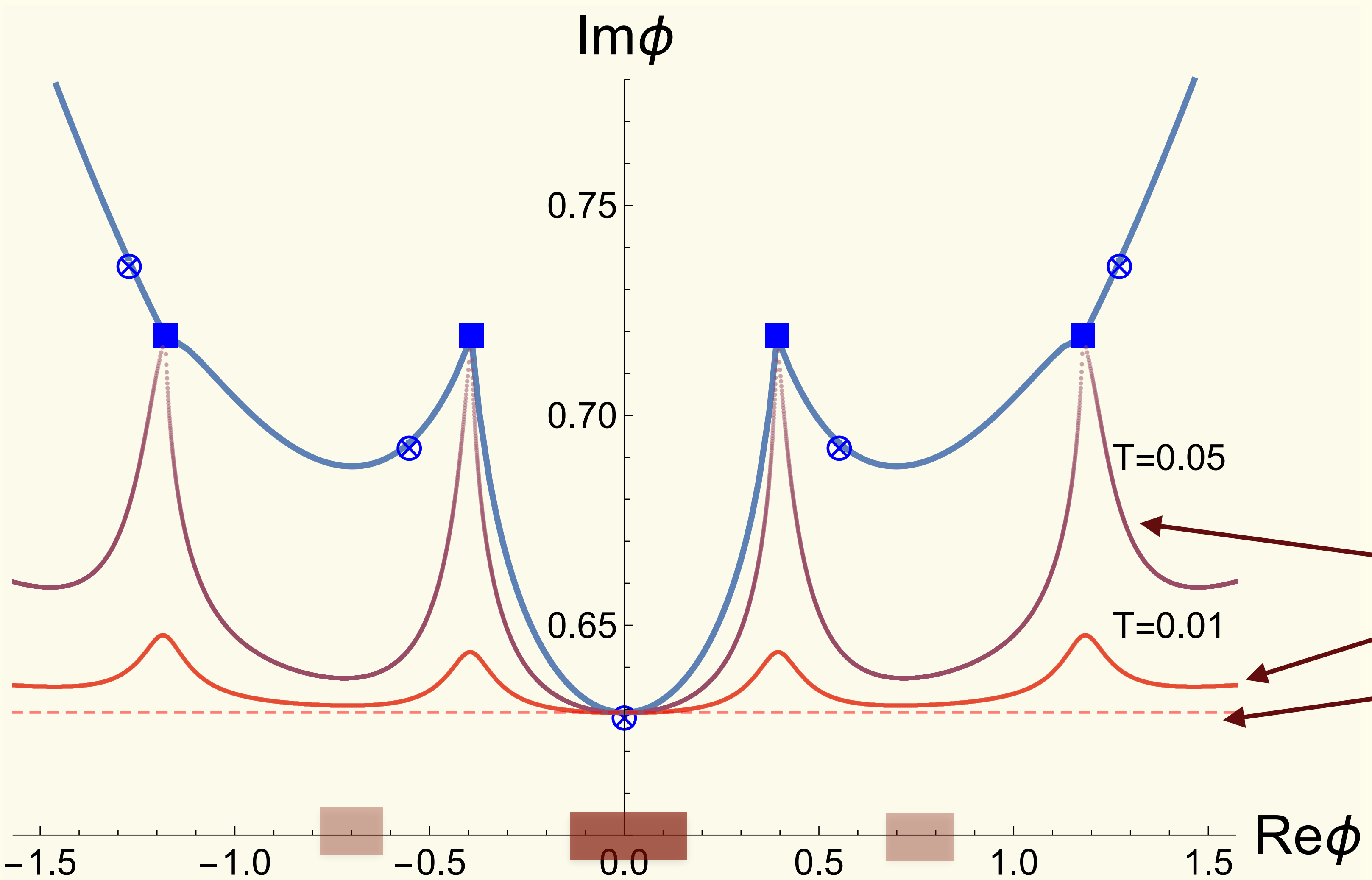


A projection of the thimbles: $\phi = \frac{1}{L^2} \sum_x A_0(x)$



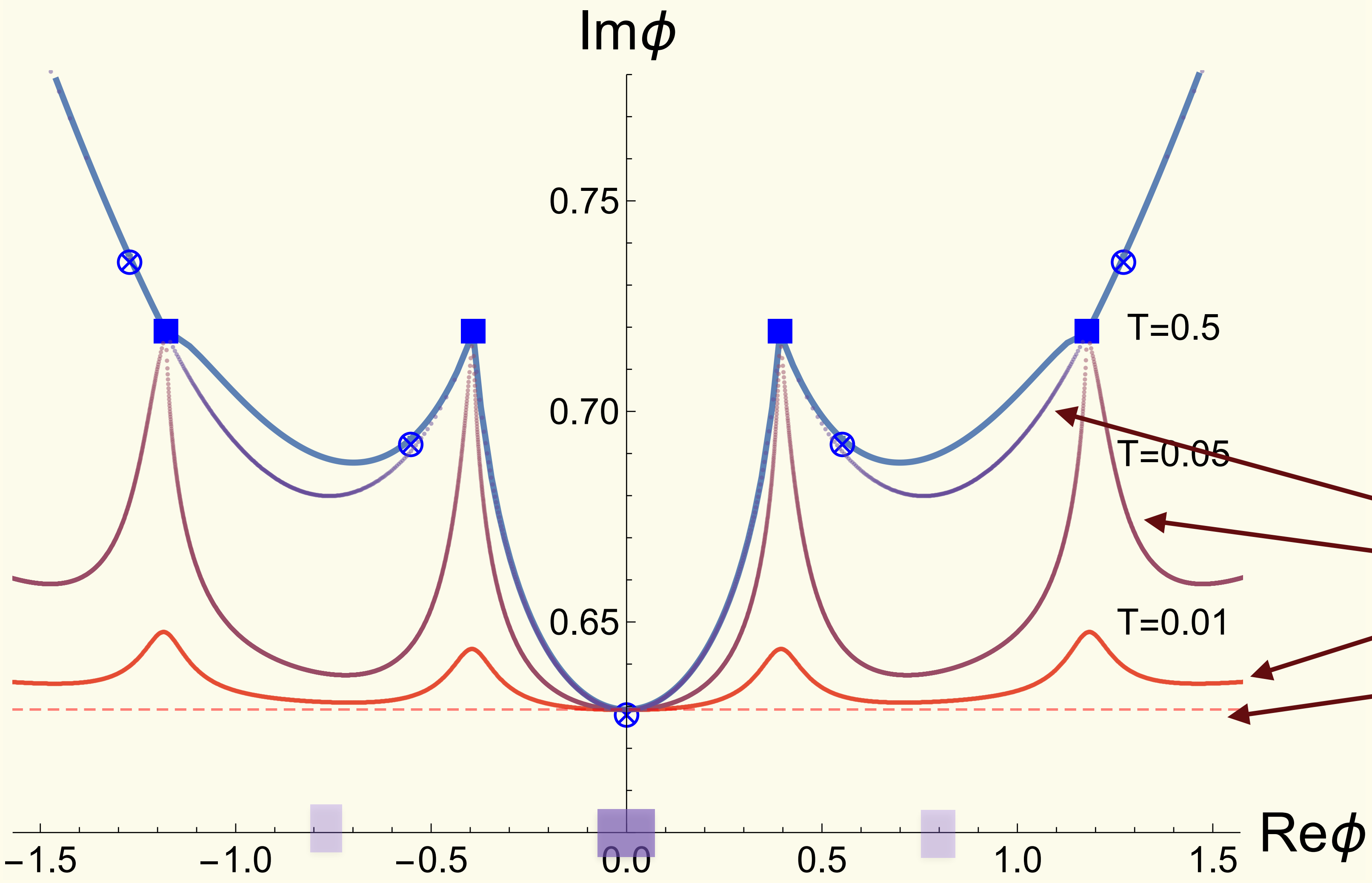
same homological class

A projection of the thimbles: $\phi = \frac{1}{L^2} \sum_x A_0(x)$



flowed tangent space

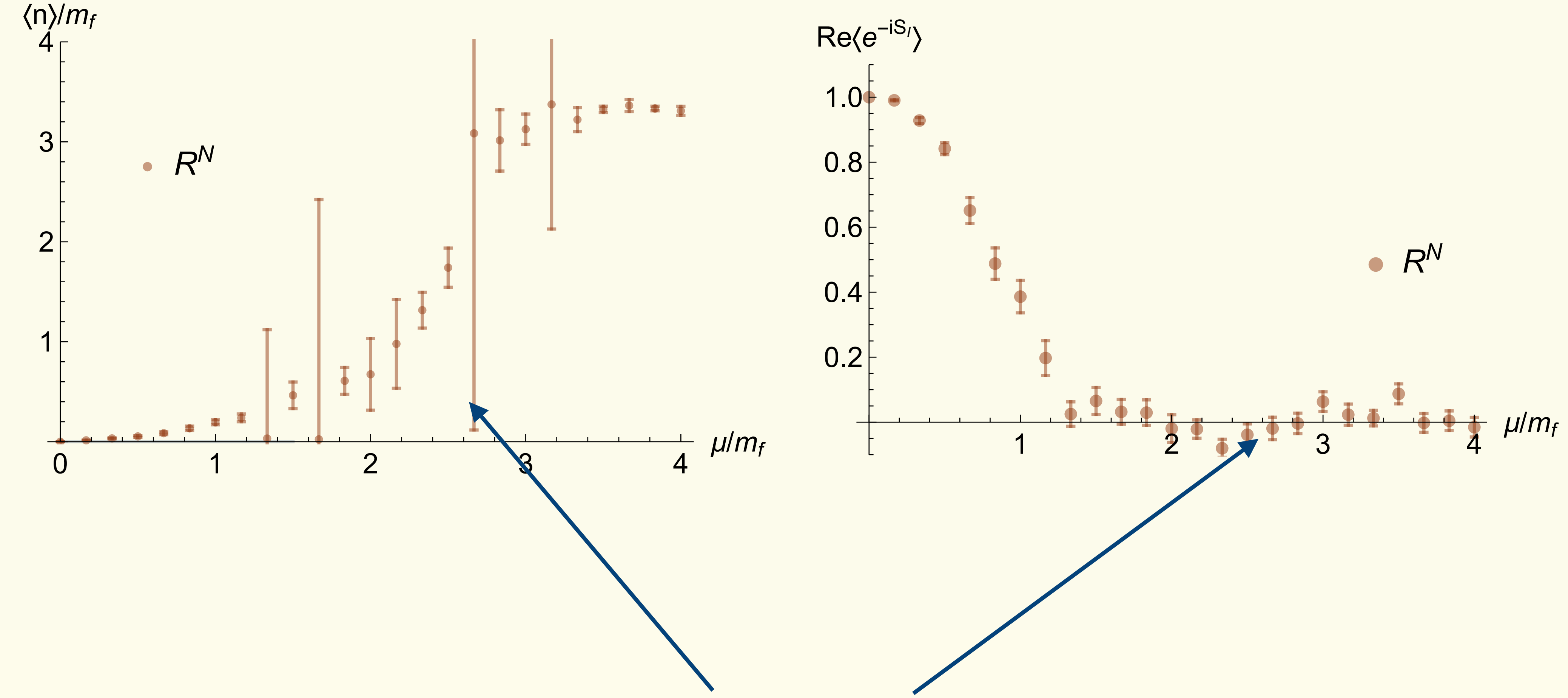
A projection of the thimbles: $\phi = \frac{1}{L^2}\sum_x A_0(x)$



flowed tangent space

Case study: massive Thirring model

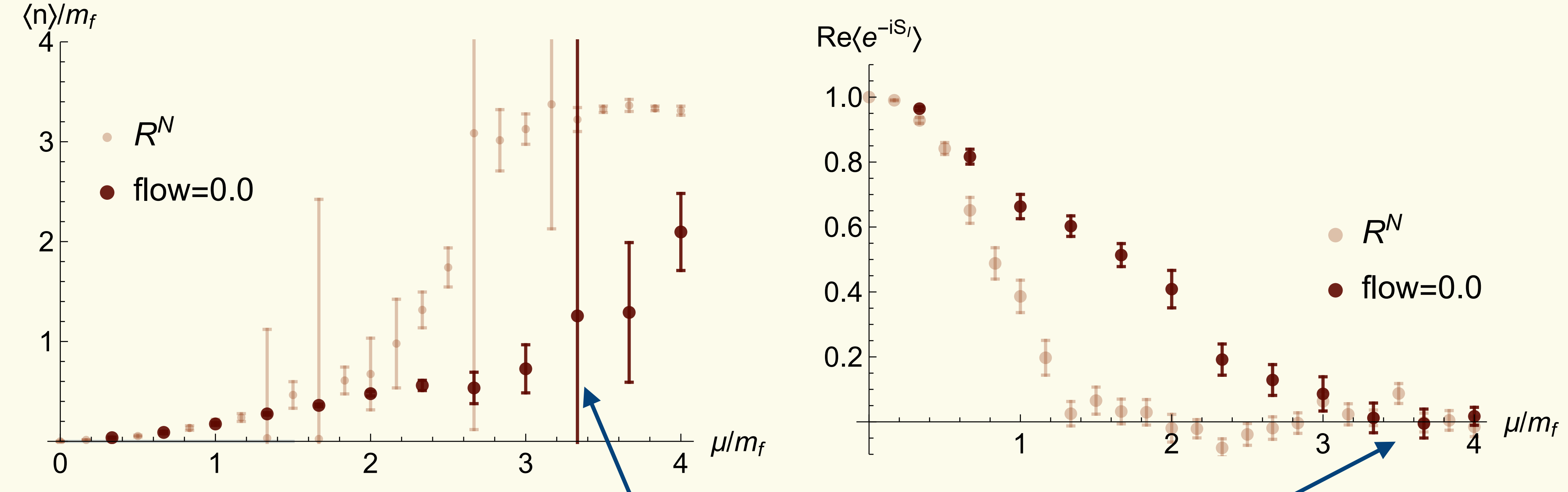
Wilson, 10 x10 lattice, N_F=2, am_f=0.3



sign problem

Case study: massive Thirring model

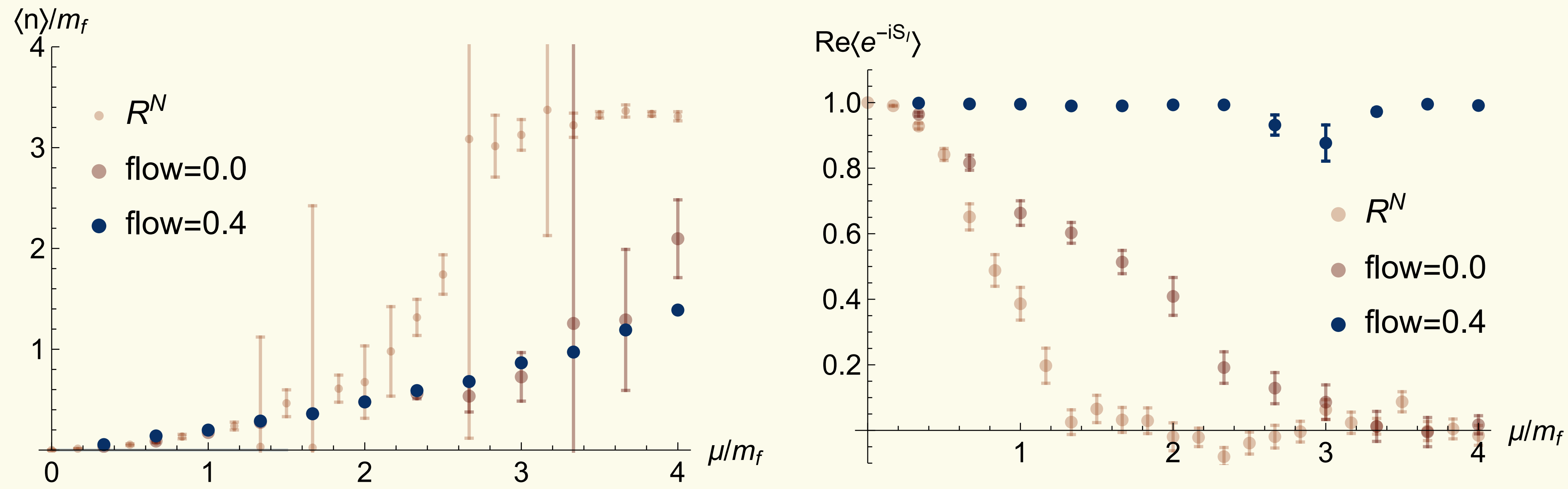
Wilson, 10 x10 lattice, N_F=2, am_f=0.3



sign problem
improved

Case study: massive Thirring model

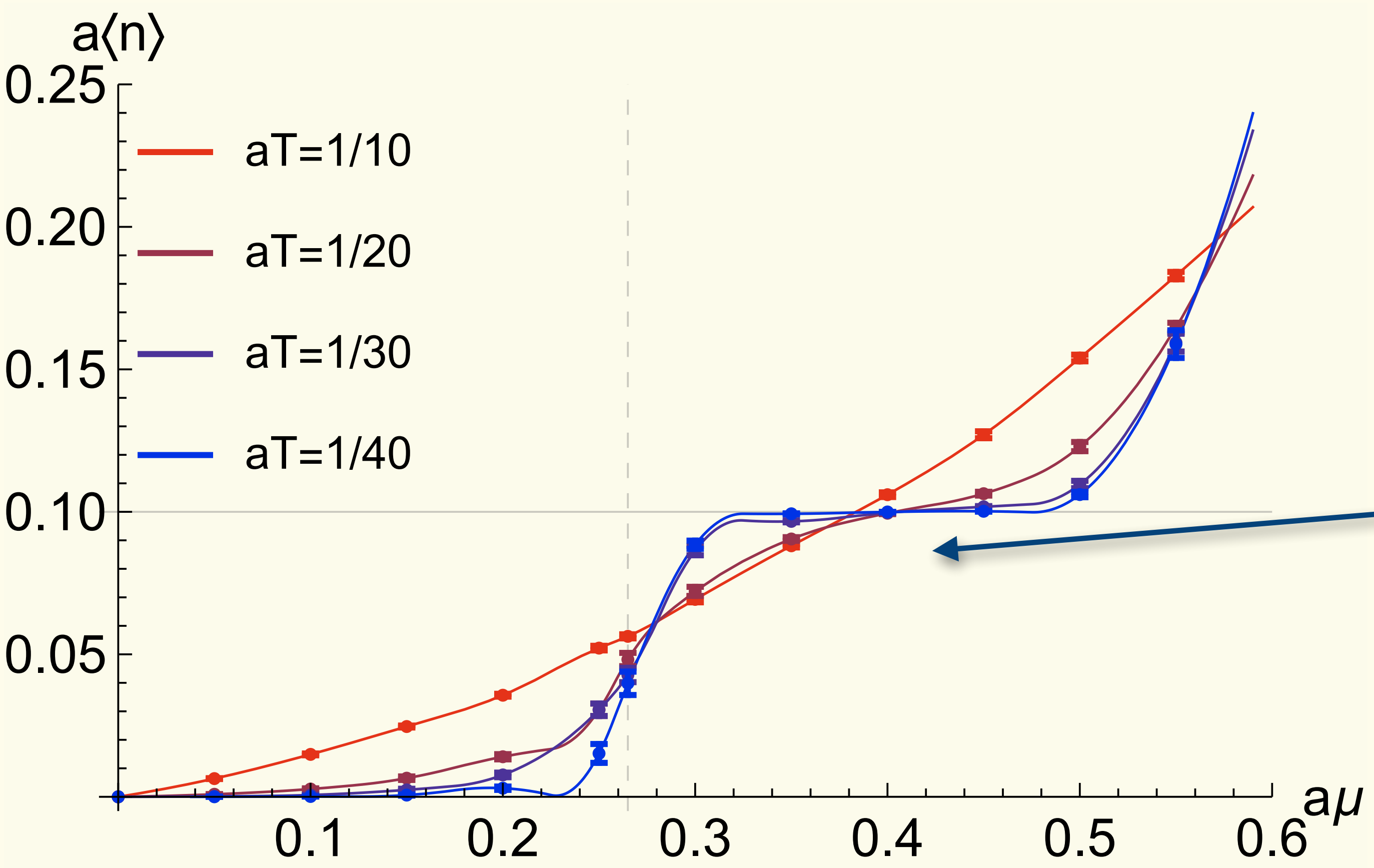
Wilson, 10 x10 lattice, $N_F=2$, $am_f=0.3$



flow done with estimators for the jacobian
(difference reweighted)
no sign problem

Case study: massive Thirring model

Staggered, N_F=2, am_f=0.265

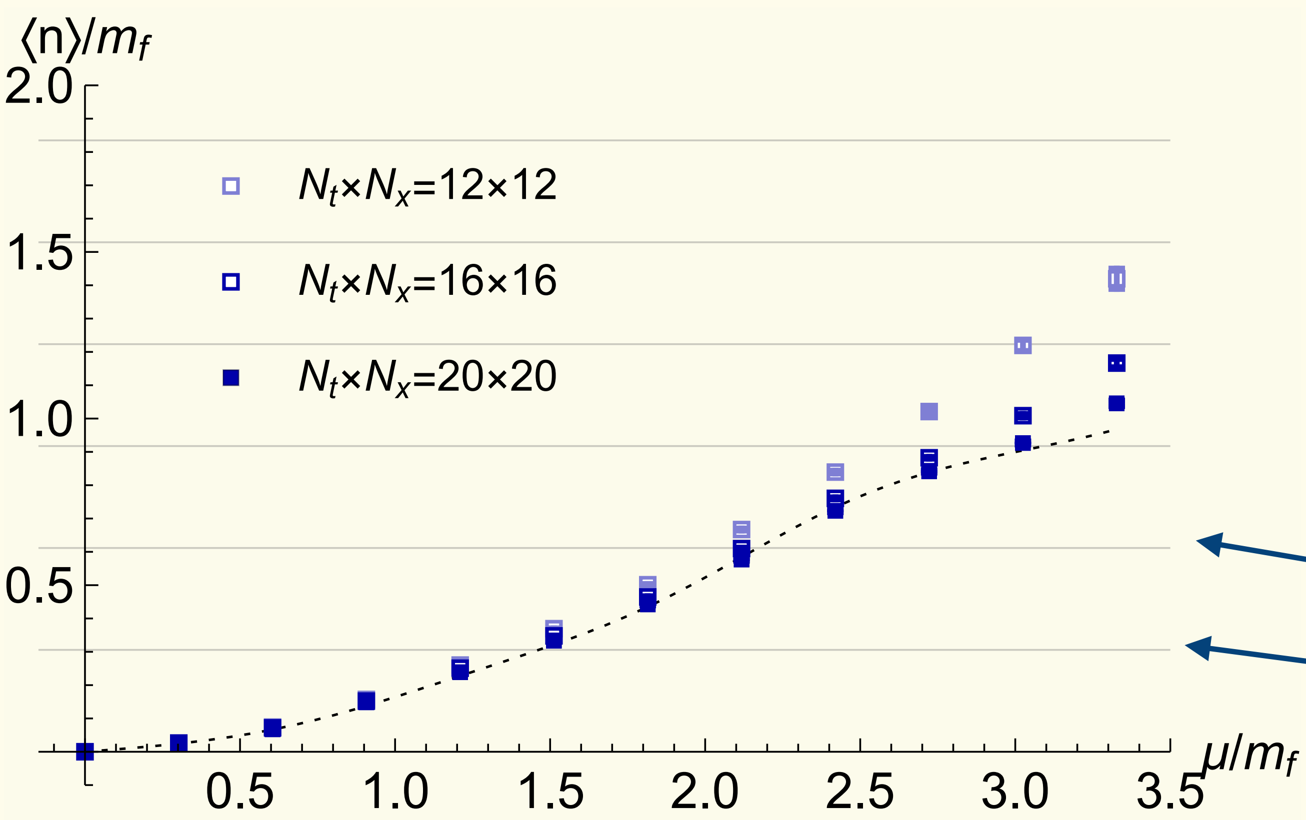


step is missed in a one thimble calculation

cold limit

Case study: massive Thirring model

Staggered, N_F=2, T/m_f=0.302, $m_f L$=3.31

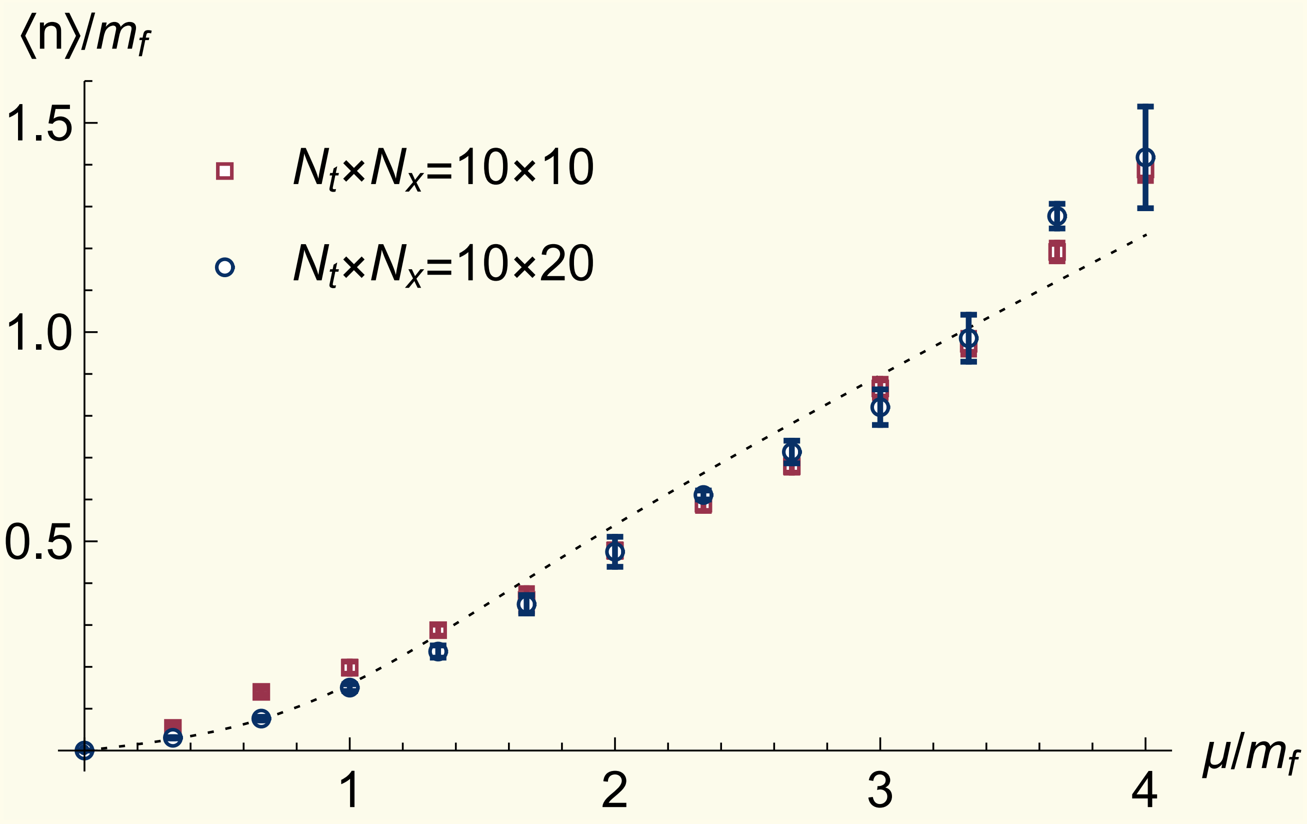


integer particle number

continuum limit

Case study: massive Thirring model

Staggered, N_F=2, T/m_f=0.302

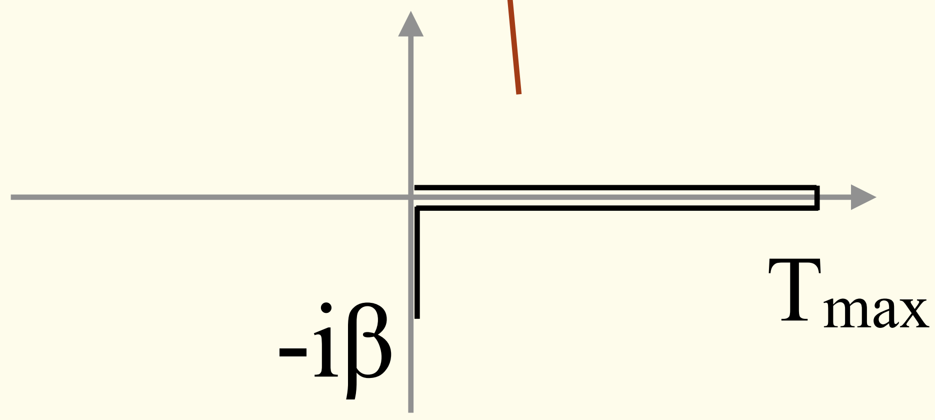


thermodynamic limit

Test case: Real Time Dynamics

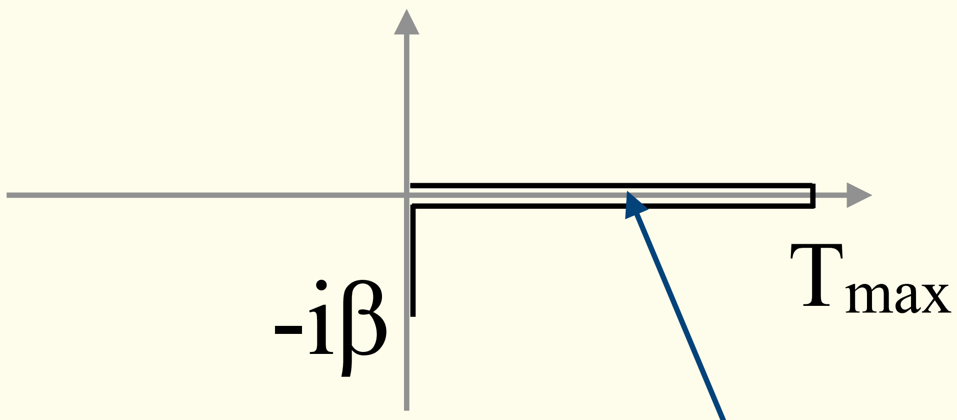
Viscosities, conductivities, … require:

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



Schwinger-Keldish contour

Test case: The Sign Problem from Hell



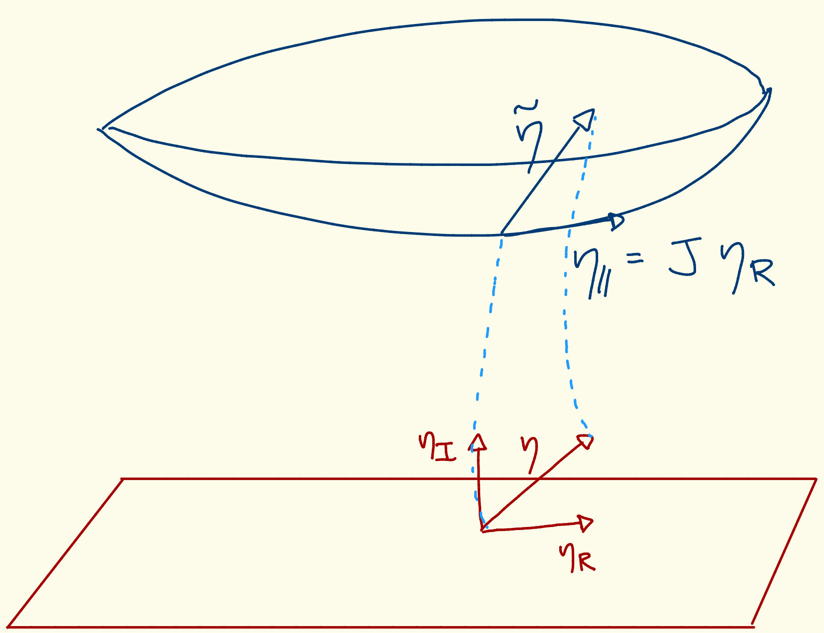
field at a point in the real axis does not contribute to the damping factor in e^{iSc}

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

Problems

- tangent space in wrong homology class
- large flow needed (from R^N)
- jacobian expensive
- anisotropic proposals

"Grady algorithm" for the jacobian (Grady '85, Creutz '92)

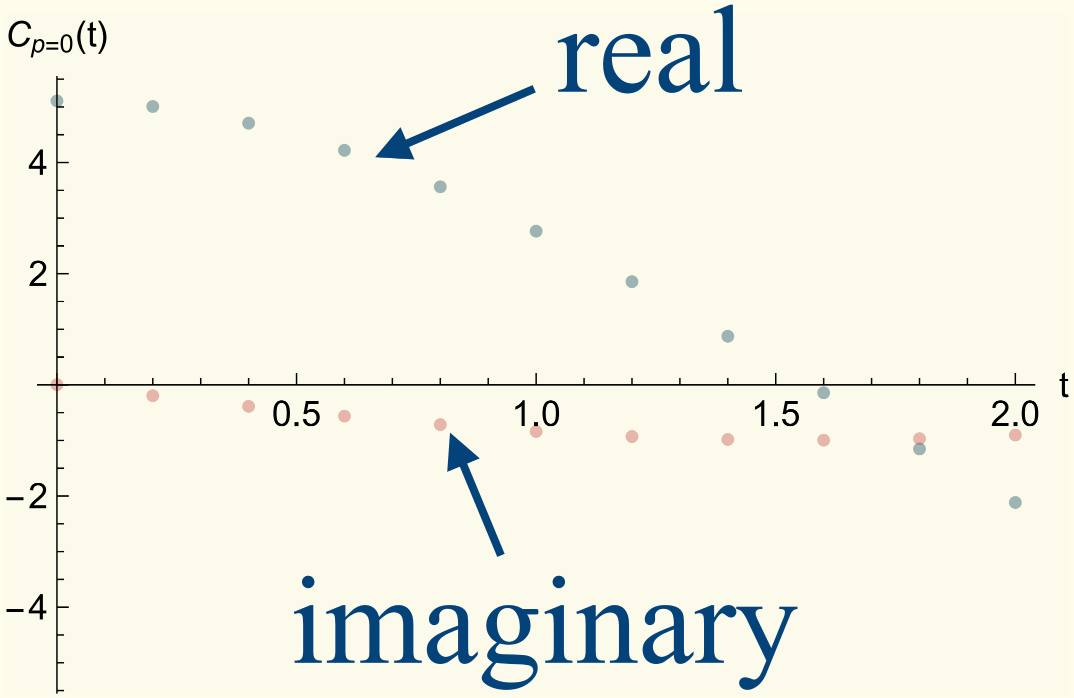


$$J_0\eta = \tilde{\eta} \qquad \tilde{\eta}_{\parallel} = J_0 Re(\eta)$$

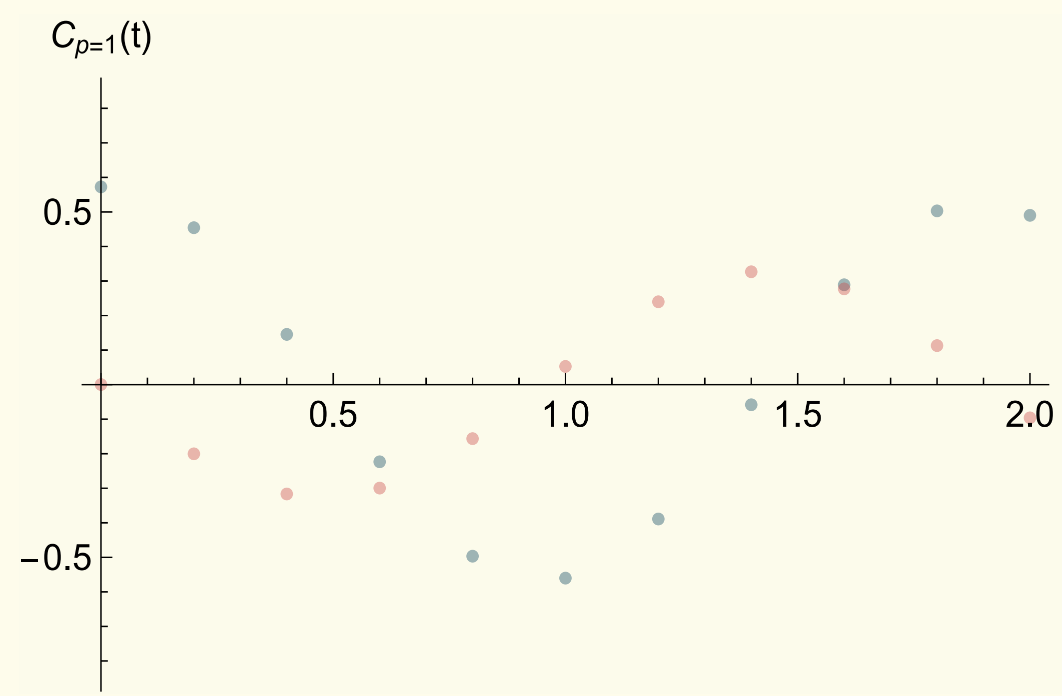
- isotropic proposal
- no need to compute $\det(J_0)$

1+1D φ^4: n_t=10, n_x=10, n_β=2, λ=0.1

weak coupling



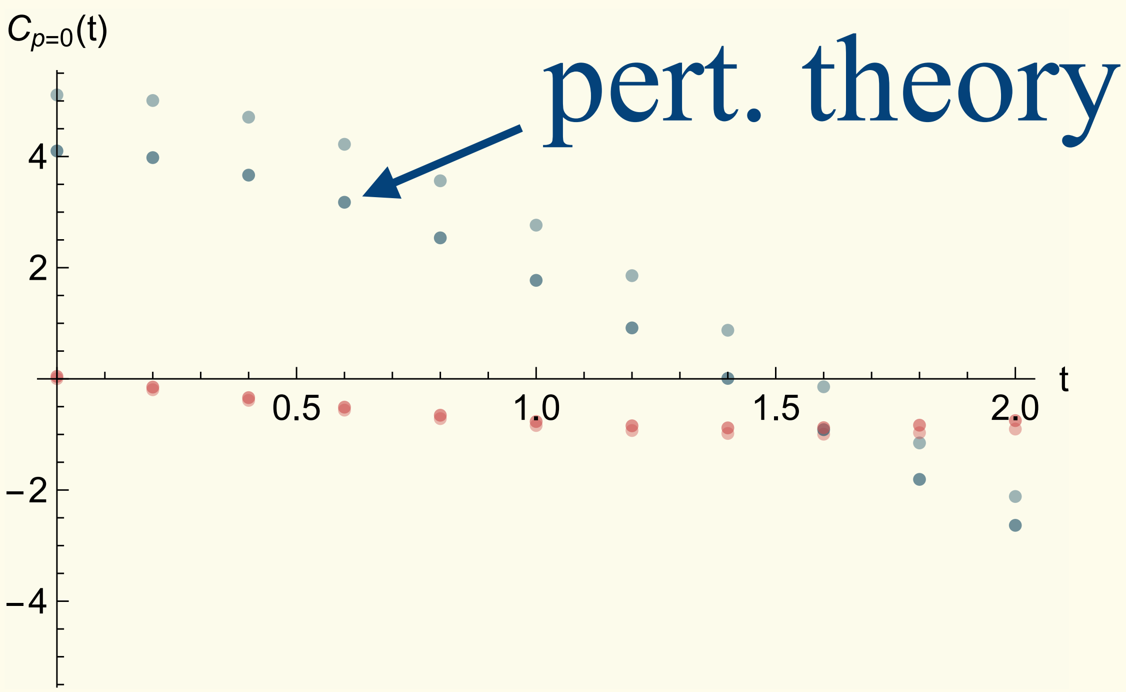
p=0

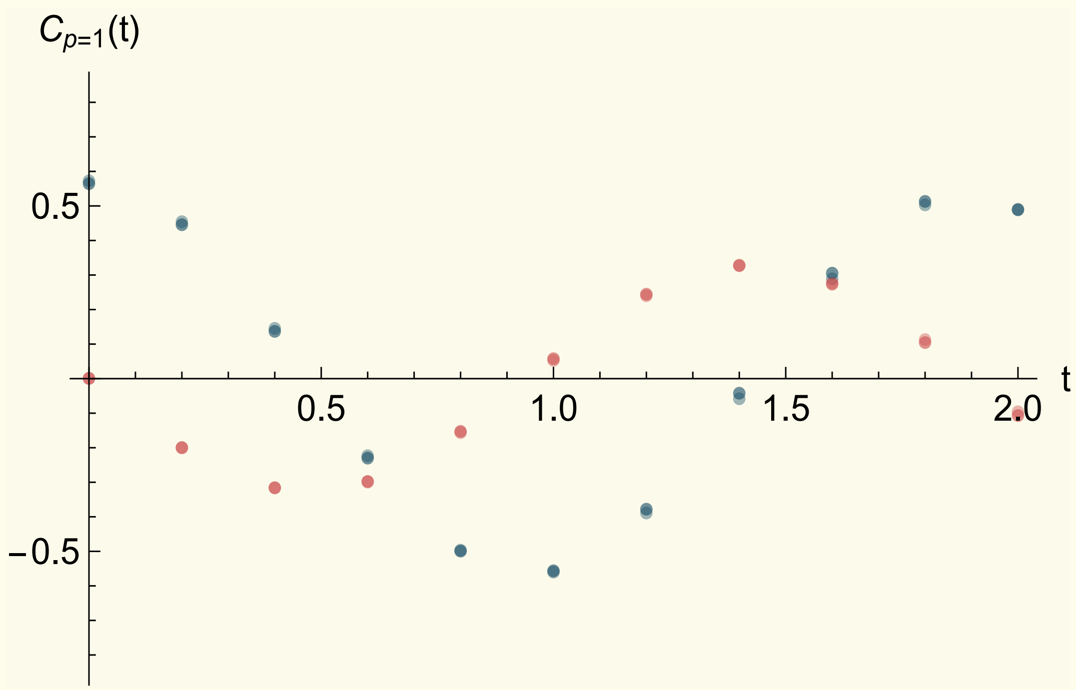


p=2π/L

1+1D φ^4: $n_t=10$, $n_x=10$, $n_\beta=2$, $\lambda=0.1$

weak coupling



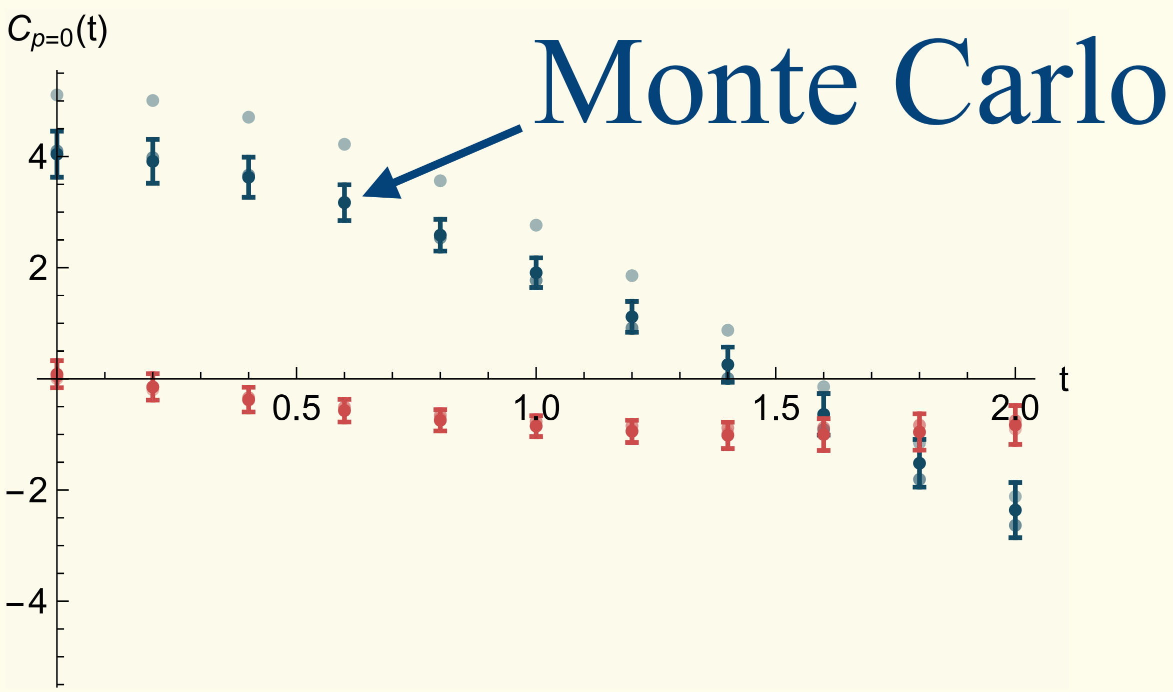


$p=0$

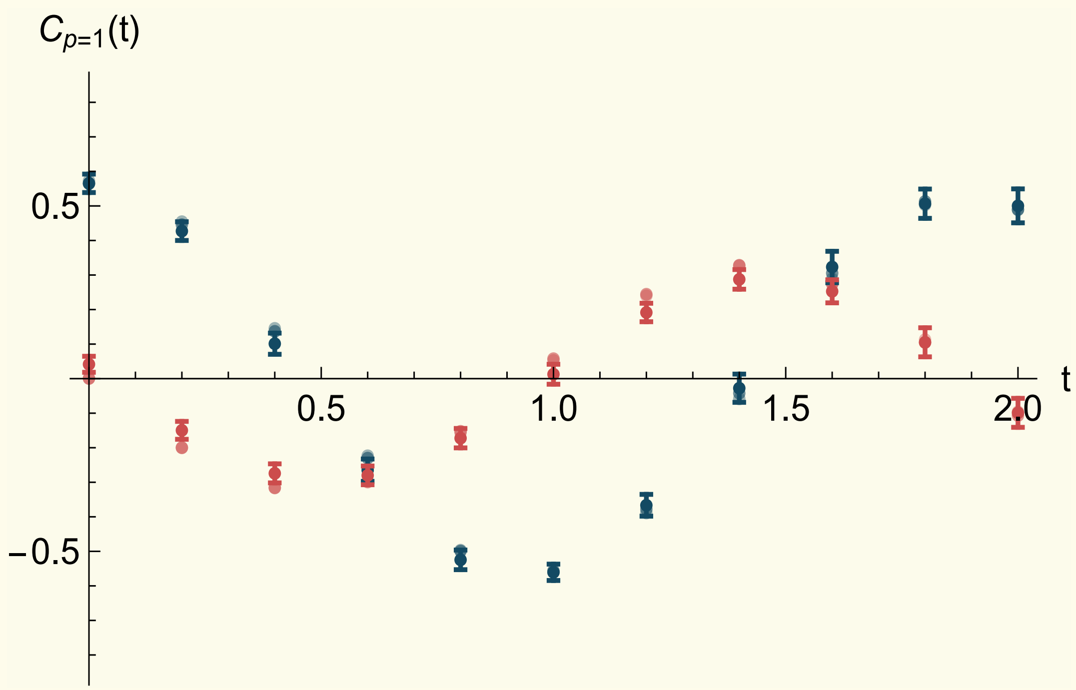
$p=2\pi/L$

1+1D φ^4: n_t=10, n_x=10, n_β=2, λ=0.1

weak coupling



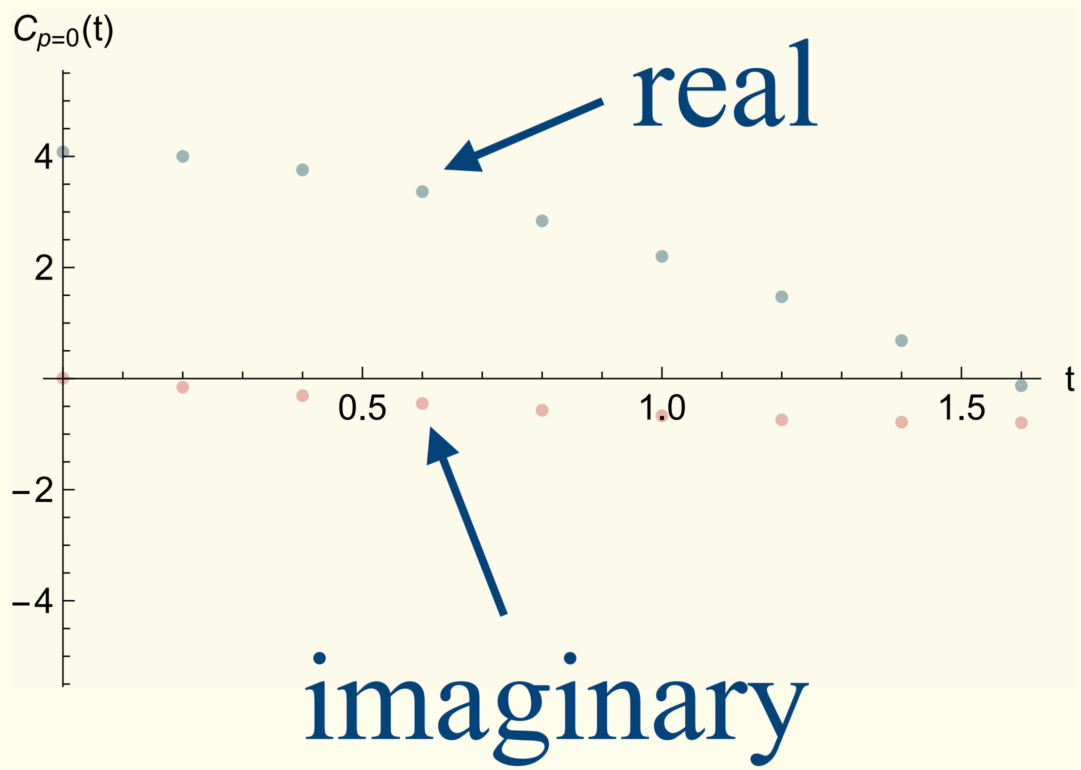
p=0



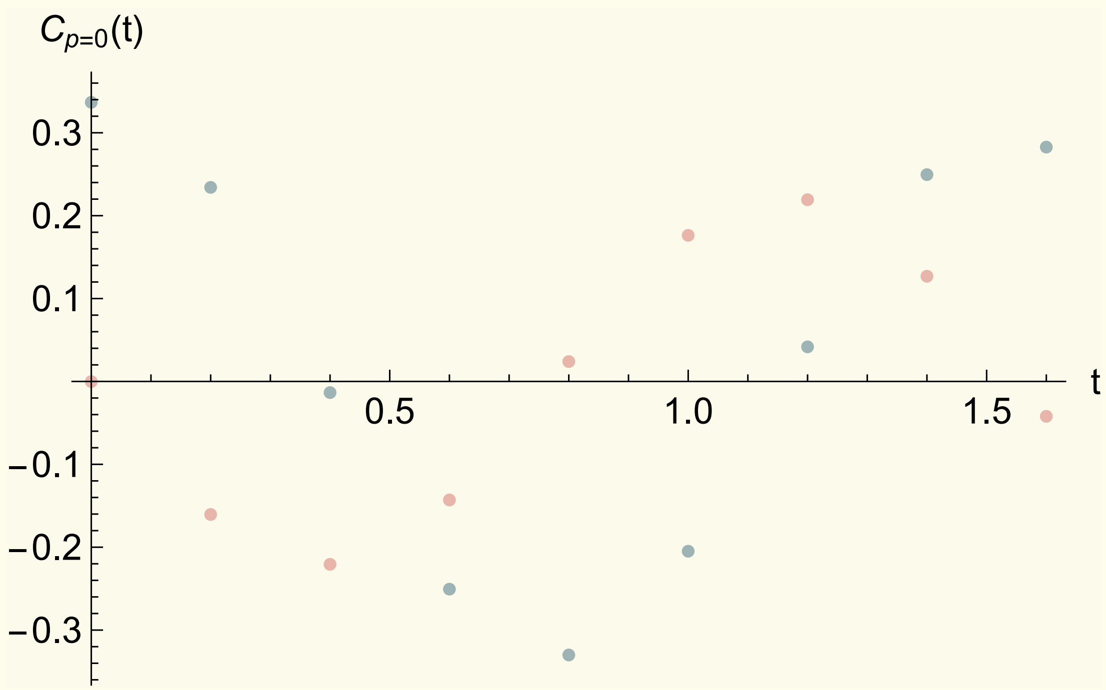
p=2π/L

1+1D φ^4: n_t=10, n_x=10, n_β=2, λ=1.0

strong coupling



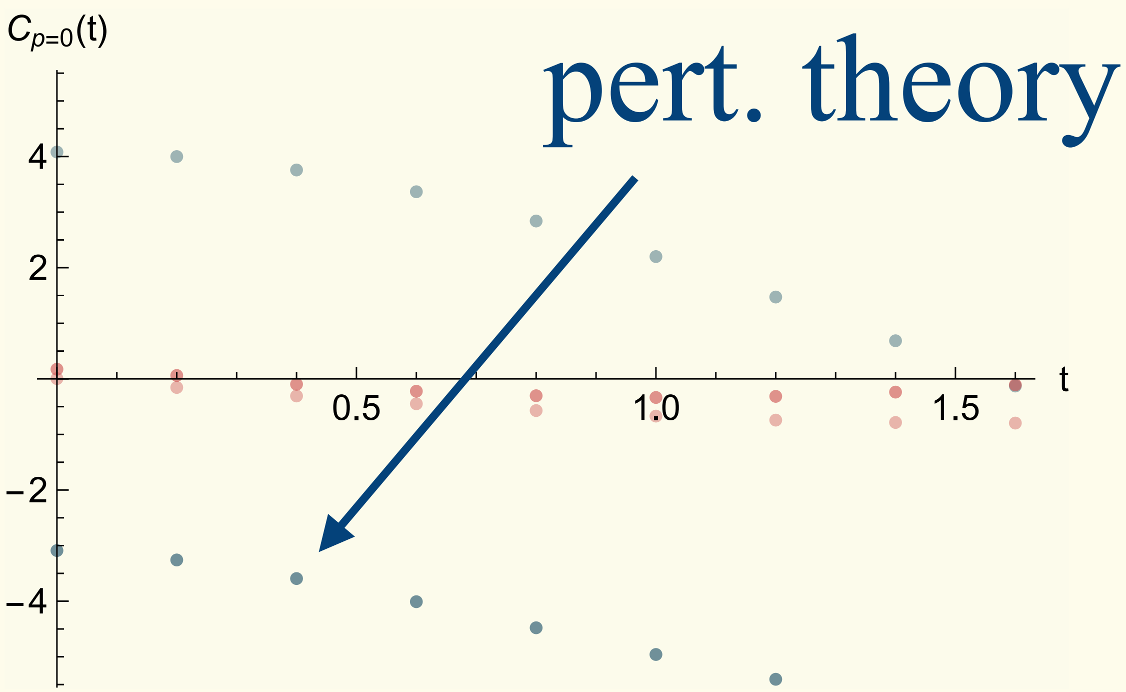
p=0



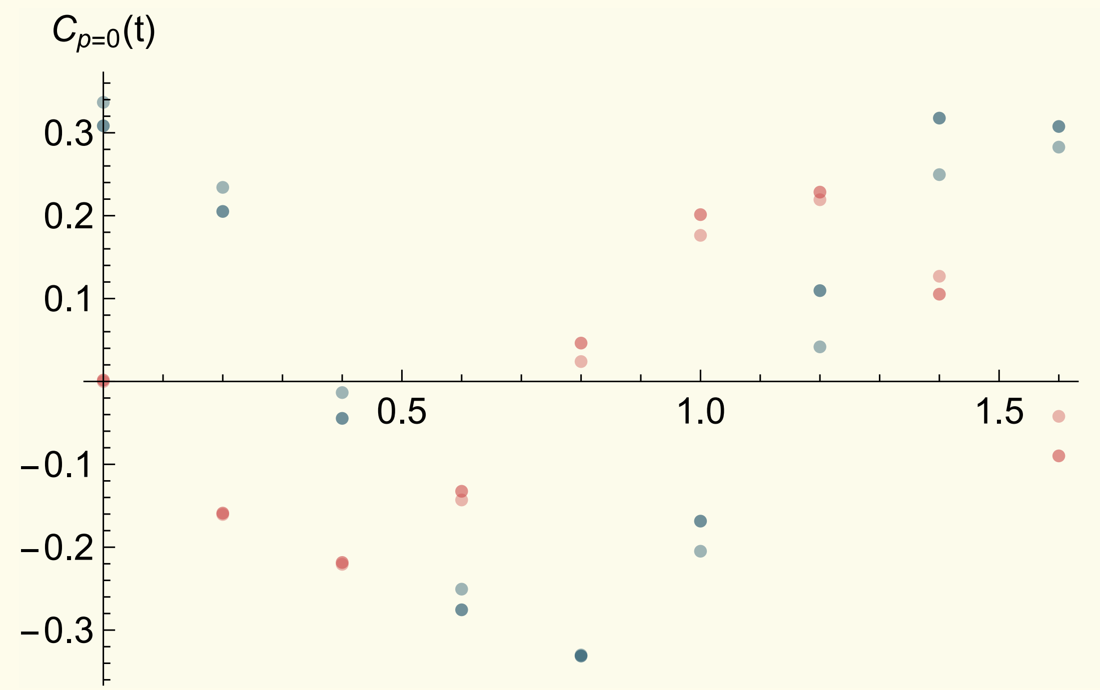
p=2π/L

1+1D φ^4: n_t=10, n_x=10, n_β=2, λ=1.0

strong coupling



p=0



p=2π/L

1+1D φ^4: n_t=10, n_x=10, n_β=2, λ=1.0

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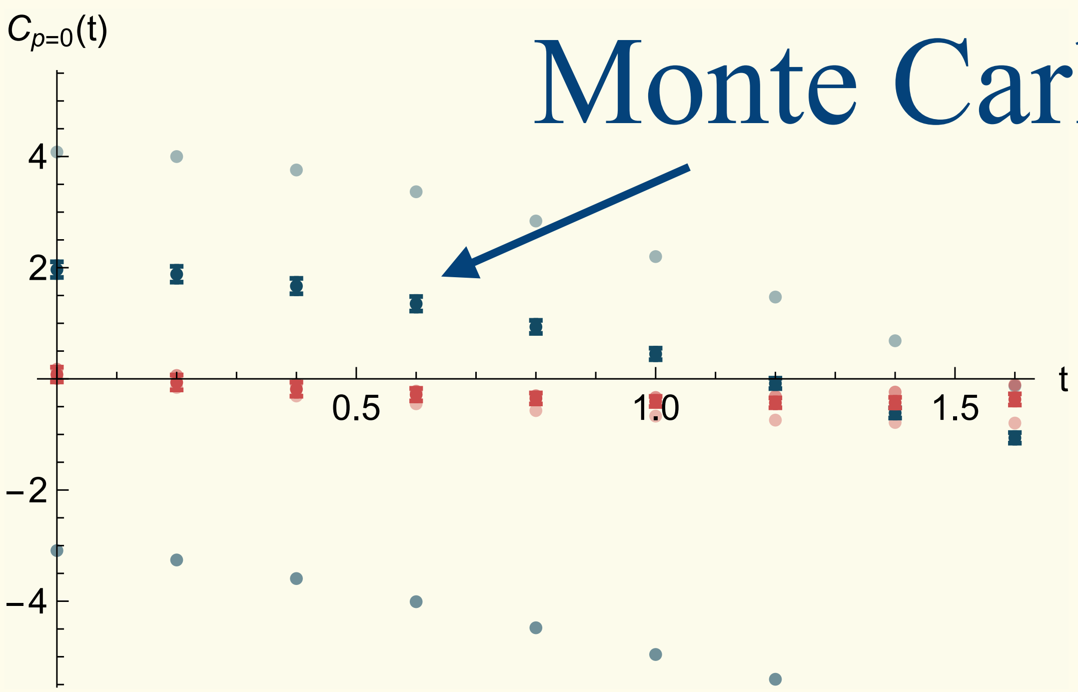
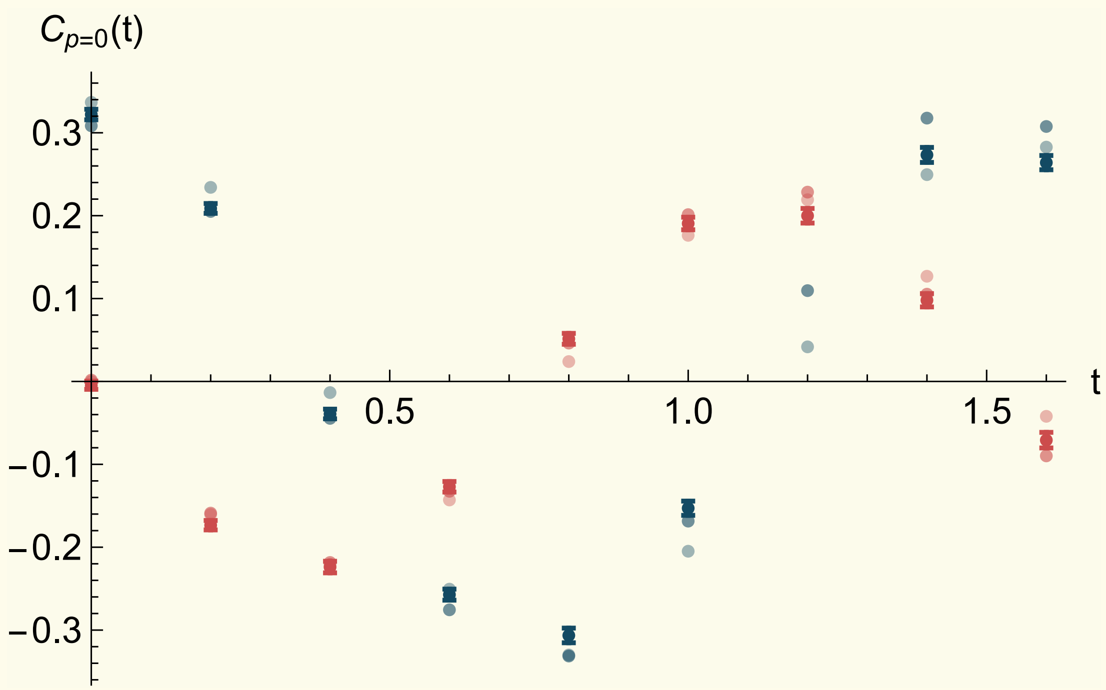


p=0



p=2π/L

To take home:

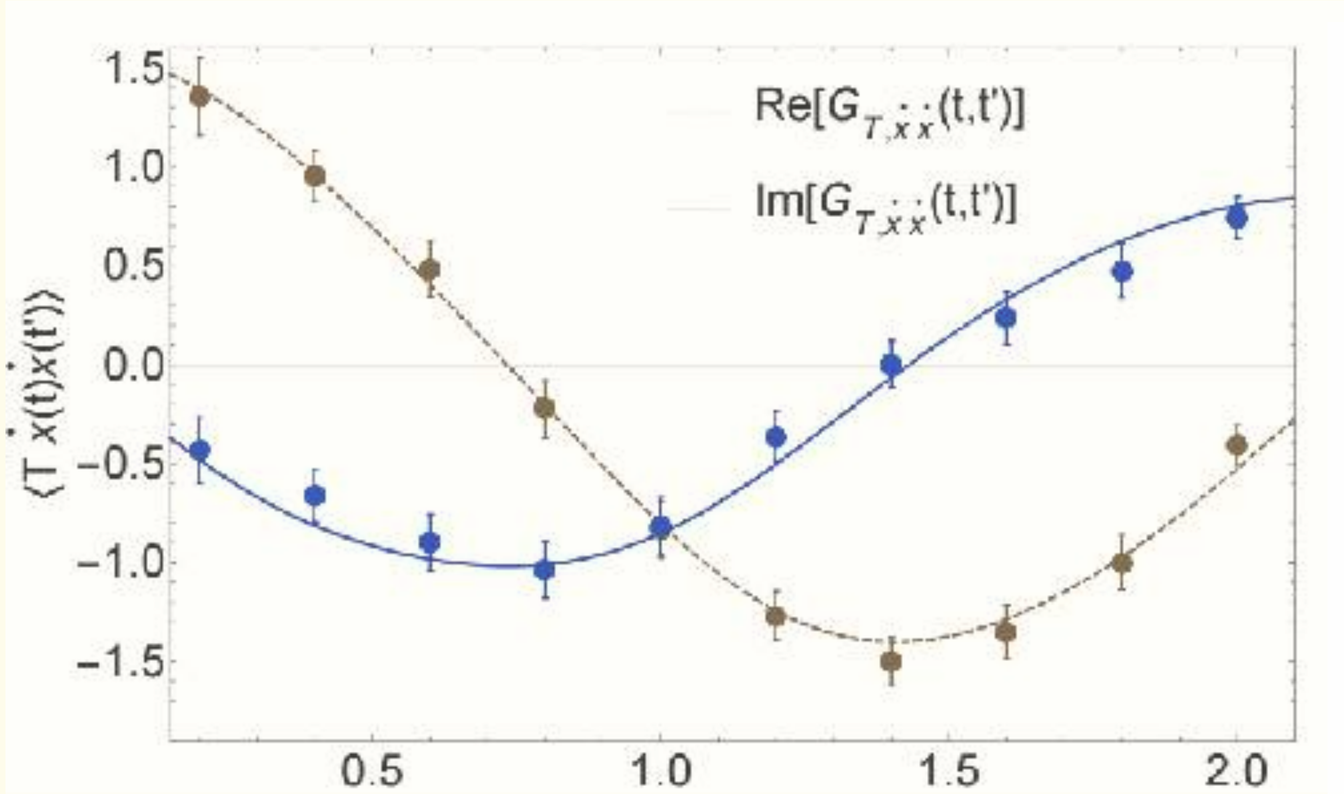
- Deforming the integration on complex space is a good thing
- Thimbles are just one possibility
- Jacobians are expensive: estimators, “Grady-style” algorithm, ansatze, alternative flows, machine learned manifolds, …
- Better proposals: solved at weak coupling, “Grady-style”
- Trapping: two tempered MC’s (*Fukuma&Masafumi `17, Alexandru et al. `17*), different parametrization

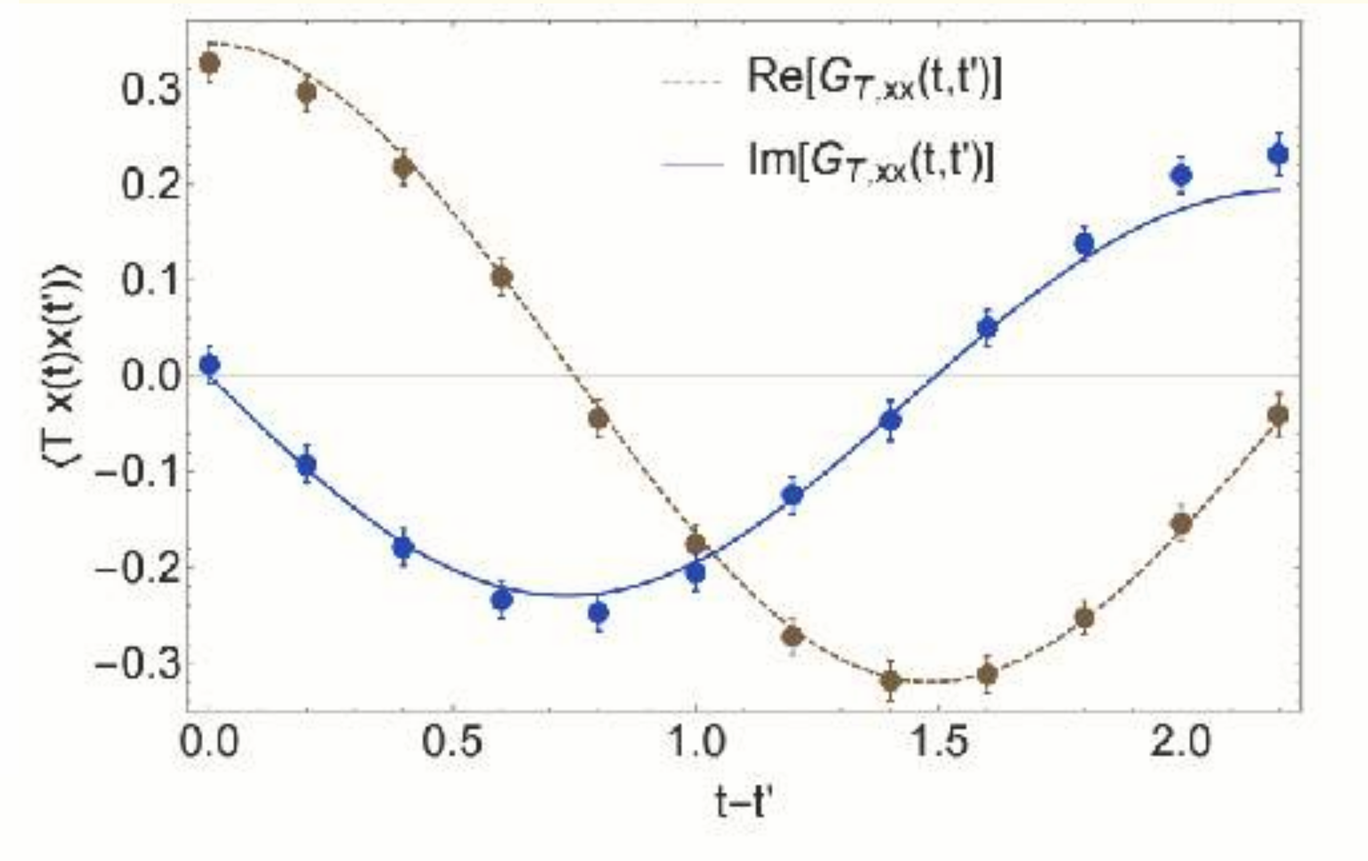
ECT* workshop

"Simulating QCD on Lefschetz thimbles"

Trento, Italy, June 28-30, 2017

Test case: anharmonic oscillator





Flowing R^N

Very slow convergence

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 ?

Complex Langevin

$$\frac{d\phi_i}{dt} = -\frac{\partial S}{\partial \phi_i} + \eta_i$$

no complex conjugation

random noise

- no general proof of convergence
- recent progress (gauge cooling) *Seiler et al., '12*
- missing phases? *Hayata et al., `15*

Similarities to Complex Langevin

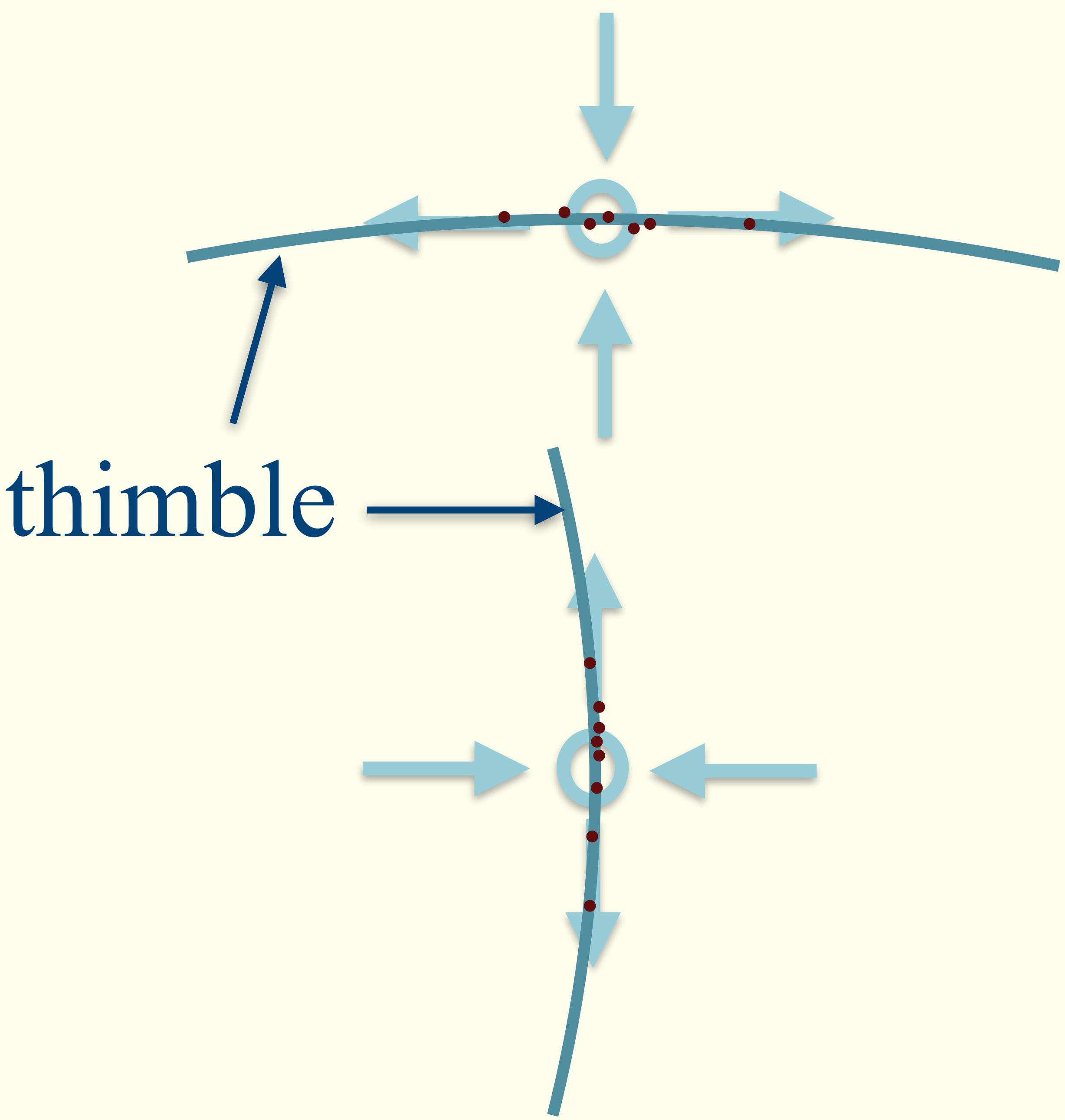
- there are complex things
- there is *a* flow

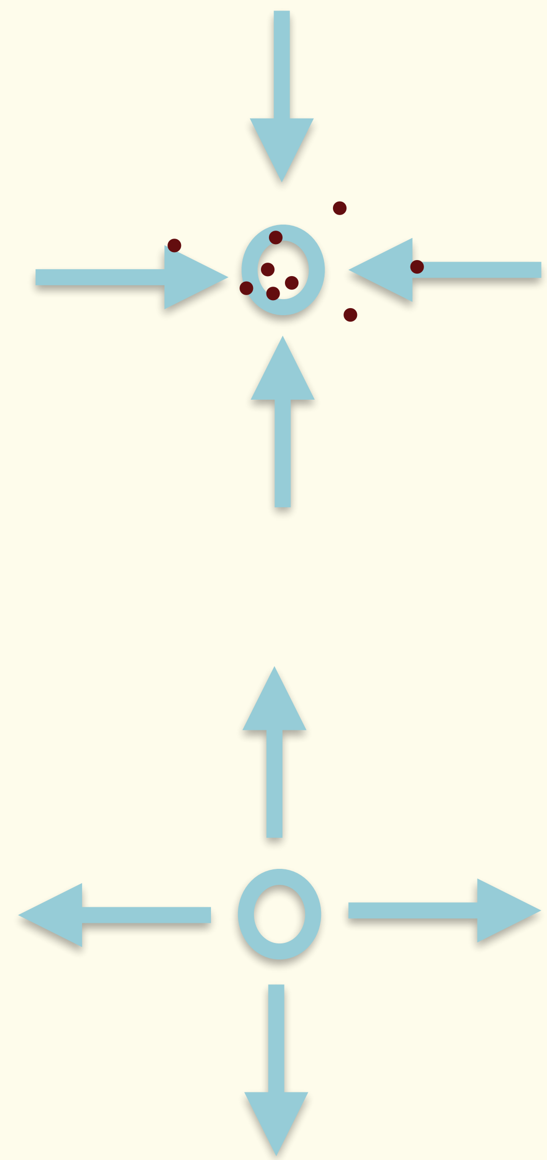
Differences from Complex Langevin

- CL has instabilities
- CL samples along the flow; we sample at the end of a different flow
- CL is not guarantee to converge to the right result
- CL has no trapping
- CL is cheaper (no need to stay on sub manifold)

holomorphic: $\frac{\partial \bar{S}}{\partial \phi_i}$

gradient: $-\frac{\partial S}{\partial \phi_i}$





Case study: massive Thirring model

$$S = \int d^2x \bar{\psi}^a(\gamma_\mu \partial_\mu + \mu\gamma_0 + m)\psi^a + \frac{g^2}{2N_F}\bar{\psi}^a\gamma_\mu\psi^a\bar{\psi}^a\gamma_\mu\psi^a$$

$$\to \frac{N_F}{2g^2}\int d^2x A_\mu A_\mu - N_F \log\det\left(\gamma_\mu(\partial_\mu + A_\mu) + \mu\gamma_0 + m\right)$$