A Complex Path Around the Sign Problem

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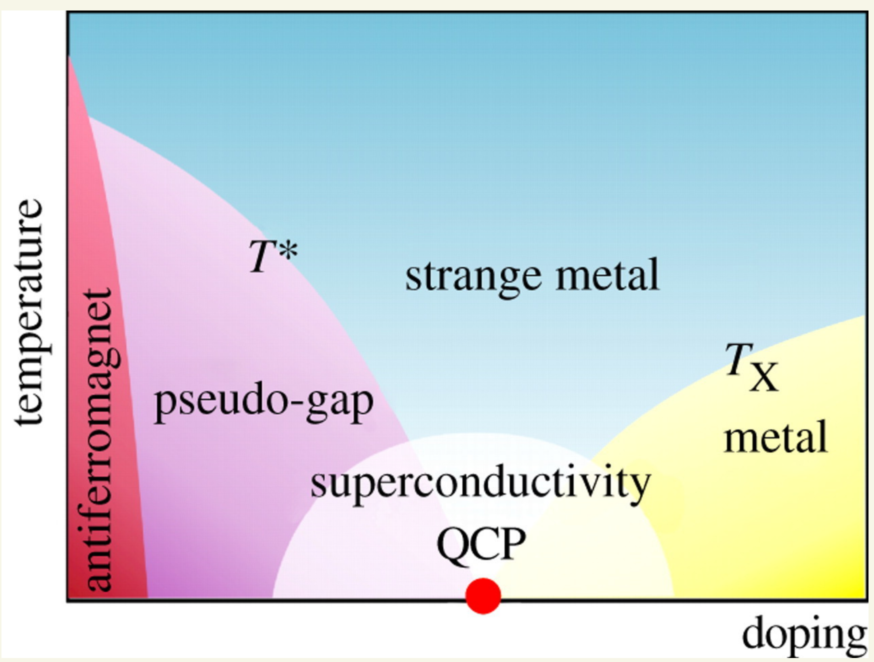
The "sign problem"

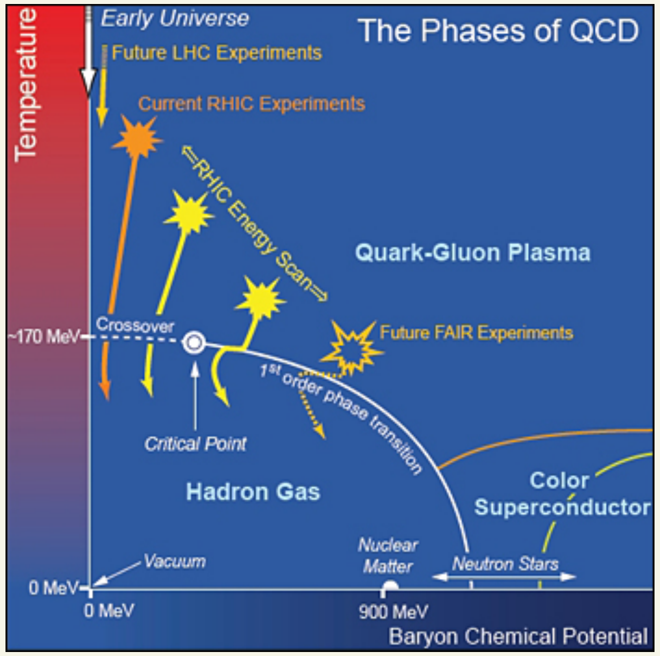
$$\langle \mathcal{O} \rangle = \frac{\int D\phi \ \mathcal{O} e^{-S[\phi]}}{\int D\phi \ e^{-S[\phi]}} \approx \frac{1}{\mathcal{N}} \sum_{n=1}^{\mathcal{N}} \mathcal{O}[\phi]$$

ϕ distributed $\sim e^{-S}$

But S is not real in a number of interesting problems:



Repulsive Hubbard model
away from half filling
(high T_c superconductivity)



QCD at finite baryon density
(neutron stars)

But S is not real in a number of interesting problems:

All "real time" observables like transport coefficients, fully non-equilibrium physics, parton distribution functions, …

$$\langle \mathcal{O}(t)\mathcal{O}(t')\rangle = f(t-t')$$

The "sign problem"

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

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$$\approx \frac{\frac{1}{\mathcal{N}} \sum_{n=1}^{\mathcal{N}} e^{-iS_I[\phi_n]} \mathcal{O}[\phi_n]}{\frac{1}{\mathcal{N}} \sum_{n=1}^{\mathcal{N}} e^{-iS_I[\phi_n]}} = \frac{\langle \mathcal{O} e^{-iS_I} \rangle_{S_R}}{\langle e^{-iS_I} \rangle_{S_R}}$$

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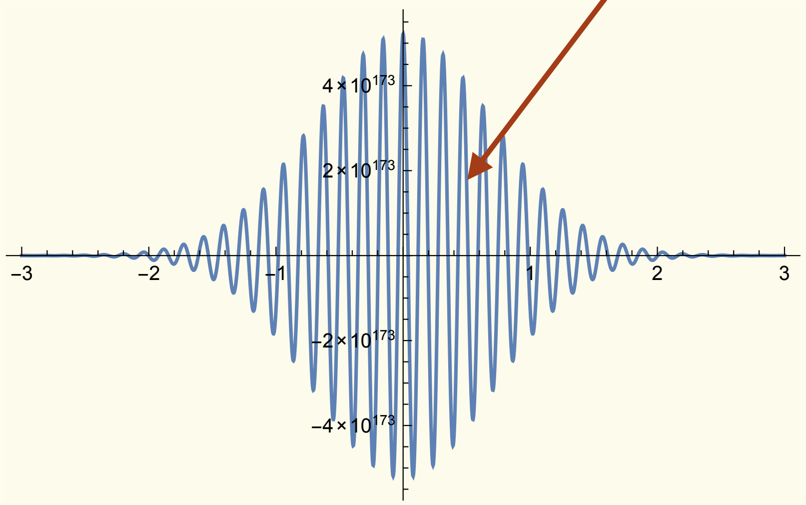
exponentially small on spacetime volume

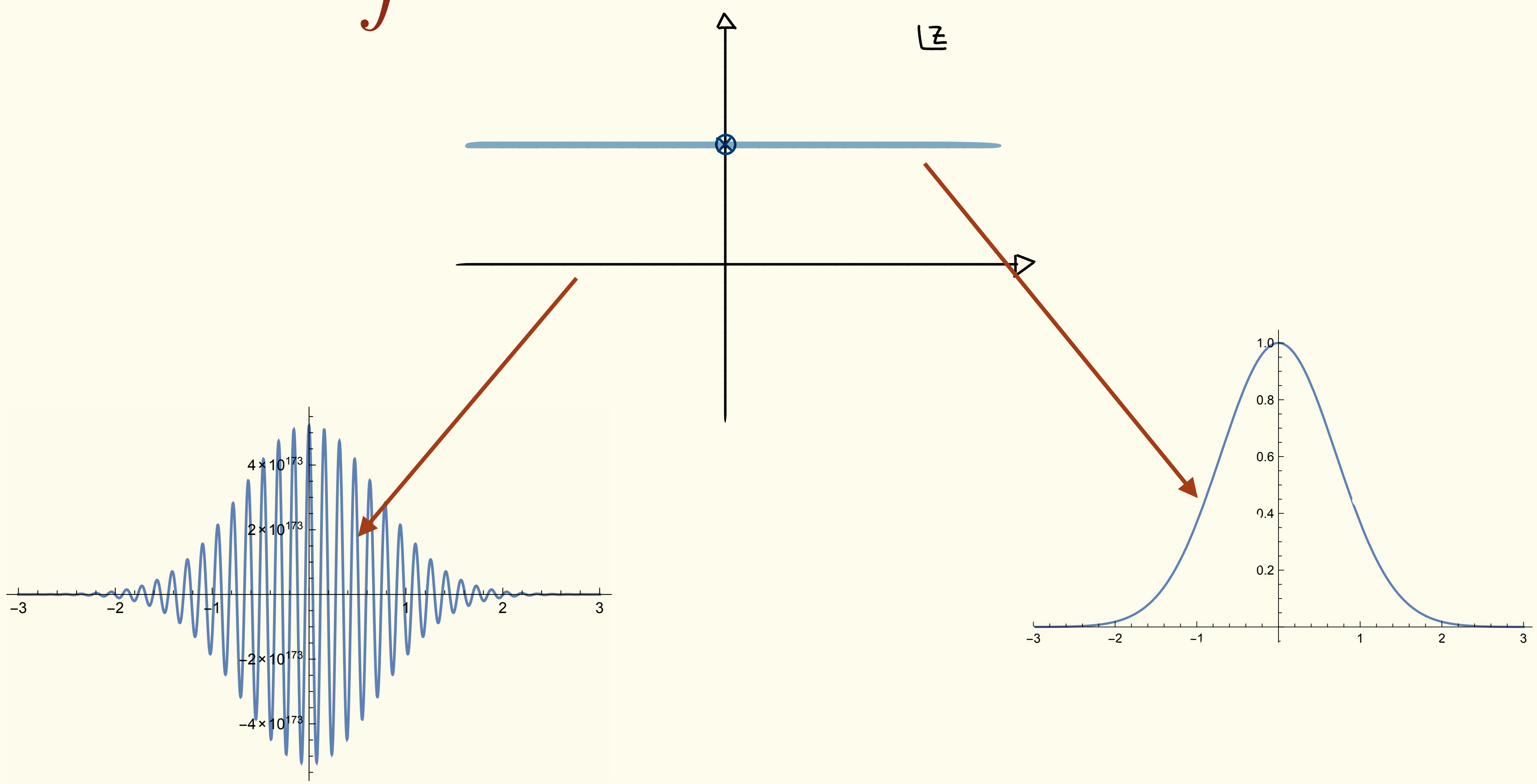
In other words, it is hard “to Monte Carlo” an oscillatory integral

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



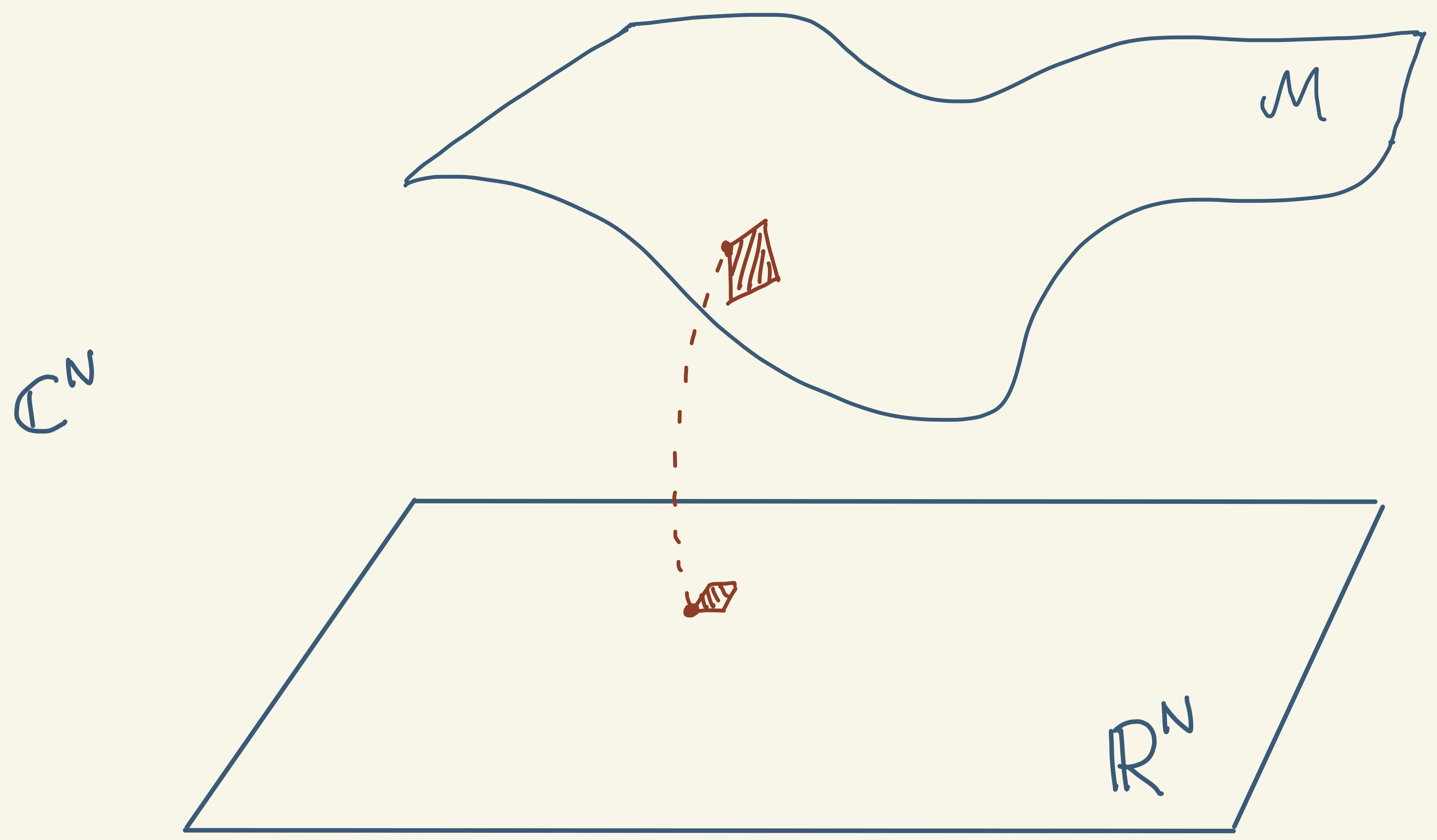
Basic Idea:
deform the domain of integration

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



Cristoforetti, DiRenzo, Scorzato, '12

Basic Idea:
deform the domain of integration

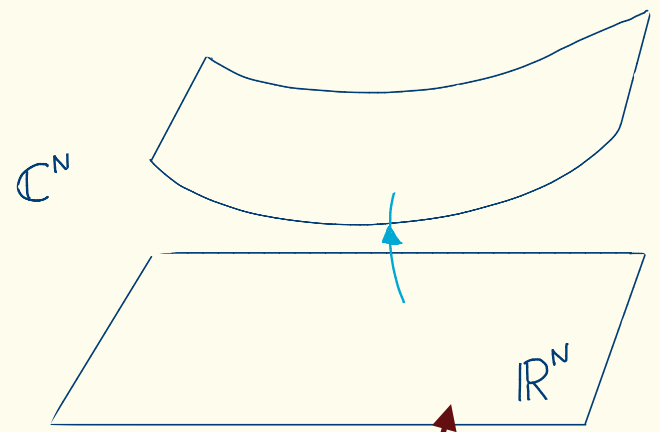


Basic Idea:
deform the domain of integration

"Cauchy-Stokes" theorem guarantees the equality of the integrals

- Integrand is always holomorphic
- Need to worry about the asymptotic directions (homology class)

Holomorphic flow is a way of finding a suitable manifold



(real) field space

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

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

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

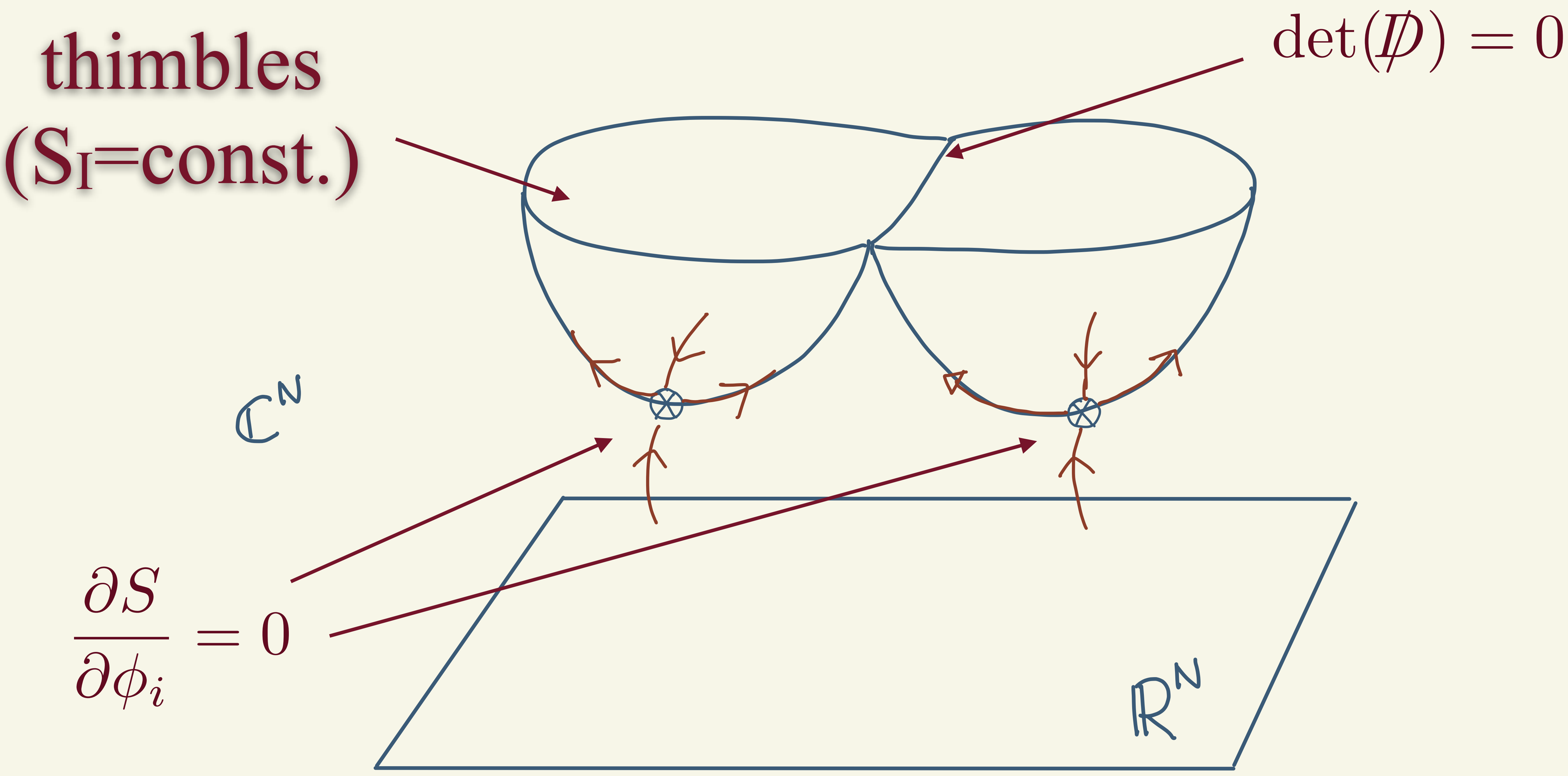
gradient flow of S_R, keeps integral well defined

hamiltonian flow of S_I, keeps phase fixed

The increase of S_R explains why the integral over the flowed manifold converges and is in the same homology class as R^N.

It takes more thinking to see that it improves the sign problem …

Initial Idea:
deform the domain of integration from R^N to thimbles



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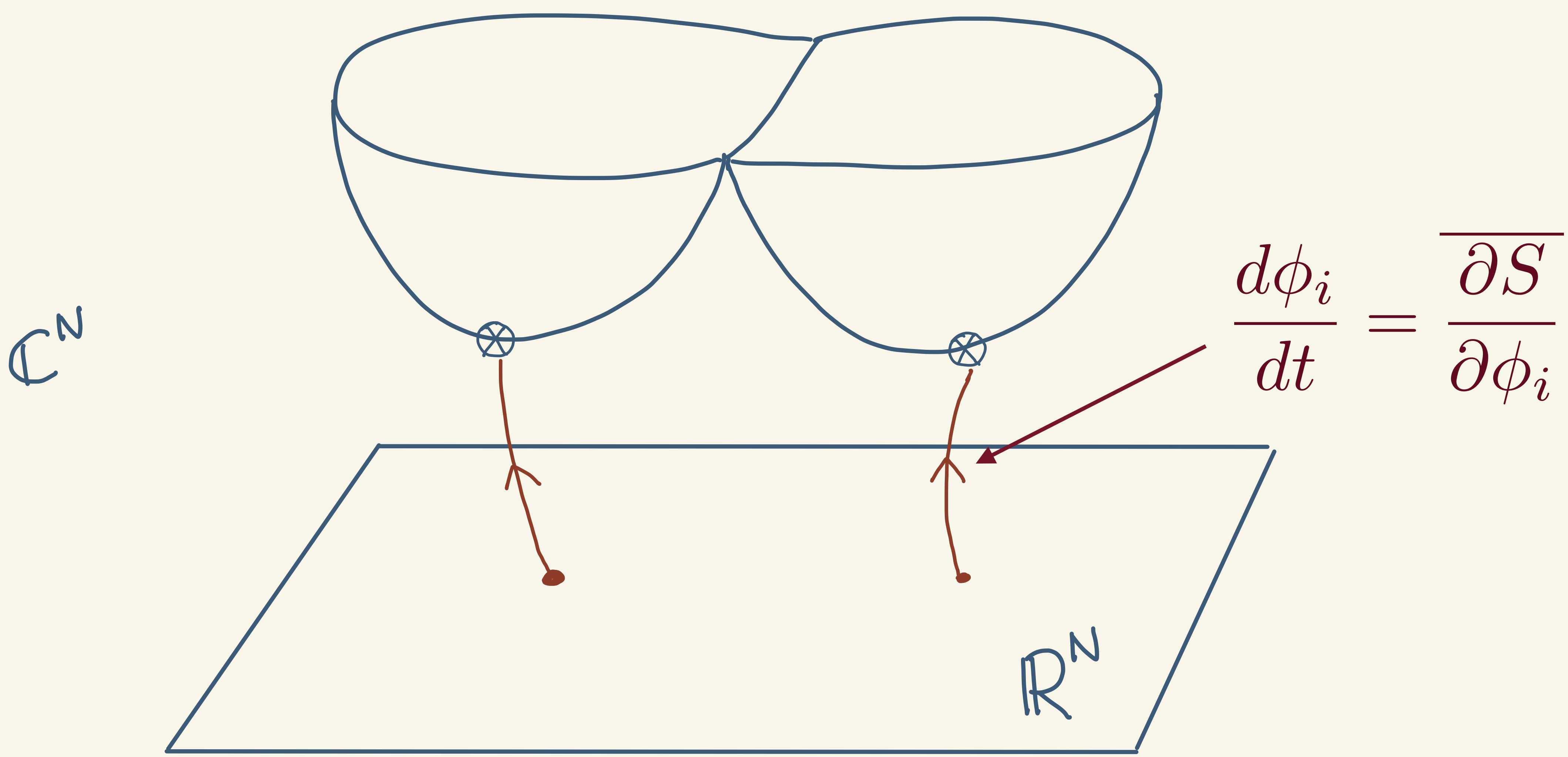
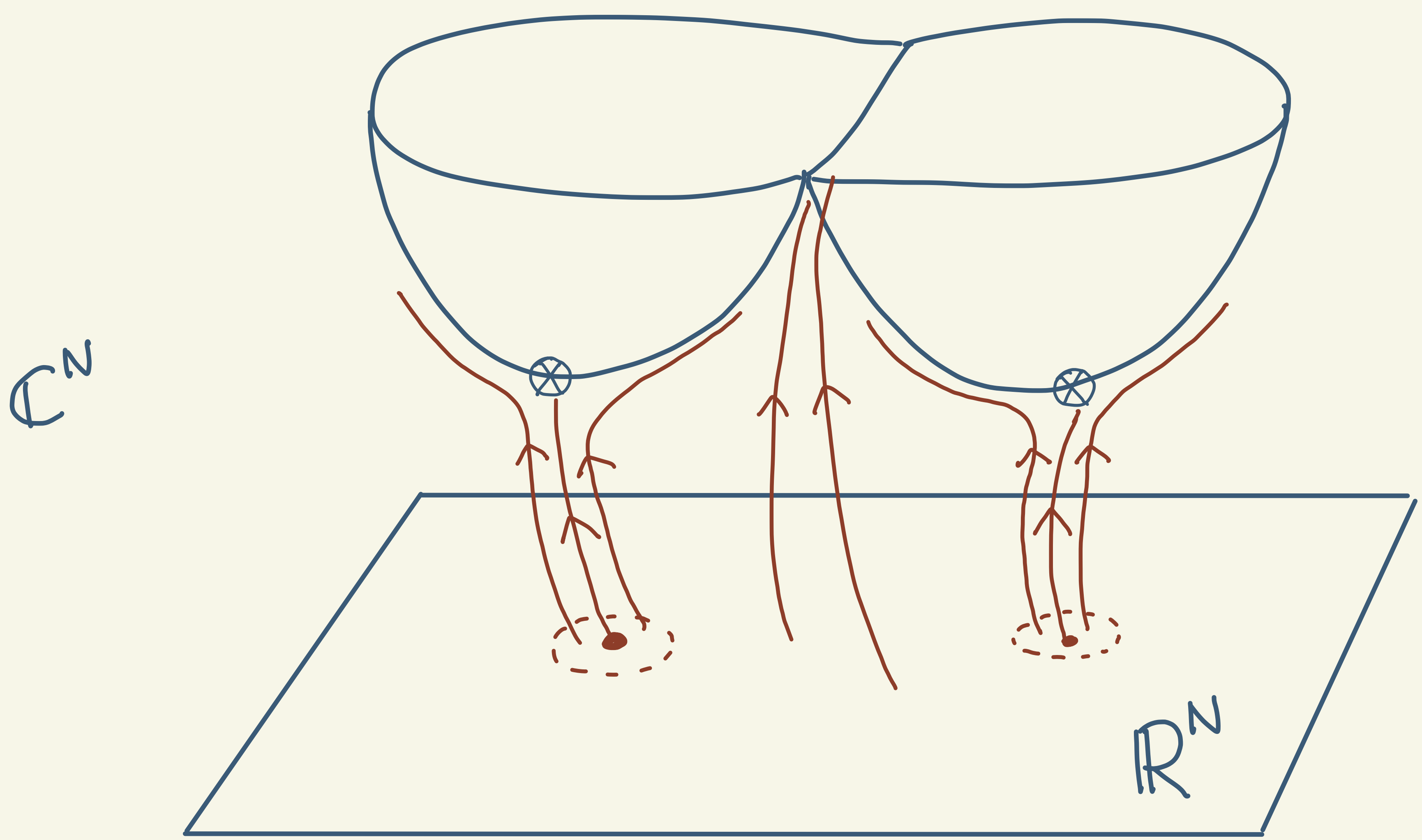


Central Idea:
deform the domain of integration from R^N to thimbles



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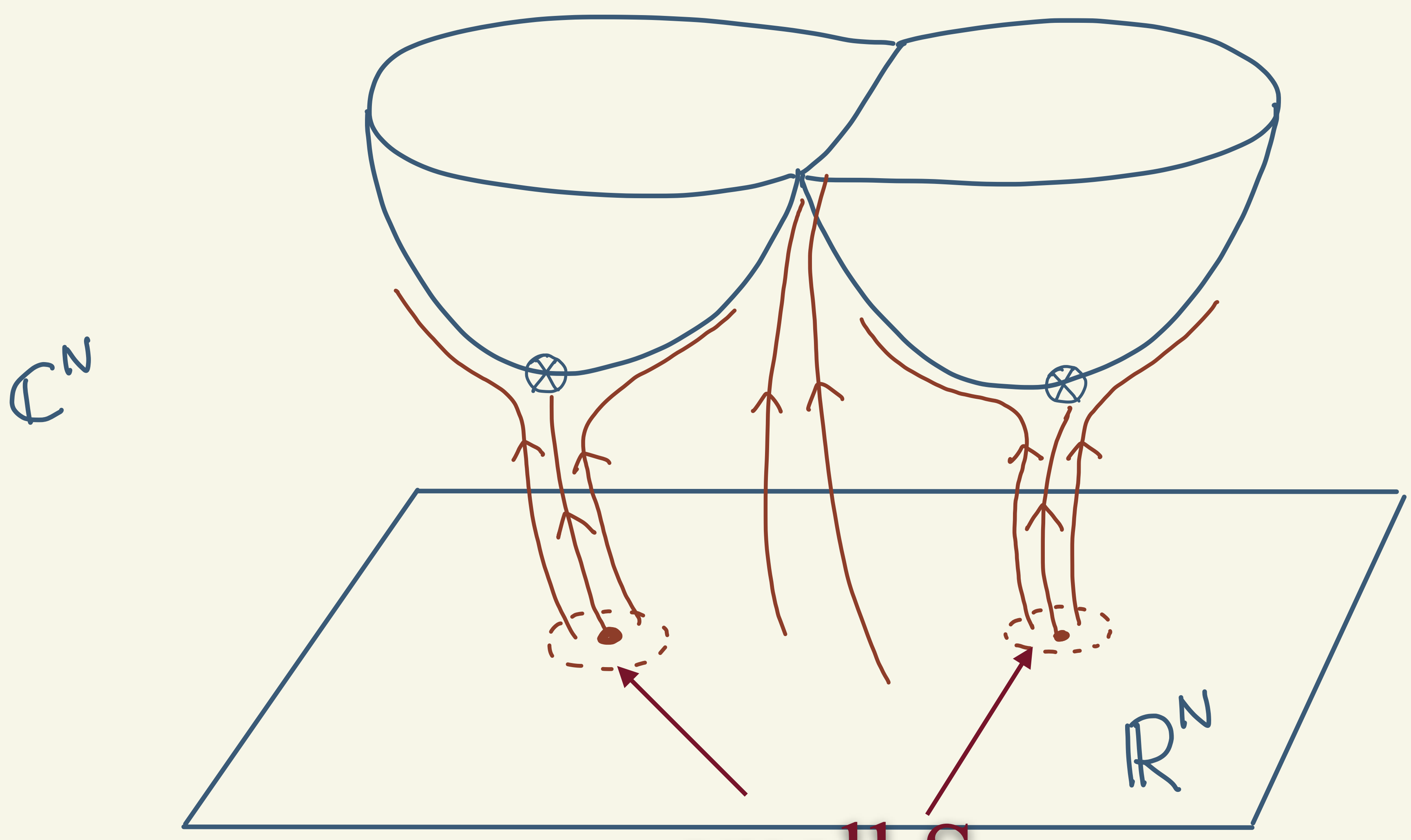
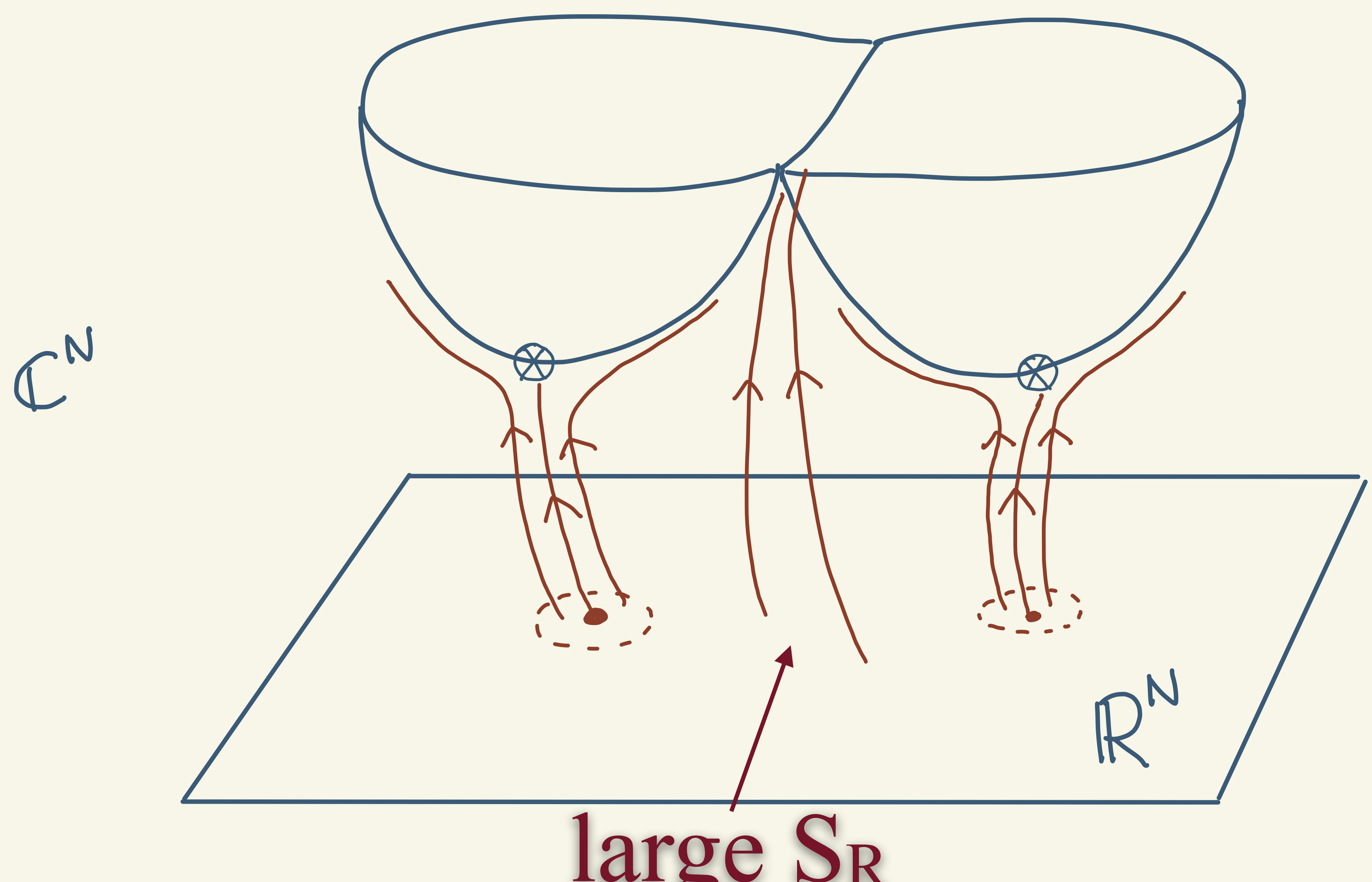


small S_R

Central Idea: deform the domain of integration from R^N to thimbles



Central Idea:
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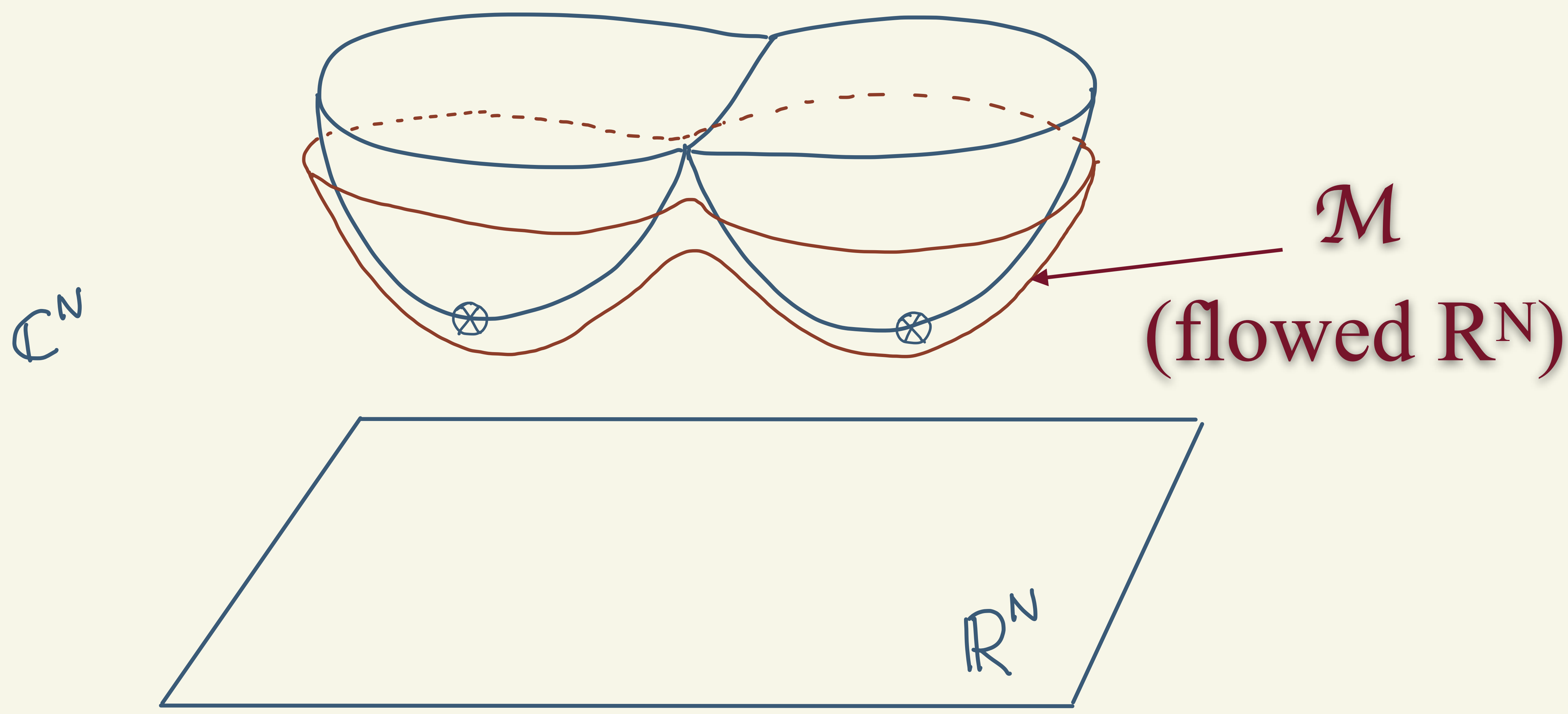


Holomorphic flow is a way of finding a suitable manifold

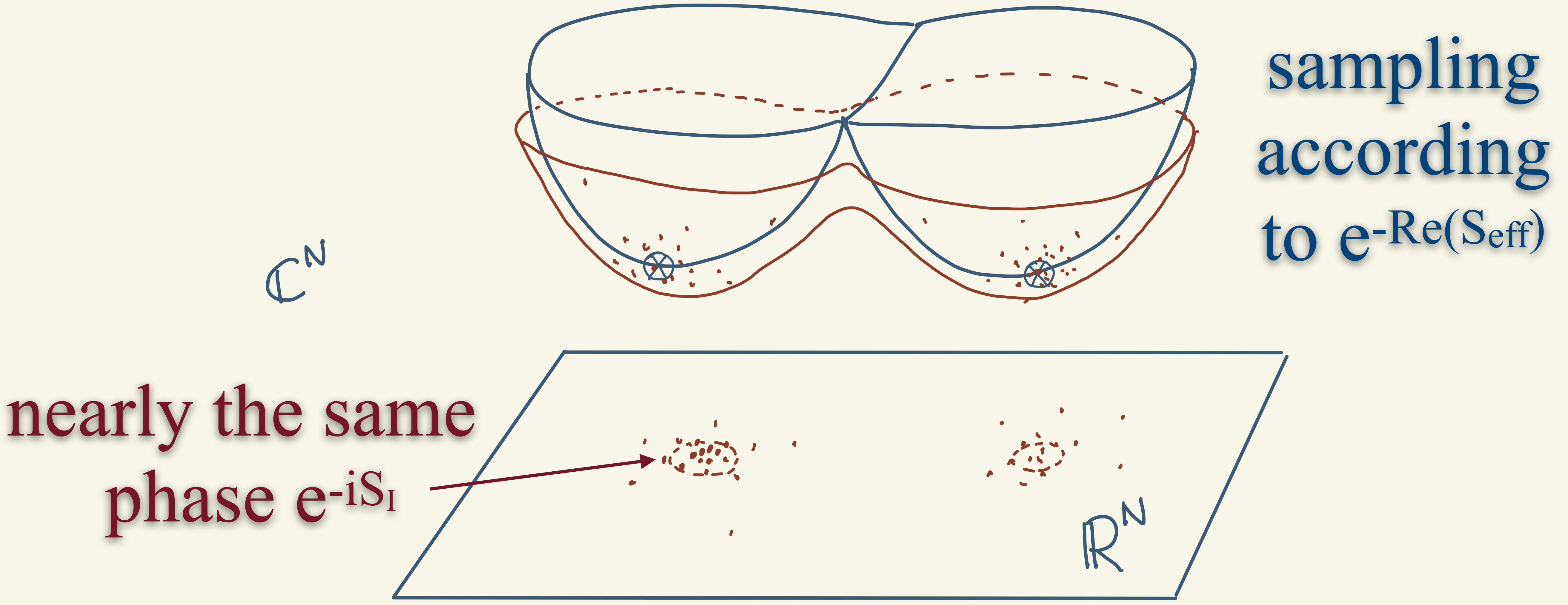
In the limit of infinite flow time:

$$\int_{R^N} D\phi \, e^{-S[\phi]} = \sum_i n_i \int_{\mathcal{T}_i} D\phi \, e^{-S[\phi]}$$

intersection numbers (n_i)

thimbles (manifolds w/ S_I=const.) ($\mathcal{T}_i$)

Central Idea: deform the domain of integration from R^N to thimbles

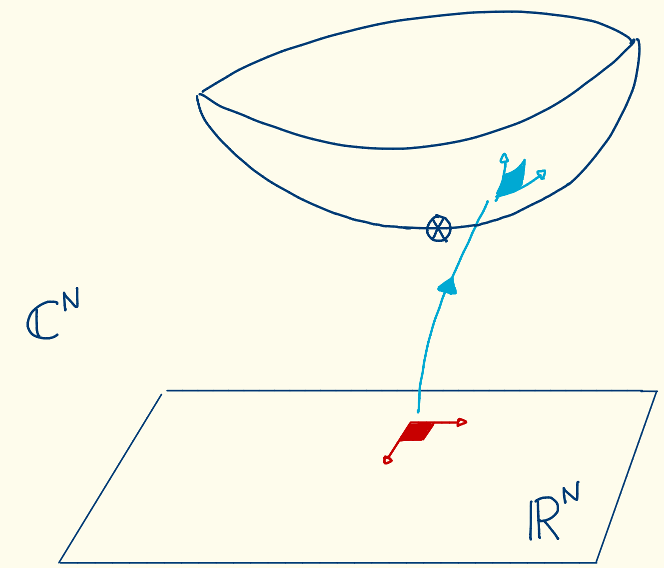


The algorithm

$$\langle \mathcal{O} \rangle = \frac{\int d\phi \mathcal{O} e^{-S_R - iS_I}}{\int d\phi e^{-S_R - iS_I}} = \frac{\int_{\mathcal{M}} d\tilde{\phi} \mathcal{O} e^{-S_R - iS_I}}{\int_{\mathcal{M}} d\tilde{\phi} e^{-S_R - iS_I}} = \frac{\int_{\mathbb{R}^N} d\phi \mathcal{O} \overbrace{\left| \frac{\partial \tilde{\phi}}{\partial \phi} \right|}^{J} e^{-S_R - iS_I}}{\int_{\mathbb{R}^N} d\phi \left| \frac{\partial \tilde{\phi}}{\partial \phi} \right| e^{-S_R - iS_I}}$$

$$= \frac{\int_{\mathbb{R}^N} d\phi \mathcal{O} e^{-iS_I + iIm \ln J} e^{-(\overbrace{S_R - Re \ln J}^{S_{eff}})}}{\int_{\mathbb{R}^N} d\phi e^{-iS_I + iIm \ln J} e^{-(S_R - Re \ln J)}}$$

$$= \frac{\langle \mathcal{O} e^{-iS_I + iIm \ln J} \rangle_{S_{eff}}}{\langle e^{-iS_I + iIm \ln J} \rangle_{S_{eff}}}$$



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

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

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

this is the expensive part

The algorithm

$$\langle \mathcal{O} \rangle = \frac{\int d\phi \mathcal{O} e^{-S_R - iS_I}}{\int d\phi e^{-S_R - iS_I}} = \frac{\int_{\mathcal{M}} d\tilde{\phi} \mathcal{O} e^{-S_R - iS_I}}{\int_{\mathcal{M}} d\tilde{\phi} e^{-S_R - iS_I}} = \frac{\int_{\mathbb{R}^N} d\phi \mathcal{O} \overbrace{\left| \frac{\partial \tilde{\phi}}{\partial \phi} \right|}^{J} e^{-S_R - iS_I}}{\int_{\mathbb{R}^N} d\phi \left| \frac{\partial \tilde{\phi}}{\partial \phi} \right| e^{-S_R - iS_I}}$$

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$$= \frac{\mathcal{O} \langle e^{-iS_I + iIm \ln J} \rangle_{S_{eff}}}{\langle e^{-iS_I + iIm \ln J} \rangle_{S_{eff}}}$$

algorithm

=

Metropolis in the real space,
action S_{eff} and
reweighted phase $e^{i \, Im(\ln J) - i \, Im(S)}$

This bypasses a number of problems with the original idea of integrating over thimbles

- find the thimbles and intersection numbers
- numerically integrate over a thimble(s)

see arXiv:2007.05436 for a recent review of this and other approaches

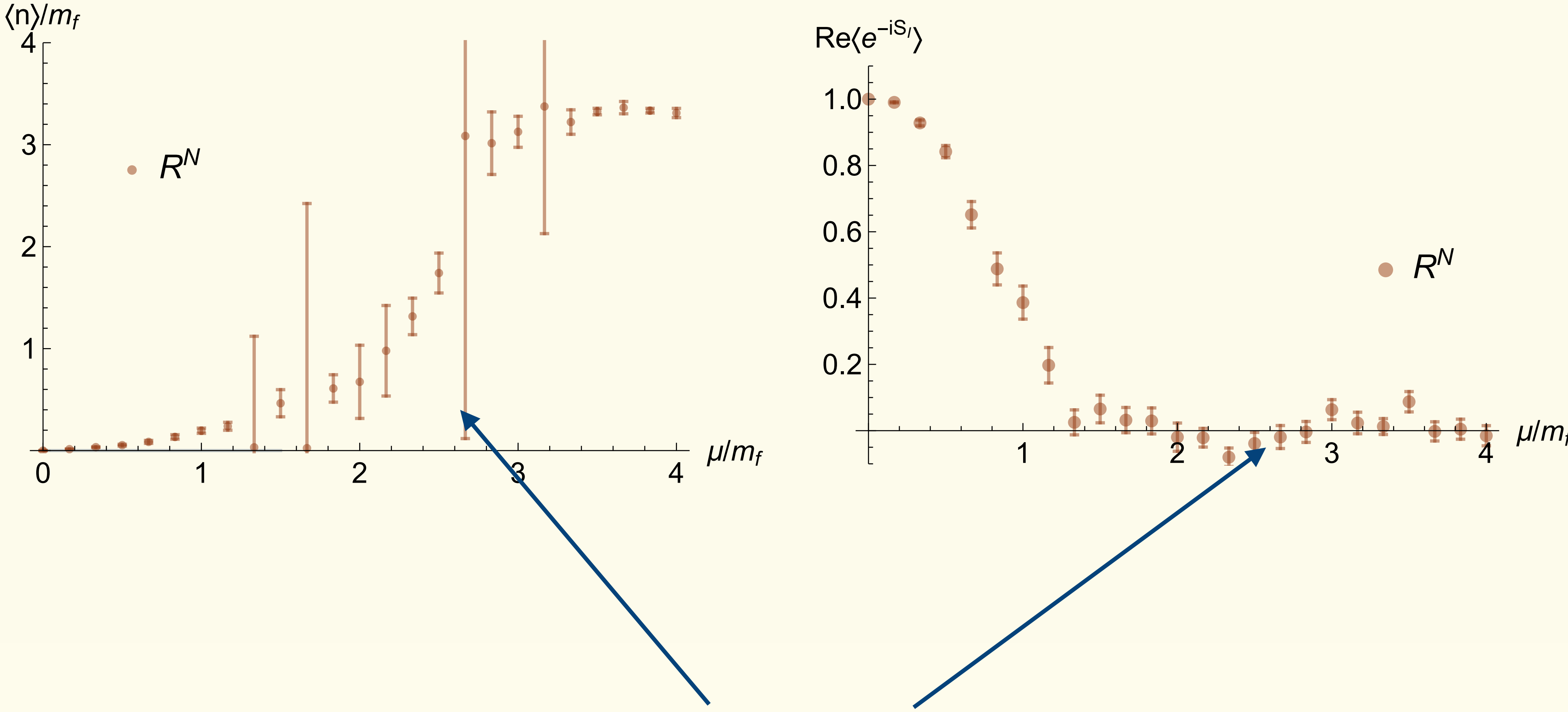
Case study: massive Thirring model

$$S = \int d^2x \; \bar{\psi}(\not{D} + m)\psi - \frac{g^2}{2}\bar{\psi}\gamma_\mu\psi\bar{\psi}\gamma_\mu\psi$$

Wilson/staggered, 10 x10 lattice, N_F=2, am_f=0.3
(close to the continuum limit, strongly coupled)

Case study: massive Thirring model

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

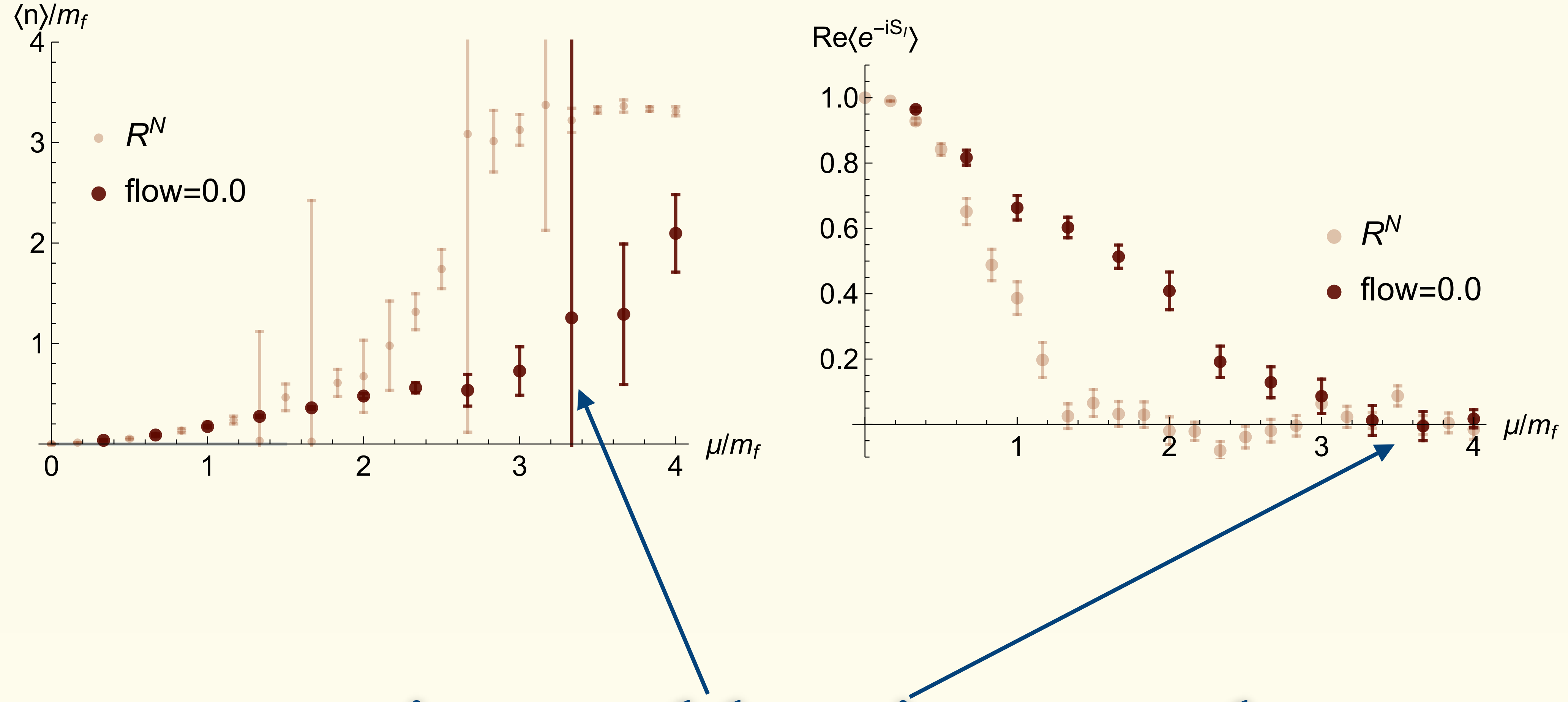


sign problem

Real field calculation

Case study: massive Thirring model

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

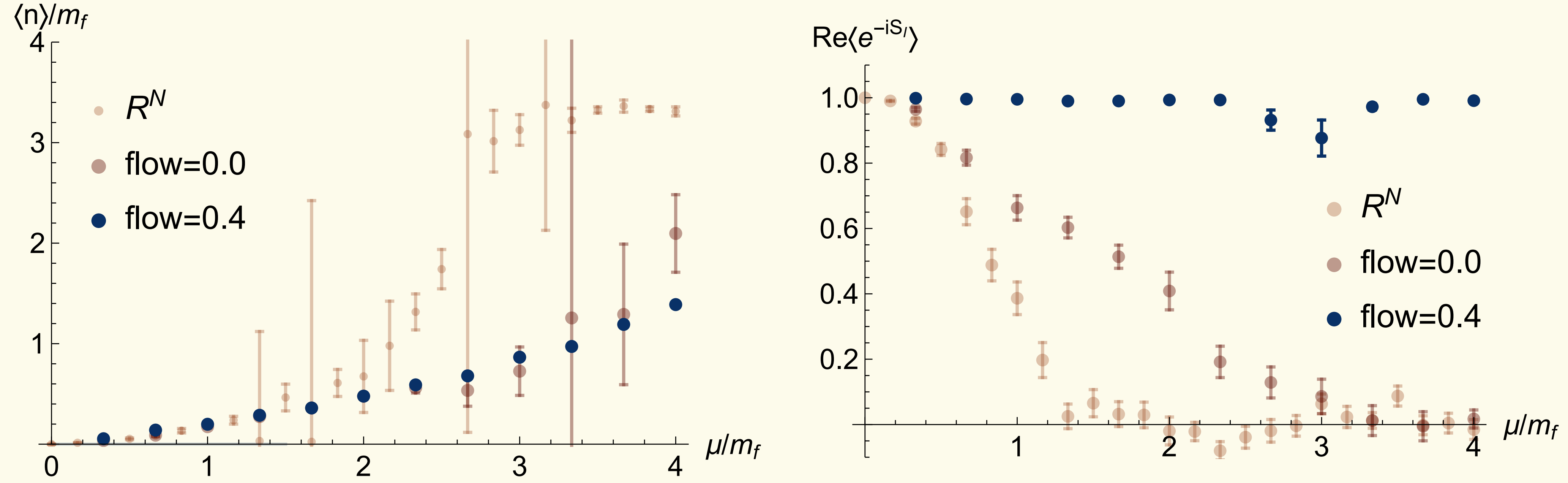


sign problem improved

tangent plane calculation

Case study: massive Thirring model

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

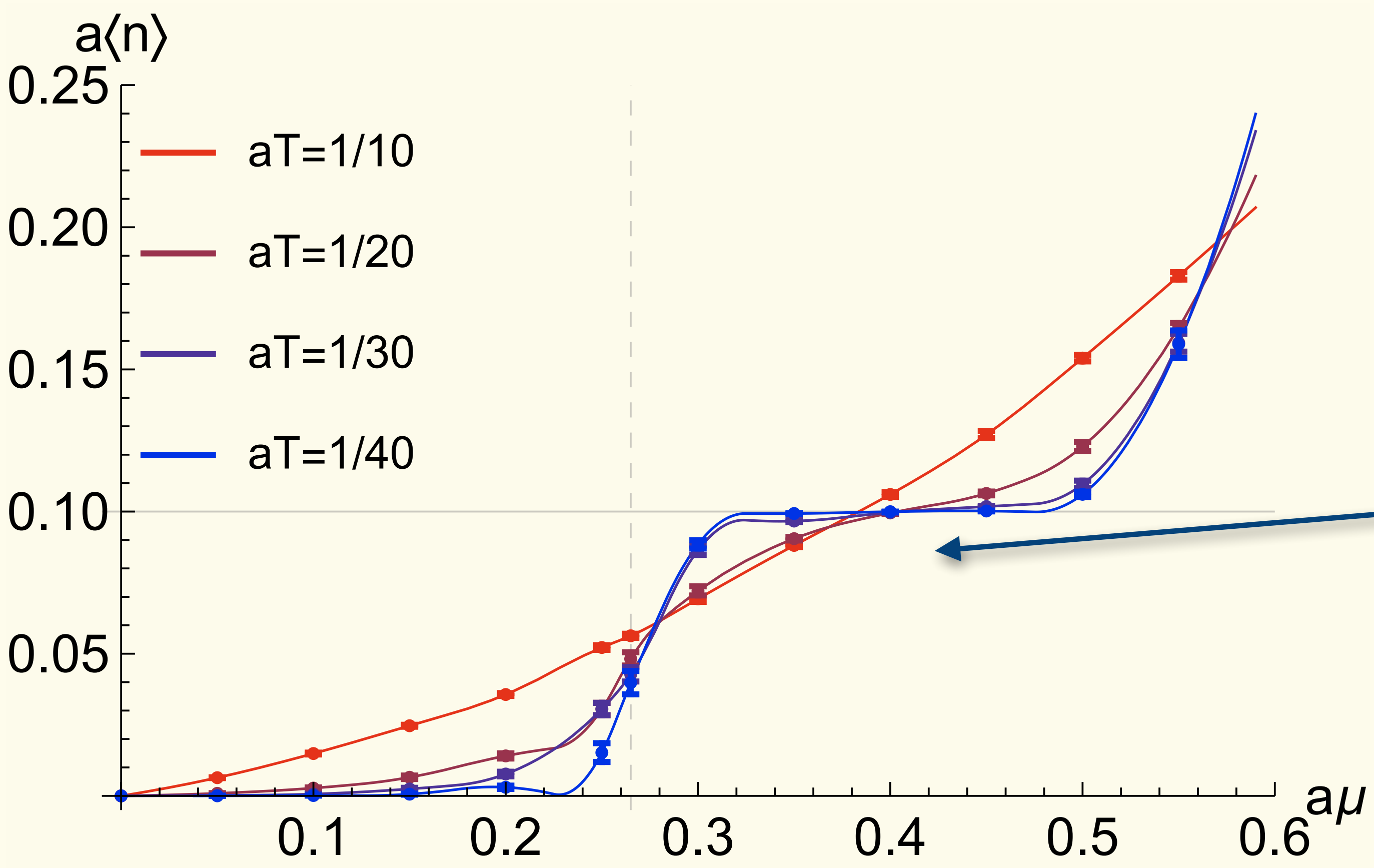


flow done with estimators for the jacobian (difference reweighted)

flowed manifold calculation

Case study: massive Thirring model

Staggered, $N_F=2$, $am_f=0.265$



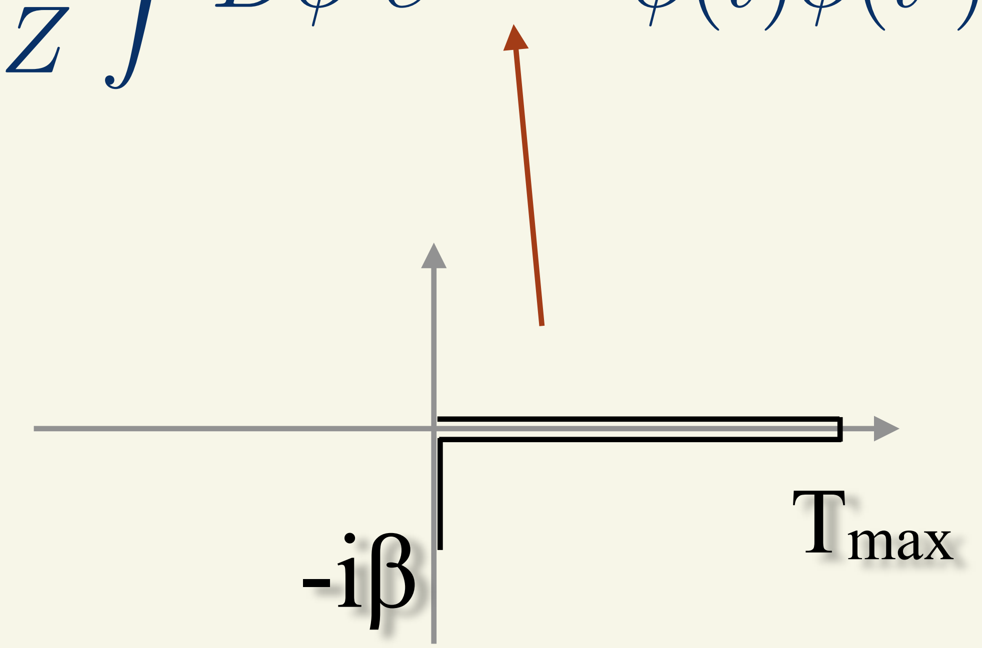
step is missed in a one thimble calculation

cold limit

Application: Real Time Dynamics

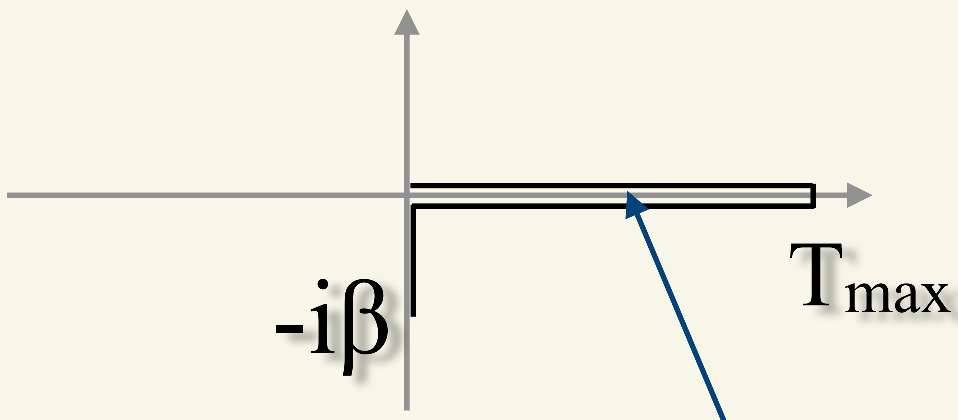
Viscosities, conductivities, … require:

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



Schwinger-Keldysh
contour
(works also out of equilibrium)

Real Time: The Mother of All Sign Problems



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

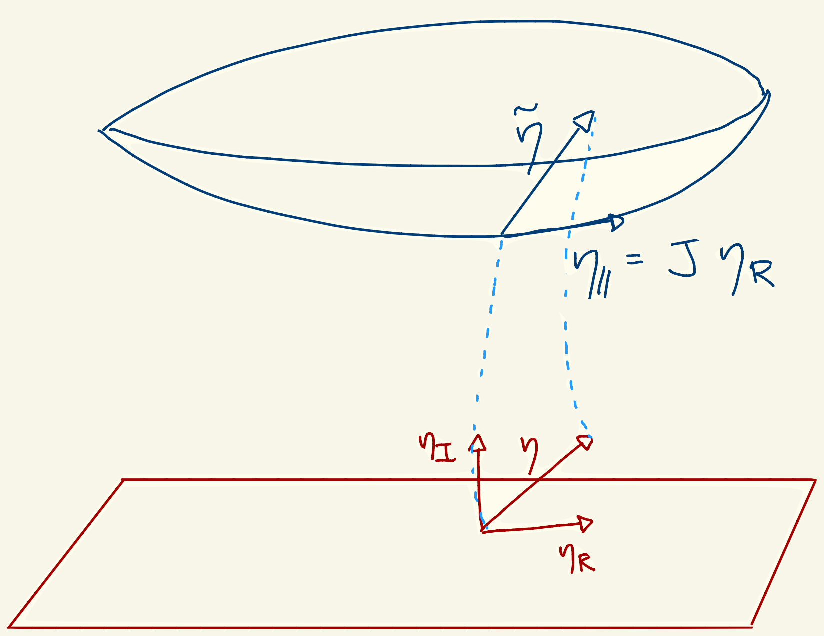
$$\langle e^{i\mathrm{Im}(iS_c)} \rangle = 0$$

Problems

- tangent space in wrong homology class
- large flow needed (from R^N)
- jacobian expensive (no known estimator)
- anisotropic proposals

"Grady algorithm" for the jacobian

(Grady '85, Creutz '92, Alexandru et al. 2018)

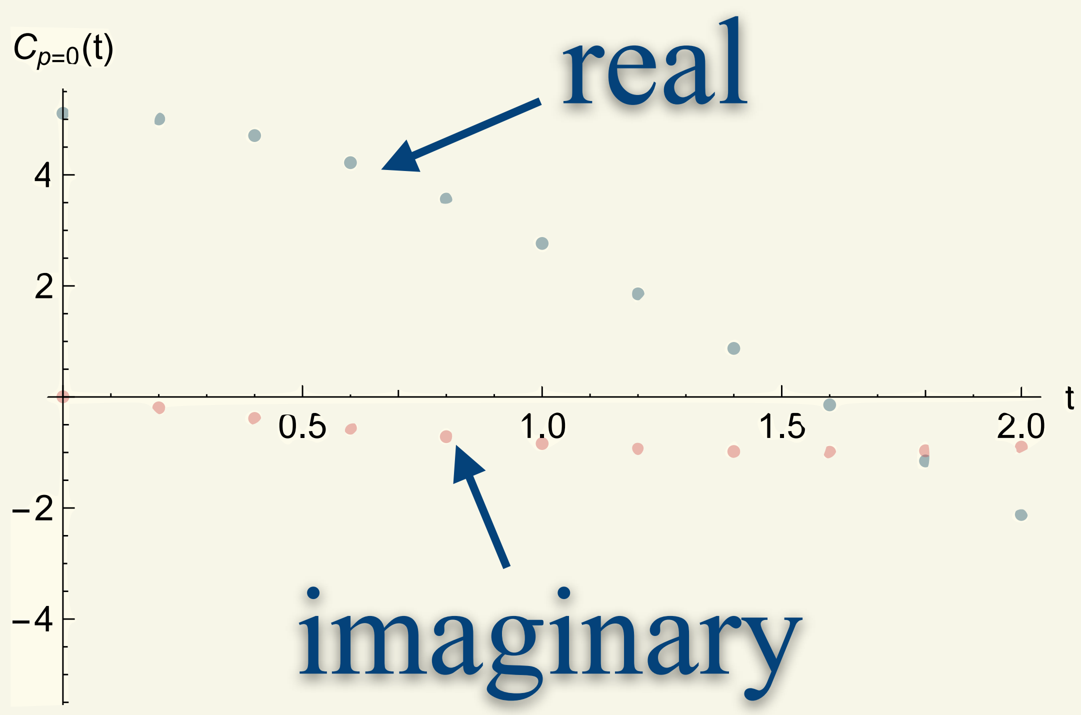


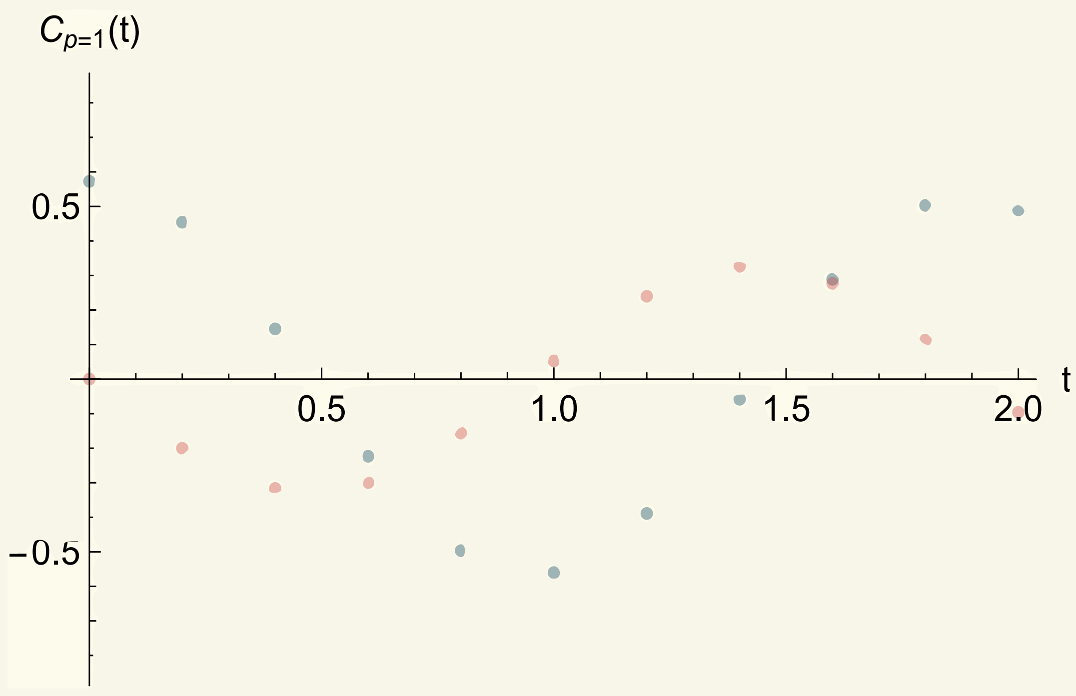
$$J\eta = \tilde{\eta} \qquad \tilde{\eta}_{||} = J Re(\eta)$$

- isotropic proposal
- no need to compute det(J)

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=0.1

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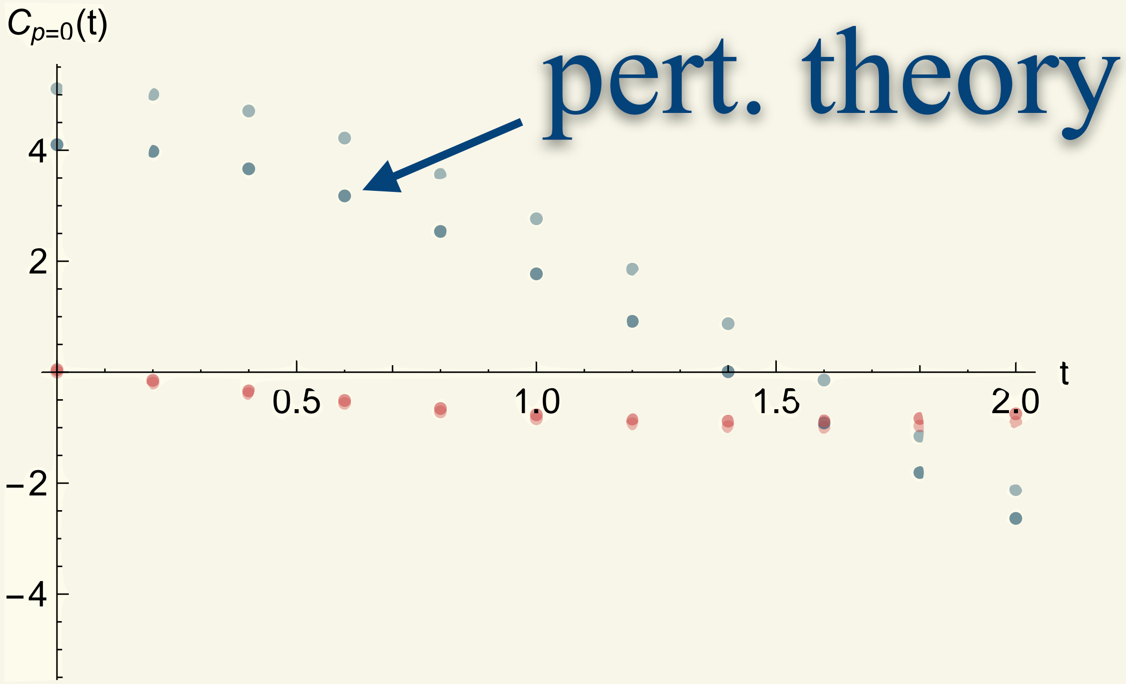

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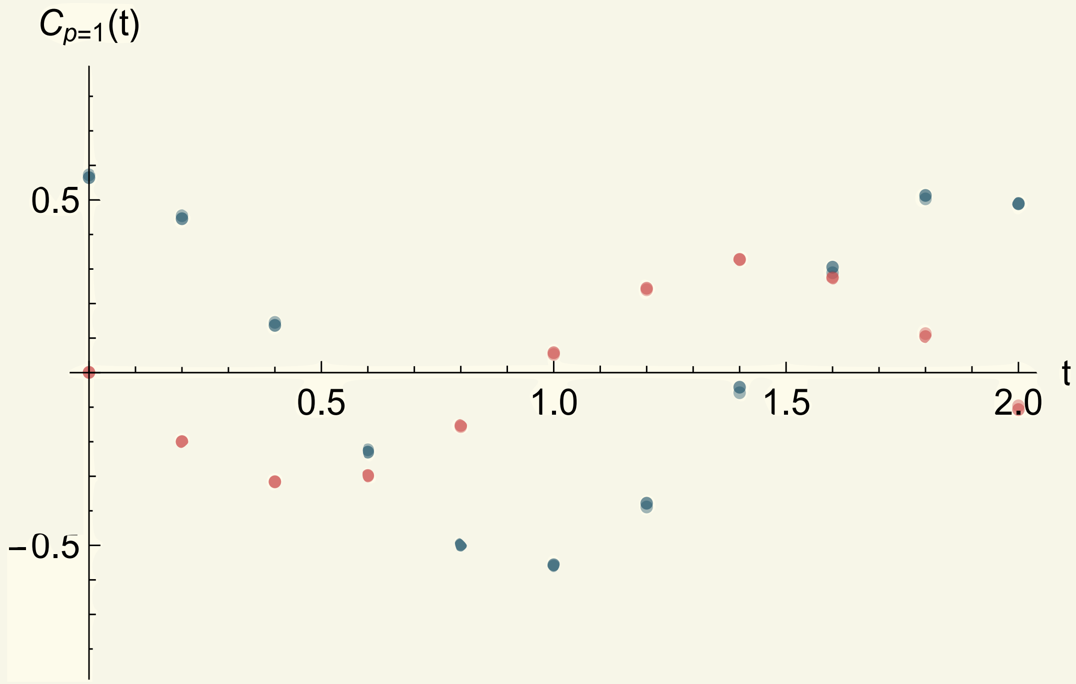

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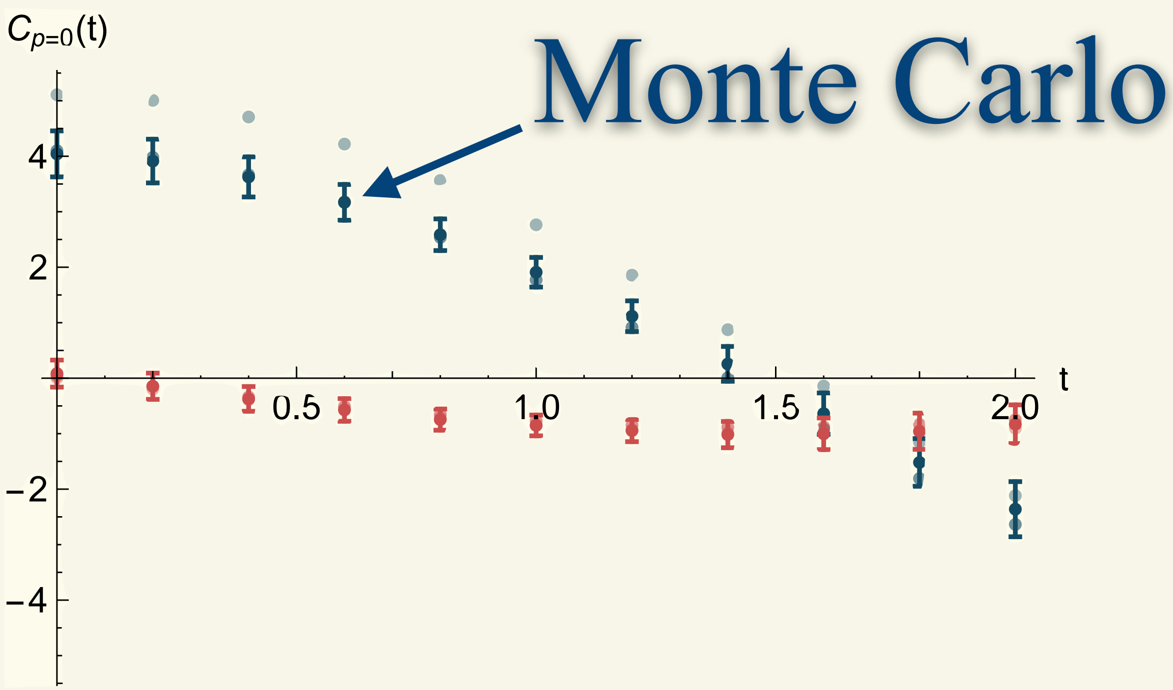

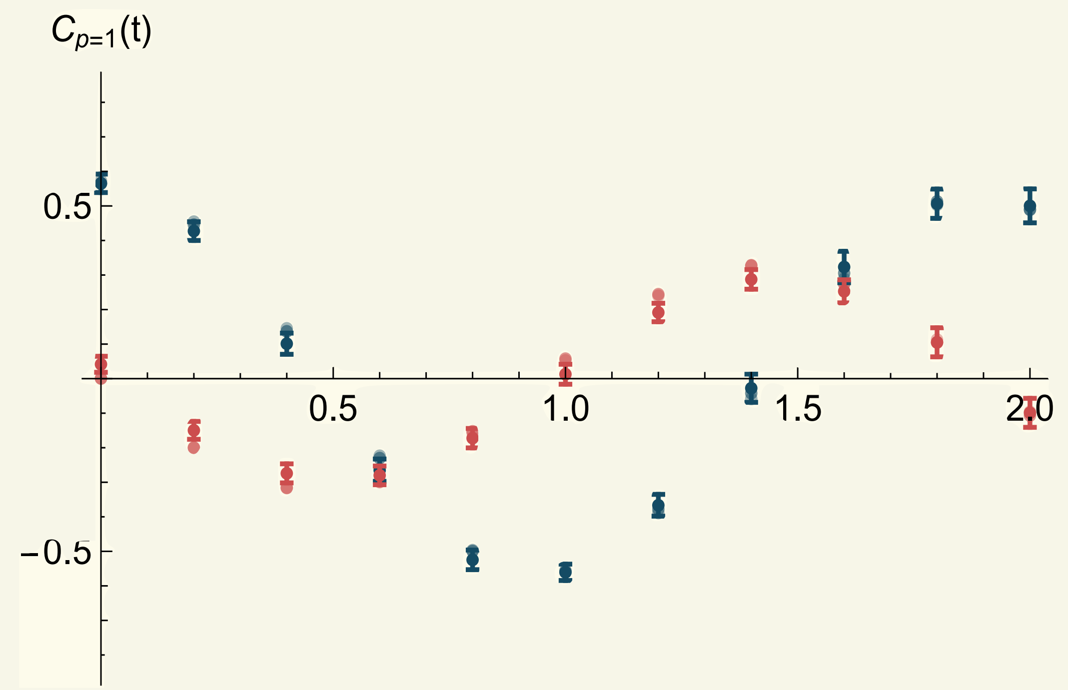

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1+1D φ^4: n_t=10, n_x=10, n_β=2, λ=1.0

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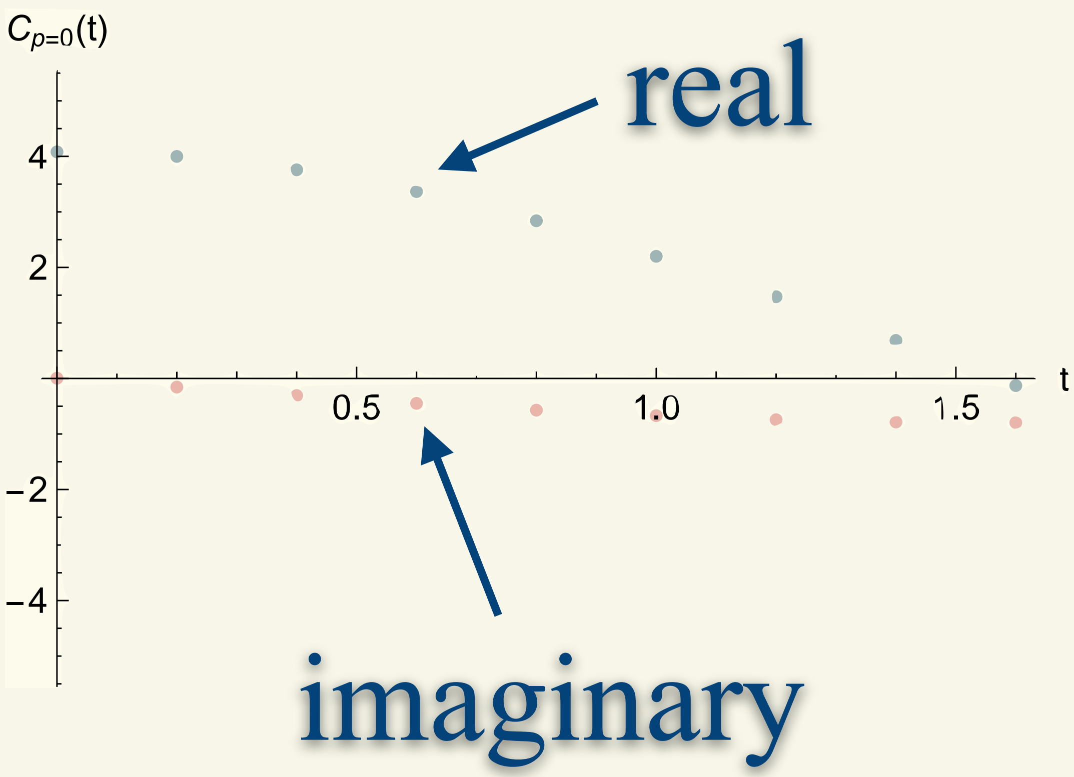
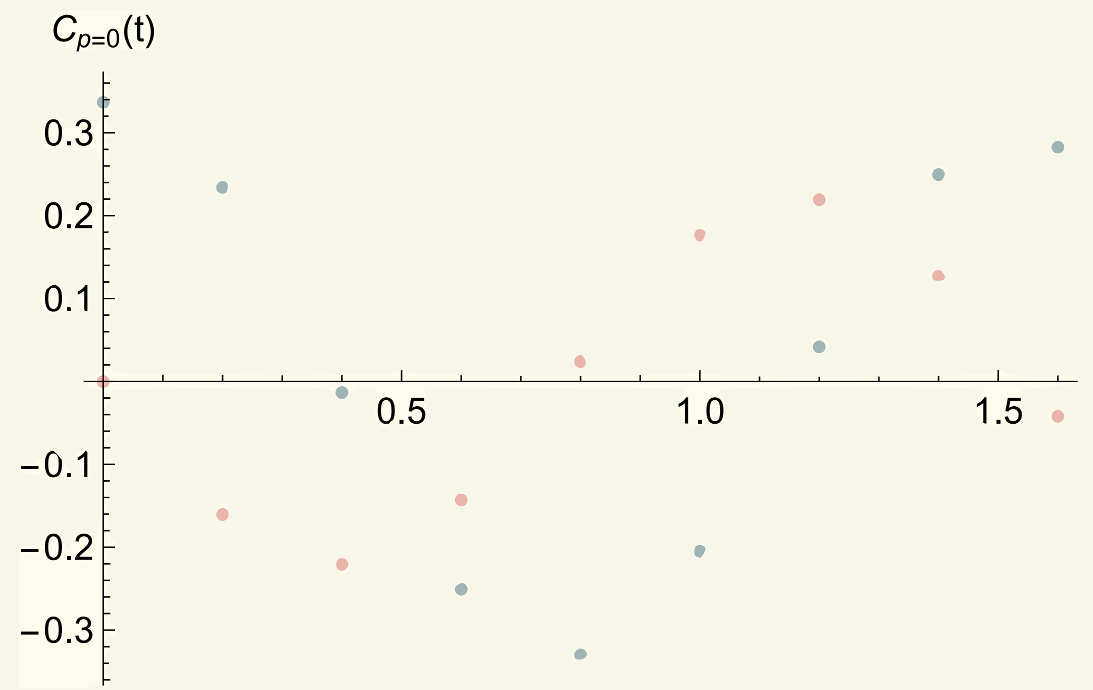


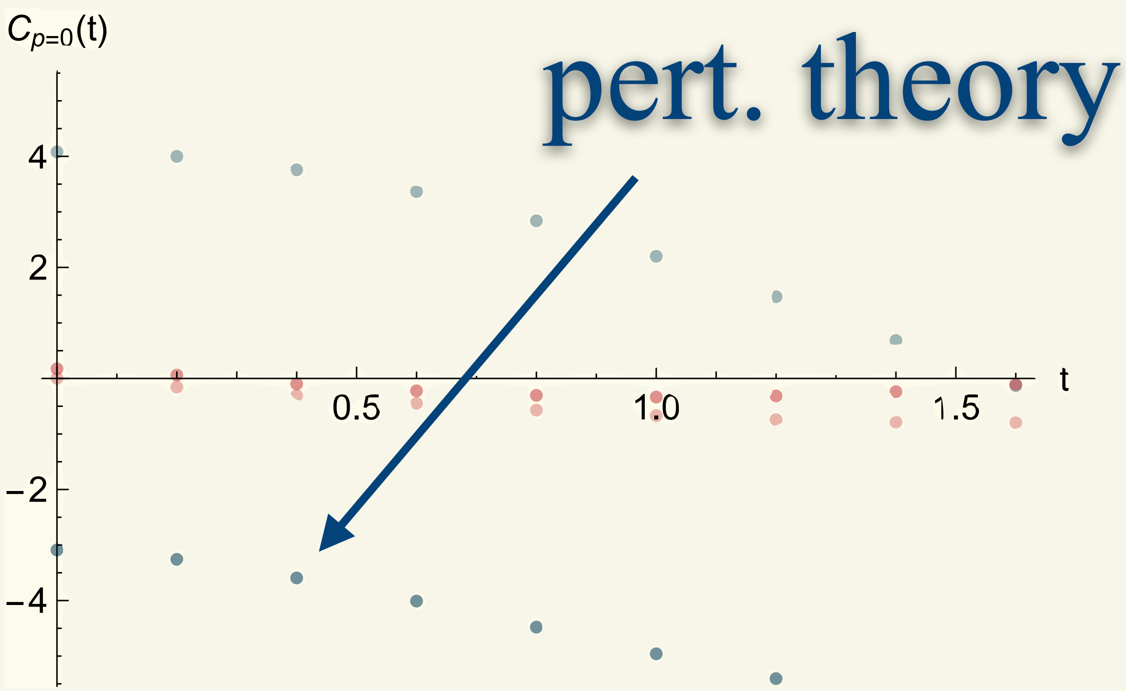
p=0



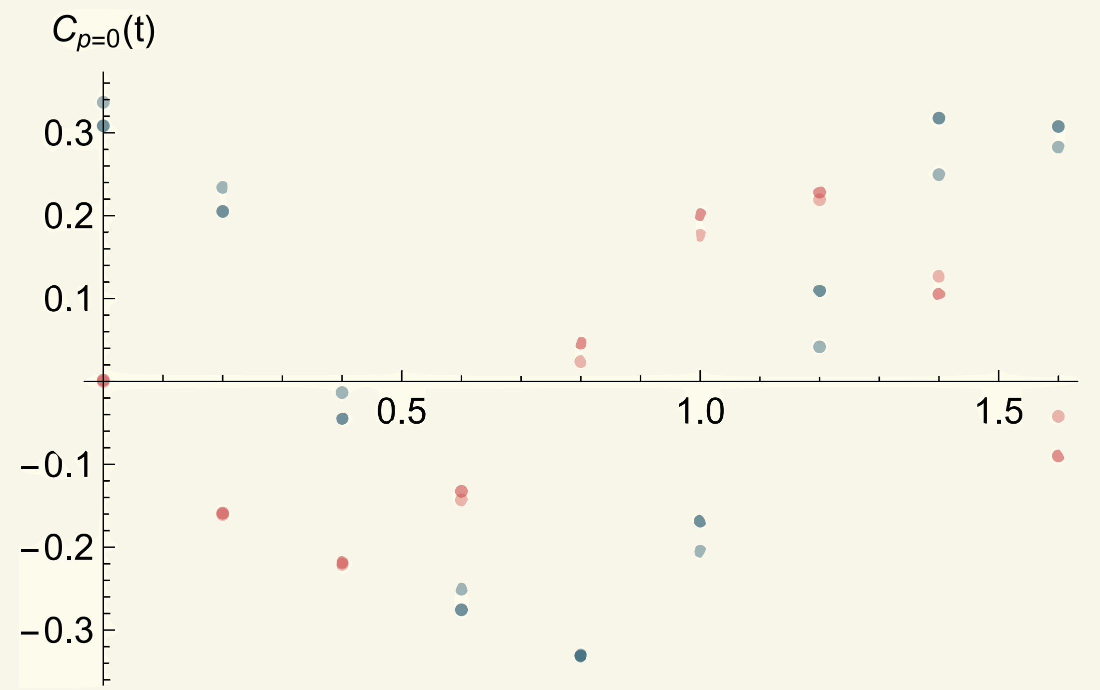
p=2π/L

1+1D φ^4: $n_t=10$, $n_x=10$, $n_\beta=2$, $\lambda=1.0$

strong coupling



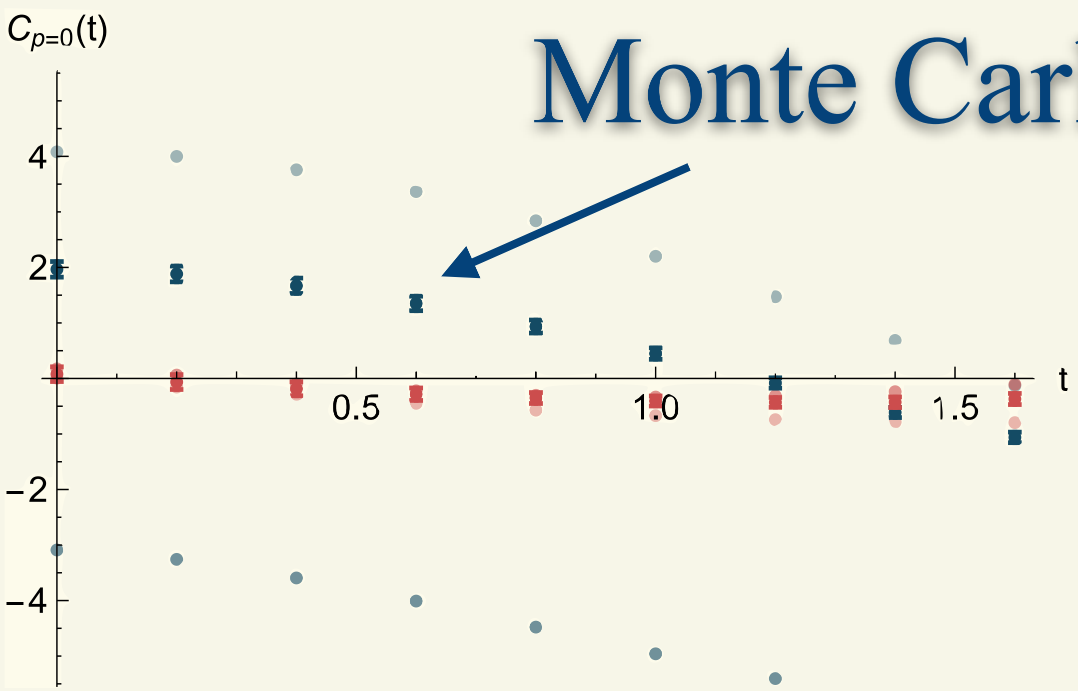
$p=0$



$p=2\pi/L$

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

strong coupling



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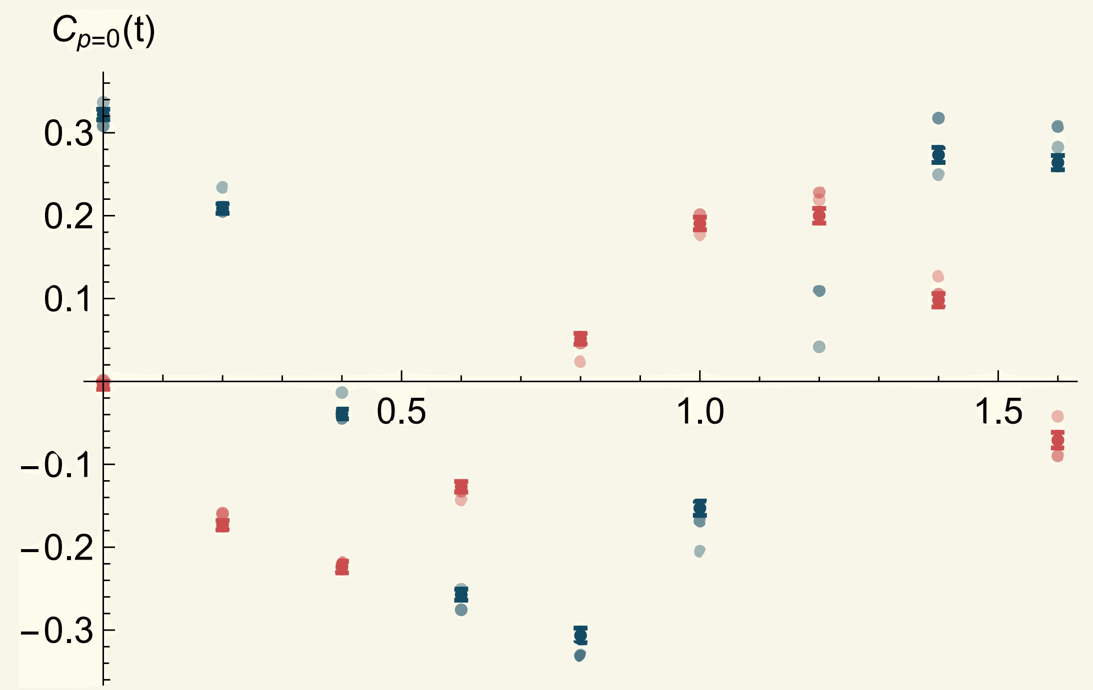


p=2π/L

Application: Real Time Dynamics

- Currently limited to small times : $t < 5/T$
- Cost increases sharply with t
- There has to be a catch:

simulation of a quantum computer performing the Schor algorithm

= nonsense

classical $O(\log^2 N)$ time factorization

The holomorphic flow is not the only way to find "good" manifolds

C^N: 2N dimensions

S_I=const : 1 constraint

tangent plane: N dimensions

↓

a lot of room to choose S_I=const manifolds

The holomorphic flow is not the only way to find "good" manifolds

maximize the average phase

$$\underbrace{\langle e^{i(S_I + ImJ)} \rangle}_{\sigma} = \frac{\int D\tilde{\phi} e^{-S - RelnJ}}{\int D\tilde{\phi} e^{-S_R - RelnJ}}$$

Mori, Kashiwa&Ohnishi, `17
Alexandru,Bedaque,Lamm&Lawrence, `17
Bursa&Kroyter, `18

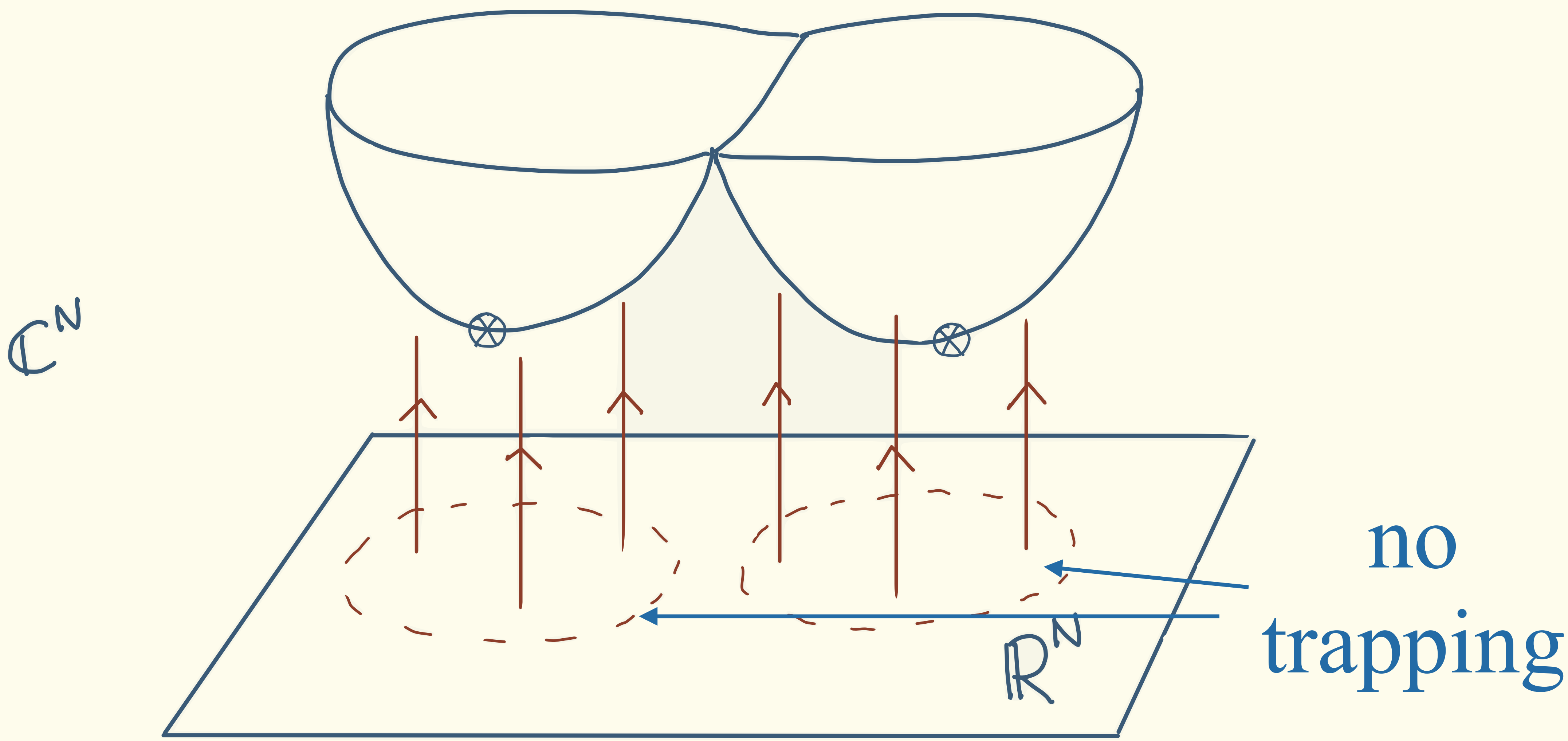
The holomorphic flow is not the only way to find "good" manifolds

$$\partial_\lambda \log |\langle \sigma \rangle| = \frac{\int_{\mathcal{M}} D\tilde{\phi}\ e^{-S_R}(\partial_\lambda S_R - Re Tr J^{-1}\partial_\lambda J)}{\int_{\mathcal{M}} D\tilde{\phi}\ e^{-S_R}}$$

no sign problem

gradient of $e^{i\alpha}$ computed by a short, sign-problem free MC run

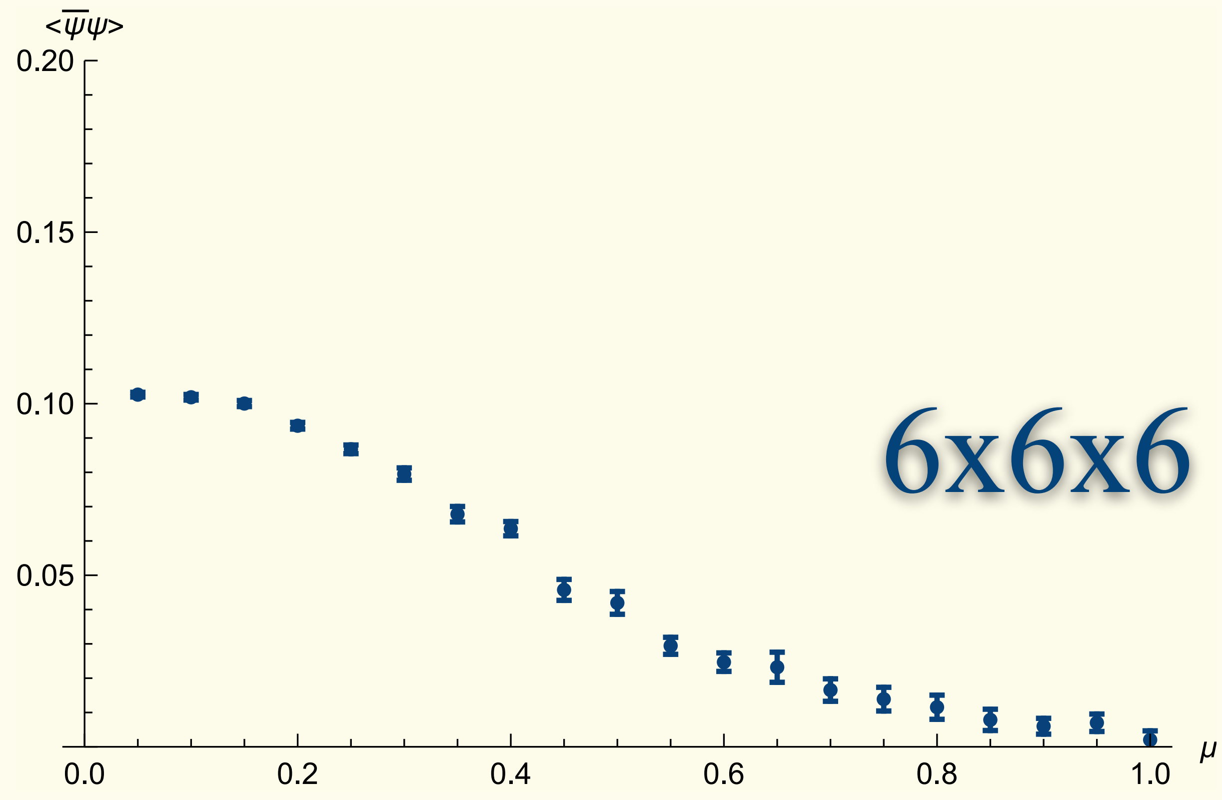
The holomorphic flow is not the only way to find "good" manifolds



simple ansatz: $\phi(x) = \phi_R(x) + i(\lambda_0 + \lambda_1 \cos(\phi_R(x)) + \lambda_2 \cos(2\phi_R(x))$

The holomorphic flow is not the only way to find "good" manifolds

2+1D Thirring model

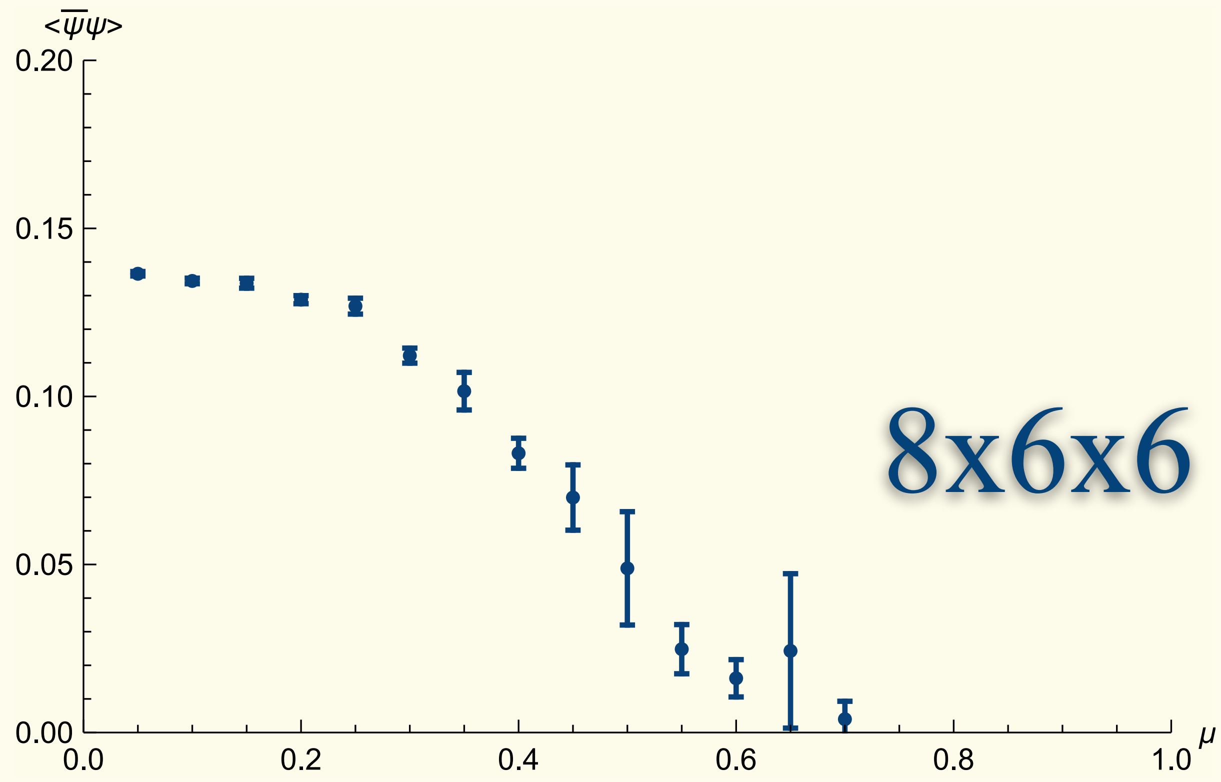


6x6x6

factorized ansatz: $\tilde{\phi}_i = \phi_i + if(\phi_i)$

The holomorphic flow is not the only way to find "good" manifolds

2+1D Thirring model

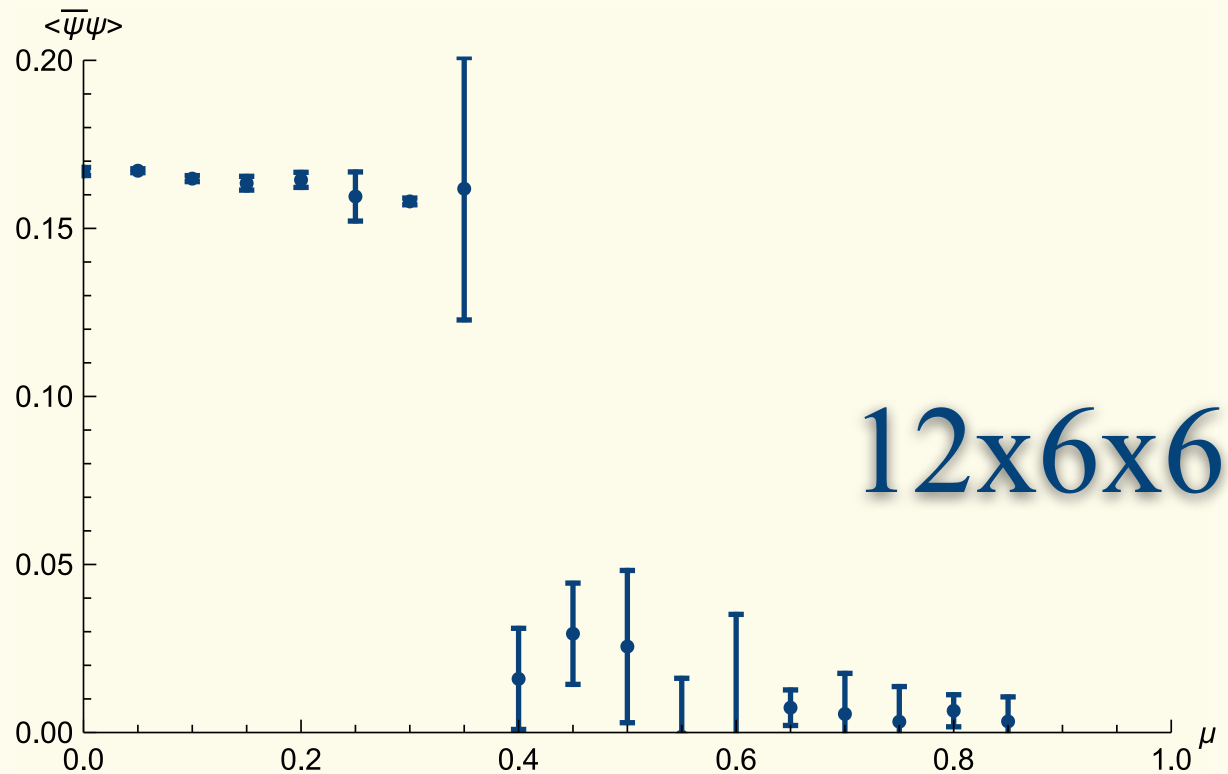


8x6x6

factorized ansatz: $\tilde{\phi}_i = \phi_i + if(\phi_i)$

The holomorphic flow is not the only way to find "good" manifolds

2+1D Thirring model

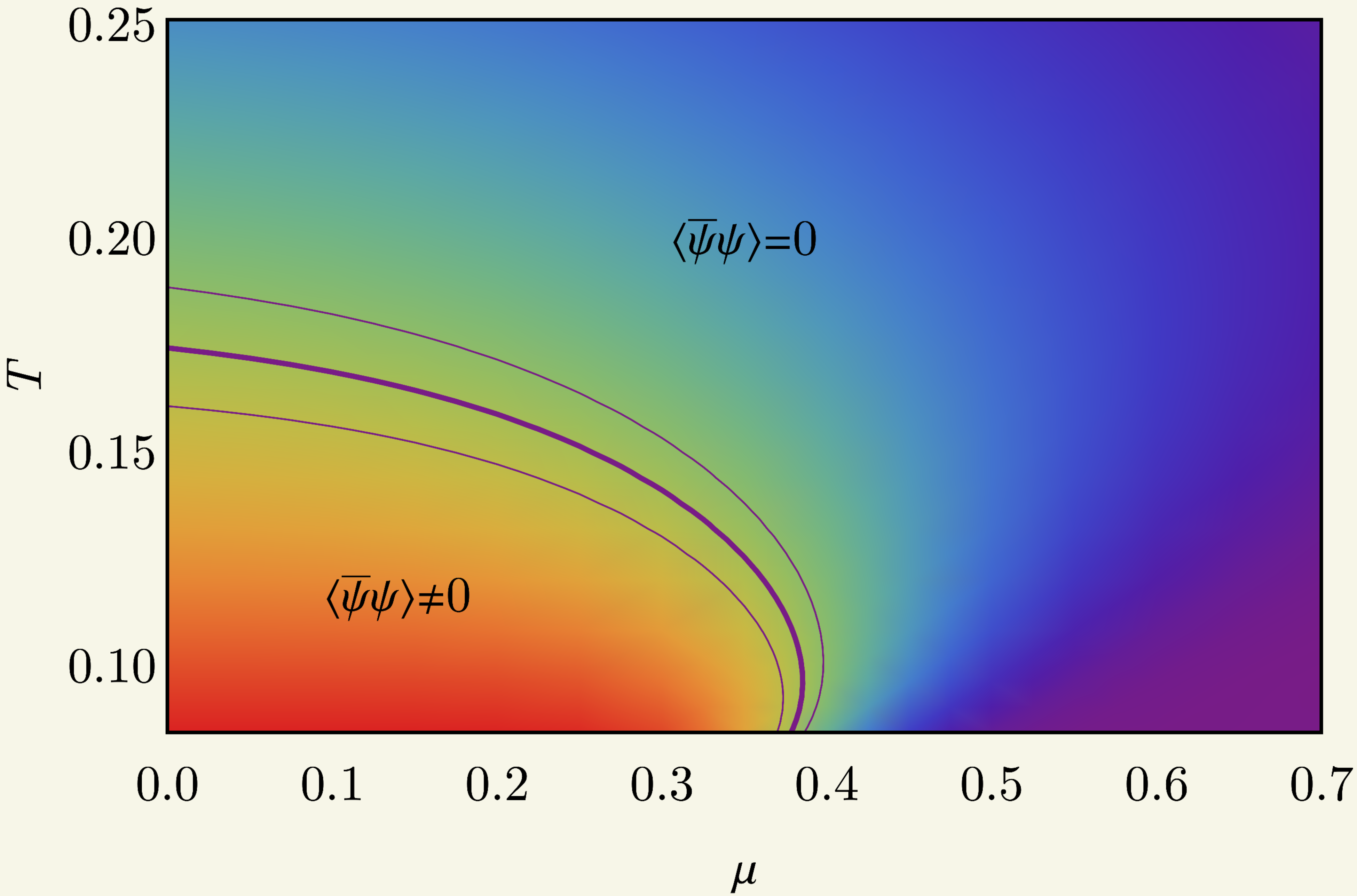


12x6x6

factorized ansatz (cheap jacobian):

$$\tilde{\phi}_i = \phi_i + if(\phi_i)$$

The holomorphic flow is not the only way to find "good" manifolds



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, … a whole new playground to attack the sign problem was opened up and remains largely unexplored
- We need more insight on complexified field theories - specially gauge theories - to design better ansatze