Generalized Thimble Method 2: The Return of the Thimbles

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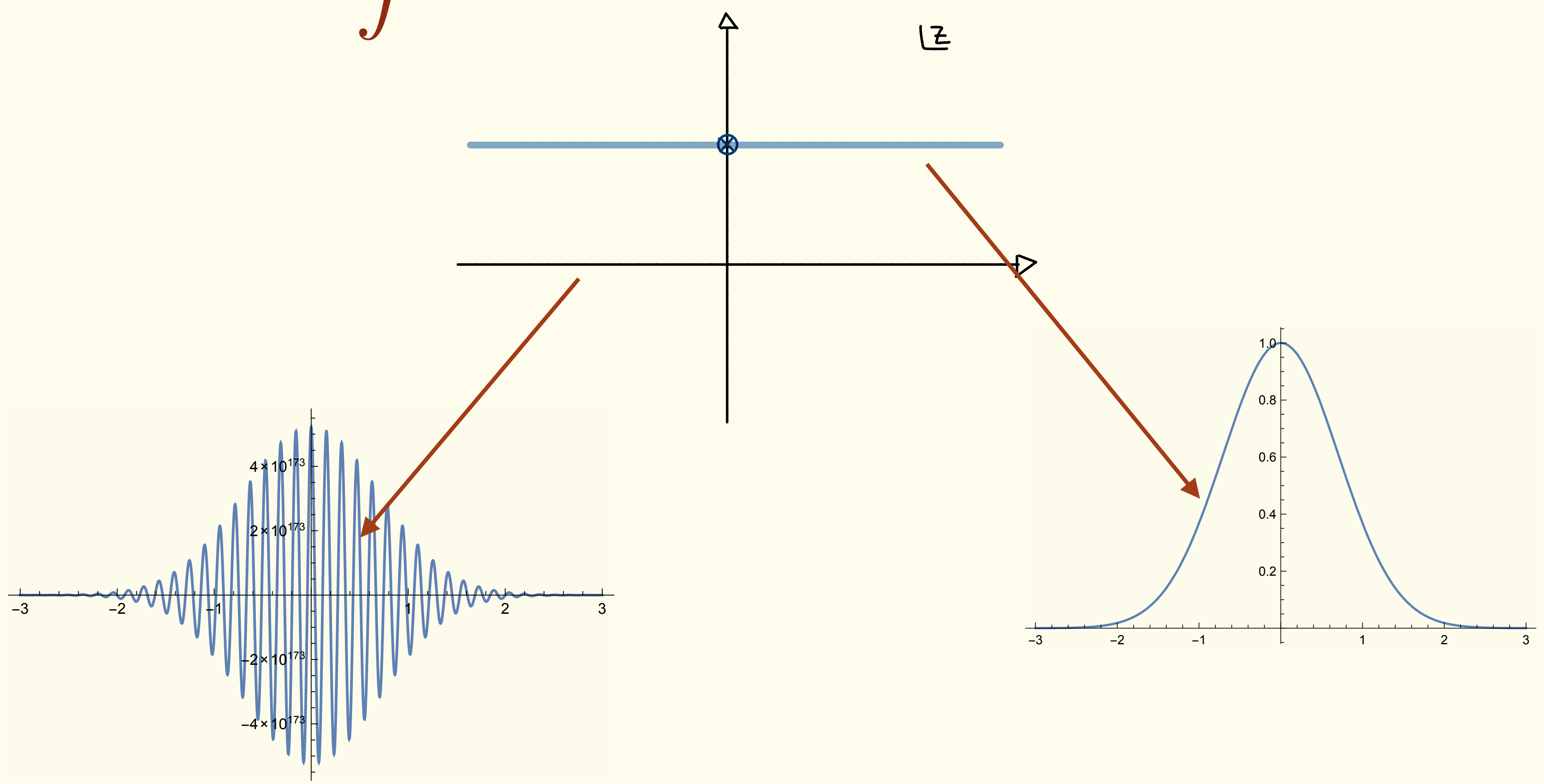
Central idea: deform the contour into the complex plane:

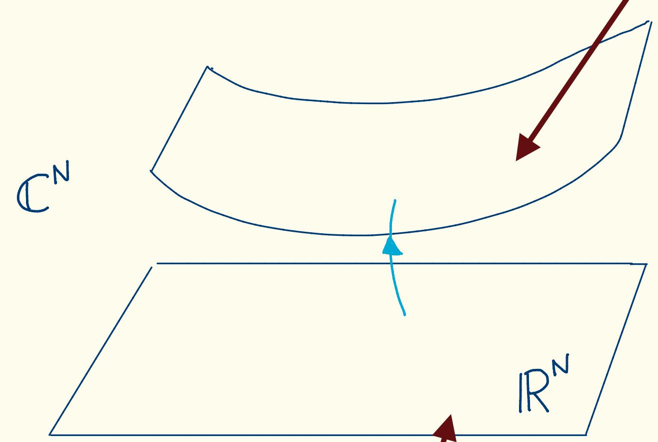
$$\int dx e^{-(z-i20)^2} = \sqrt{\pi}$$



Cristoforetti, DiRenzo, Scorzato, '12

How to find good deformations ?

new integration manifold



(real) field space

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

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

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

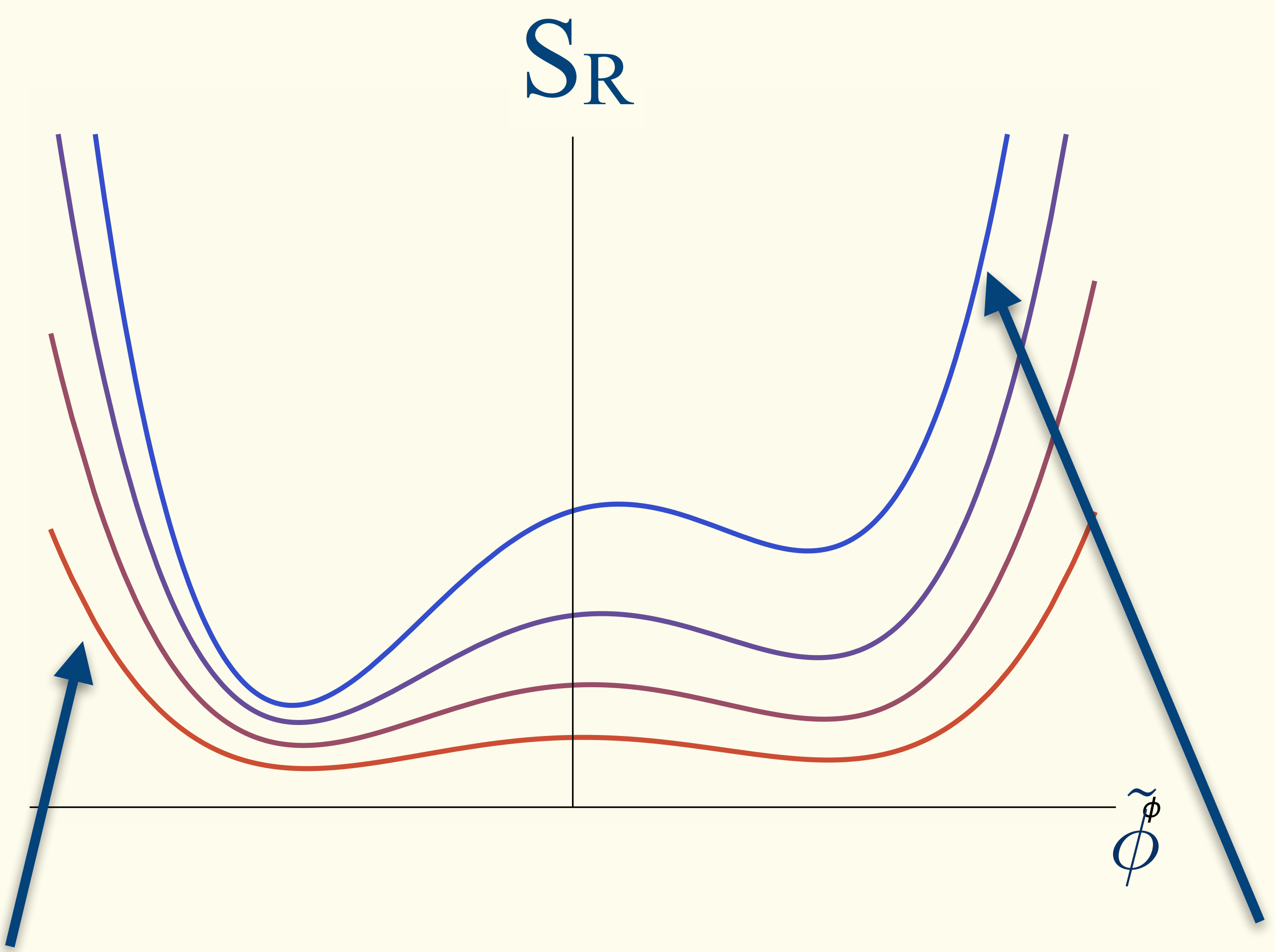
gradient flow of S^R, keeps integral well defined

hamiltonian flow of S^I, keeps phase fixed

How to find good deformations ?

S_R under the flow

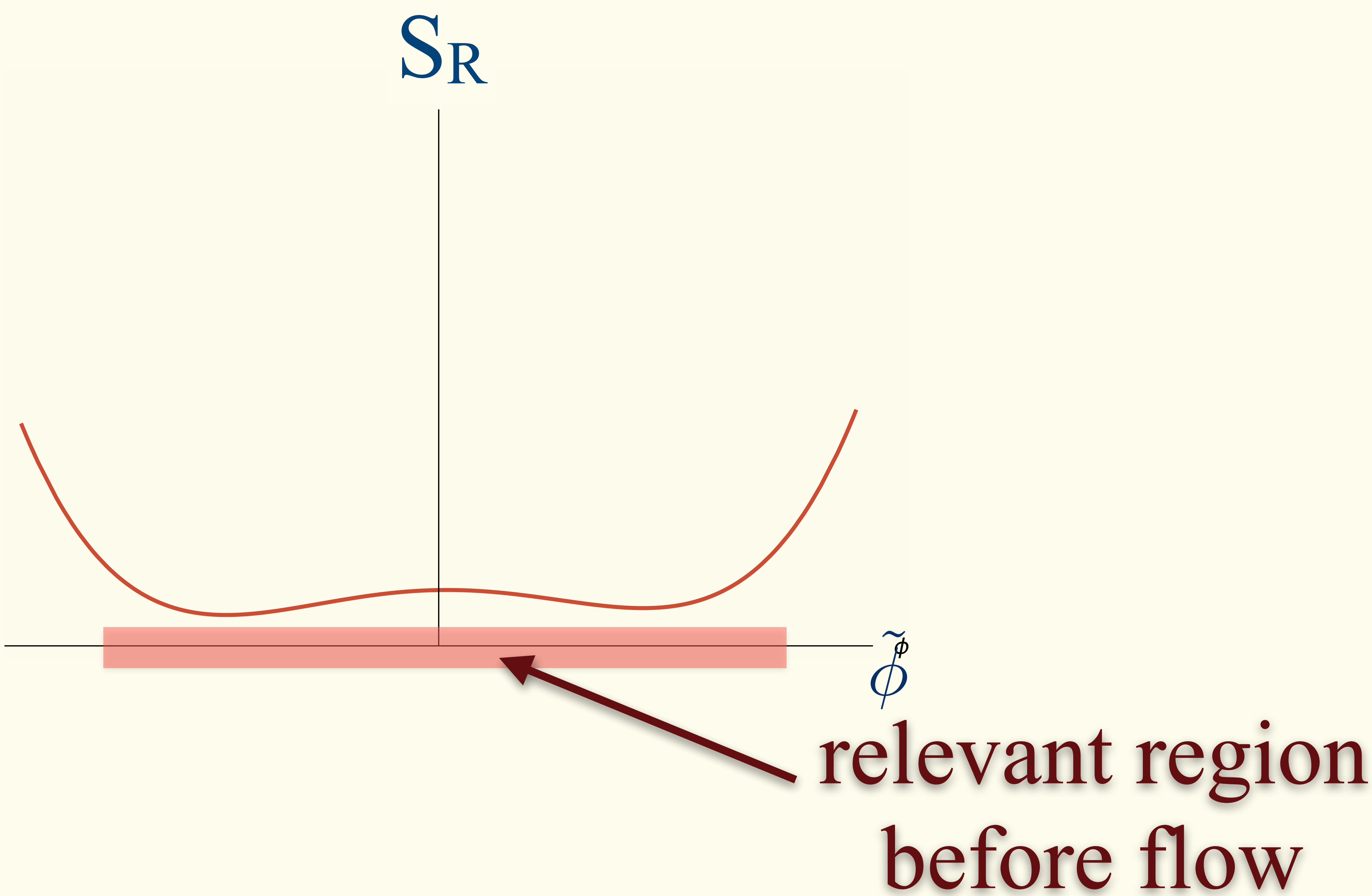
How to find good deformations ?



if this integral exists, so does that

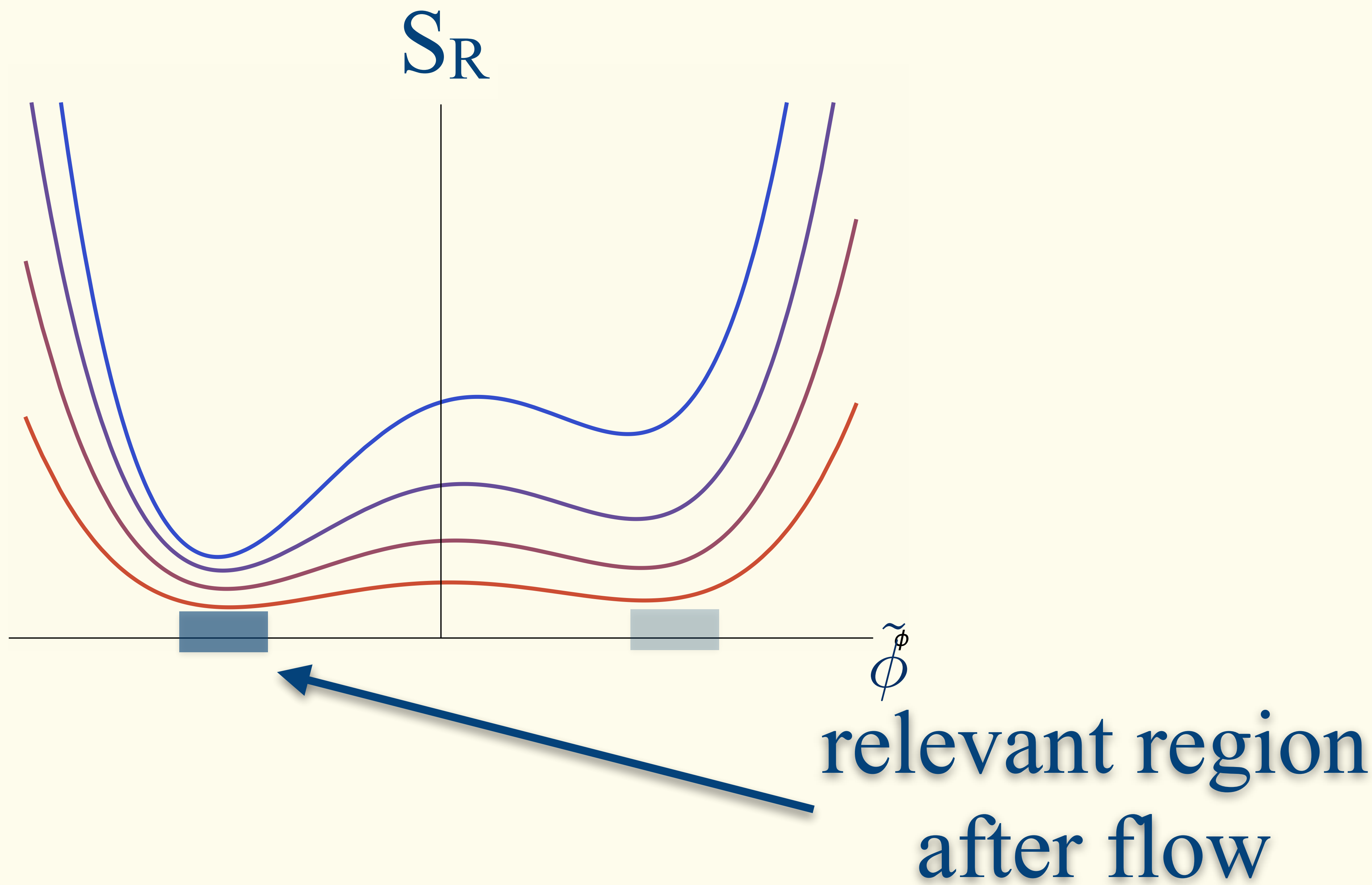
1) homology class preserved by the flow

How to find good deformations ?



S_R grows under the flow

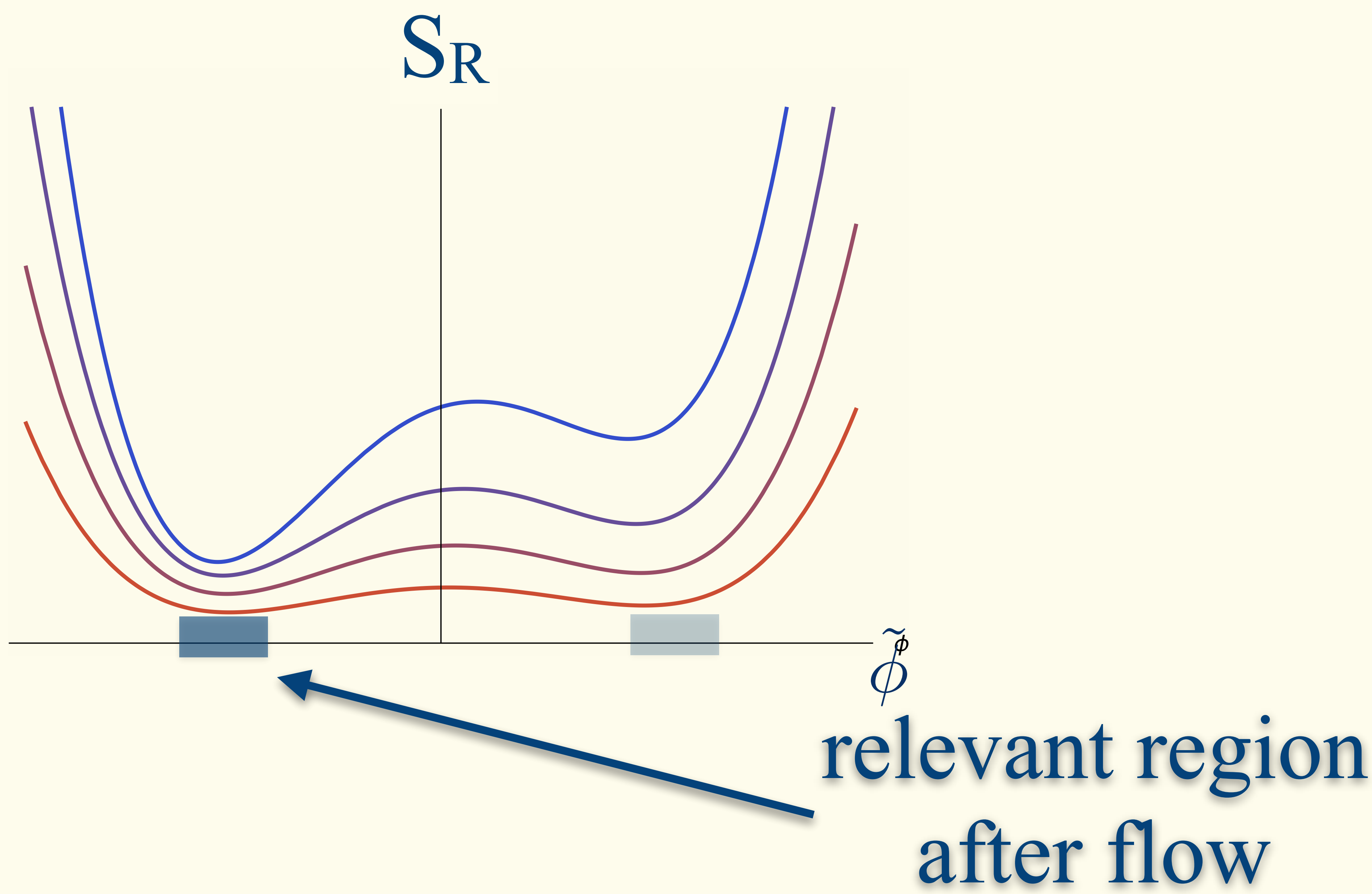
How to find good deformations ?



S_R grows under the flow

S_I stays constant

How to find good deformations ?

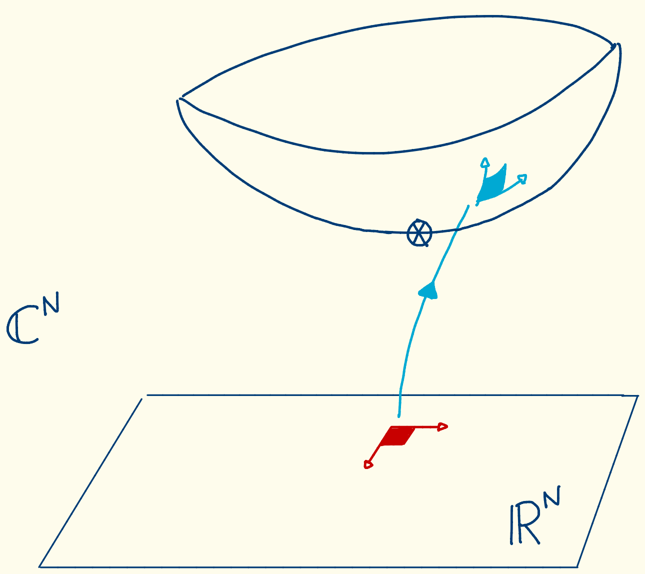


2) sign fluctuations are reduced

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

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

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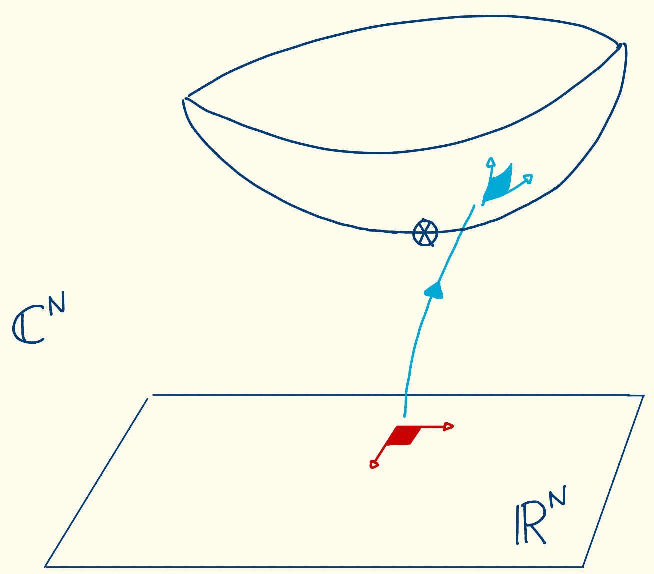


our algorithm

=

Metropolis in the real space,

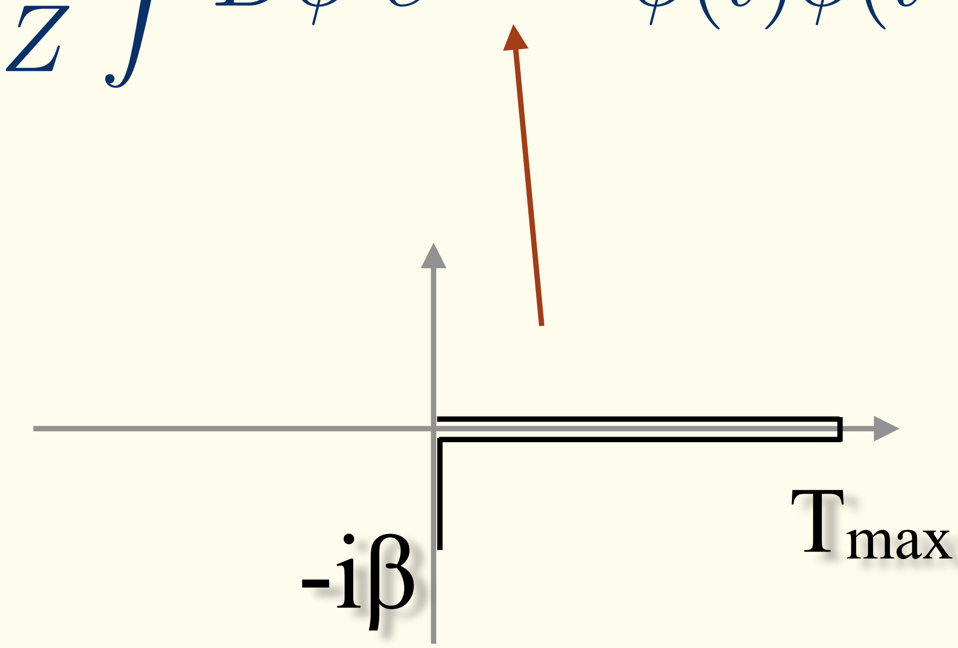
action S_{eff} and

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

Application: Real Time Dynamics

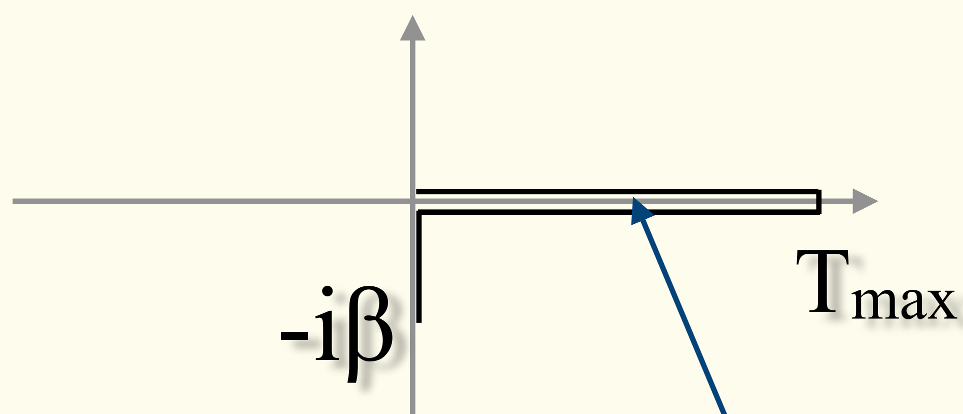
Viscosities, conductivities, … require:

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



Schwinger-Keldysh
contour
(works also out of equilibrium)

Real Time: The Mother of All Sign Problems



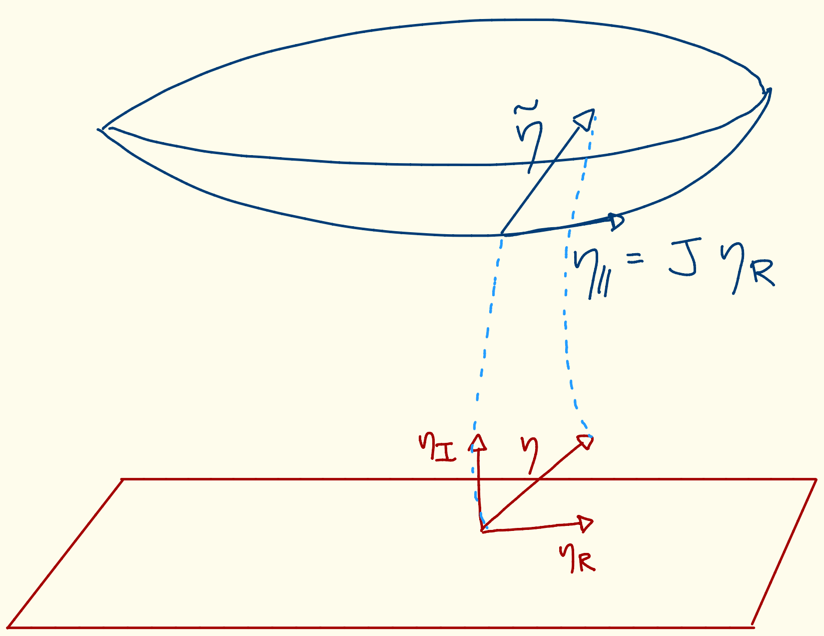
field at a point in the real axis does not contribute to the damping factor in e^{iSc}

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

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)

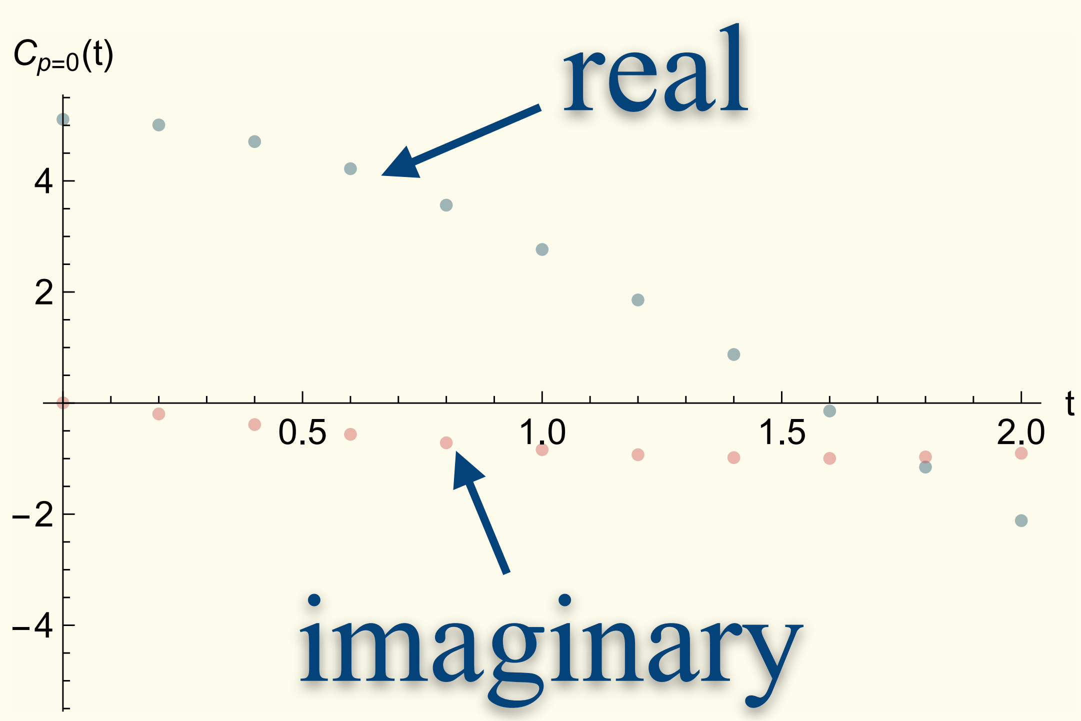


$$J\eta = \tilde{\eta} \qquad \tilde{\eta}_{\parallel} = J Re(\eta)$$

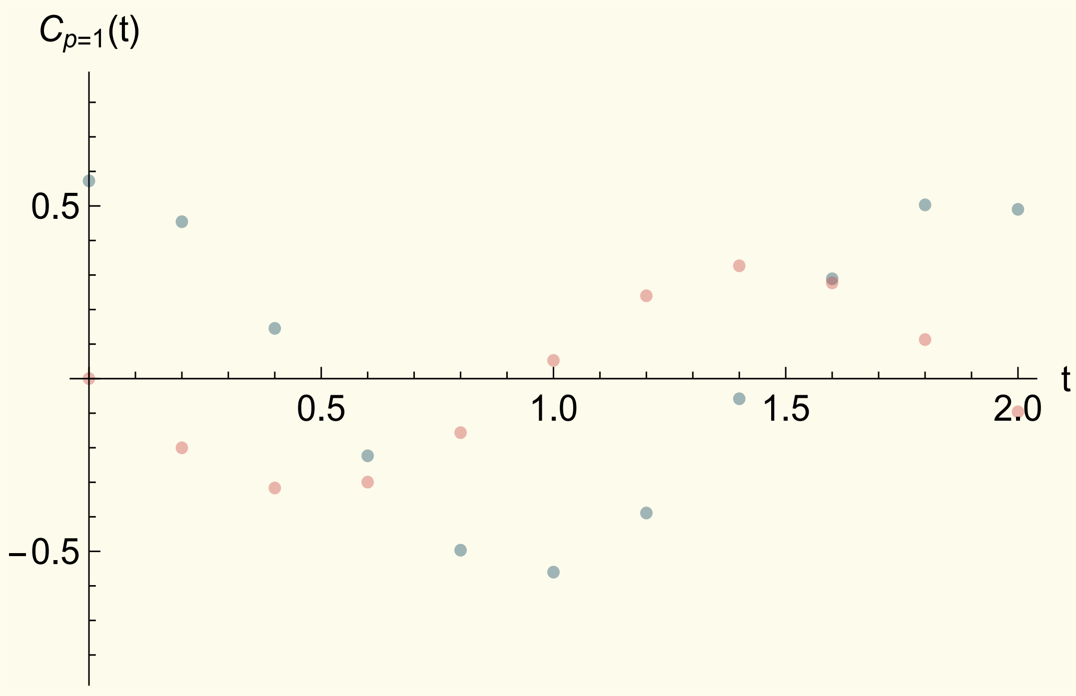
- isotropic proposal
- no need to compute det(J)

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

weak coupling



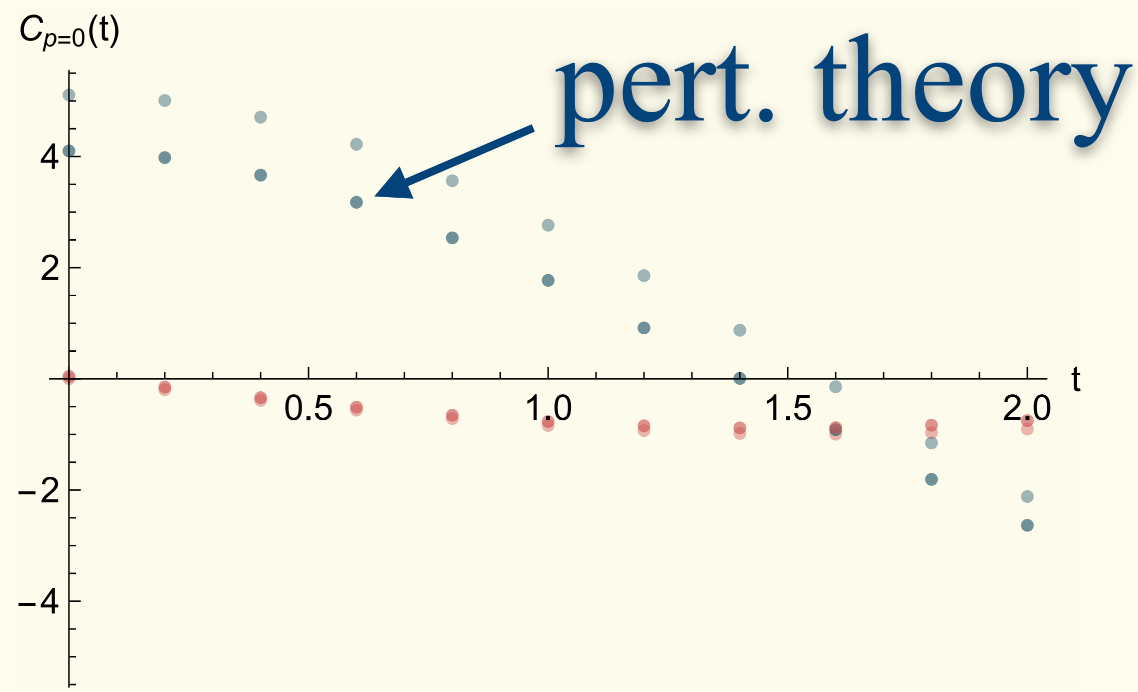
p=0

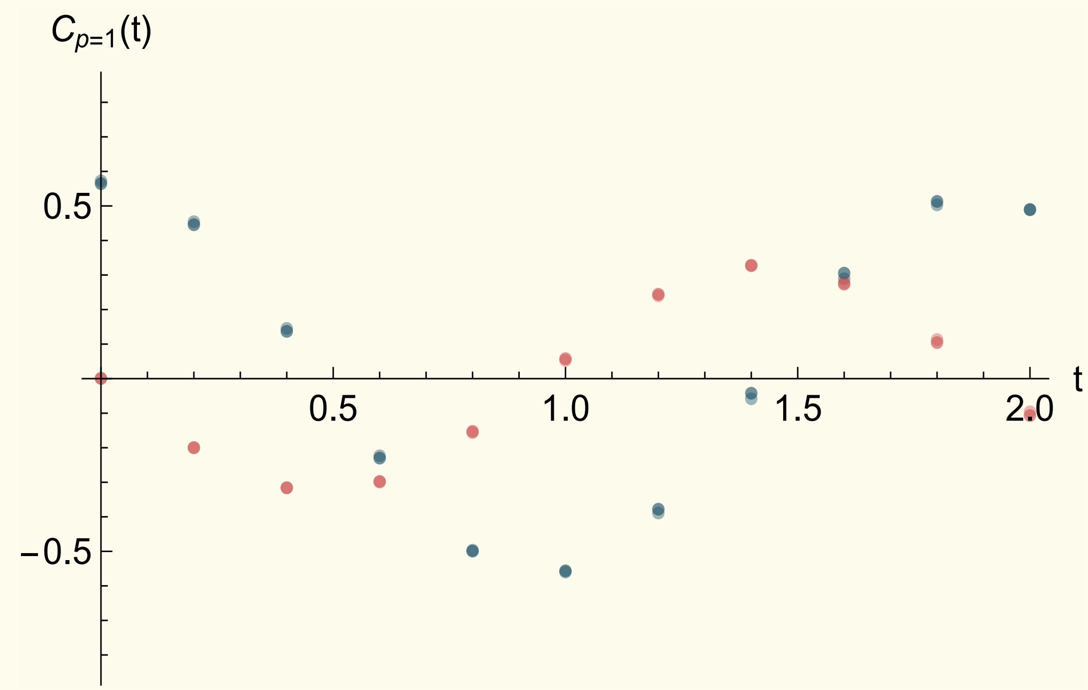


p=2π/L

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

weak coupling





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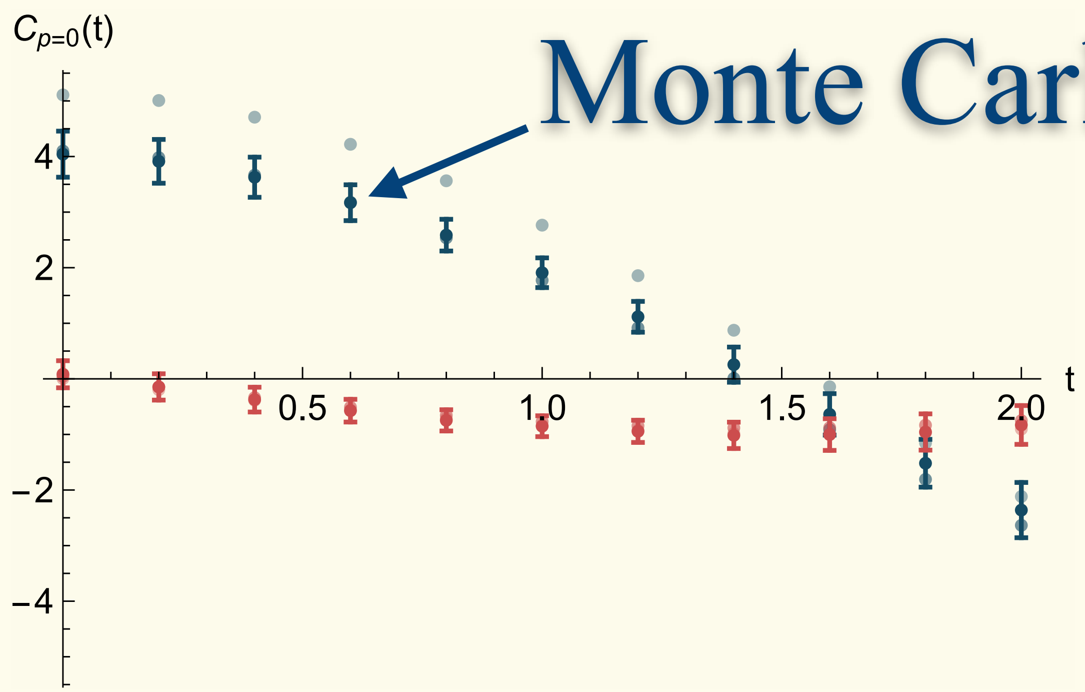
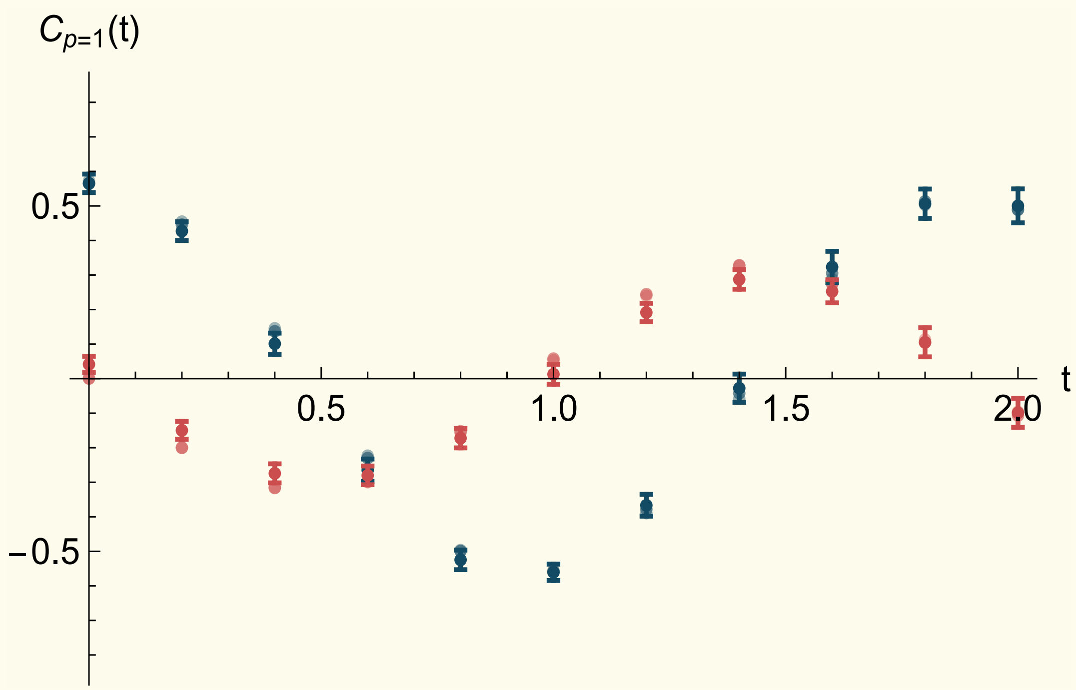


p=0



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

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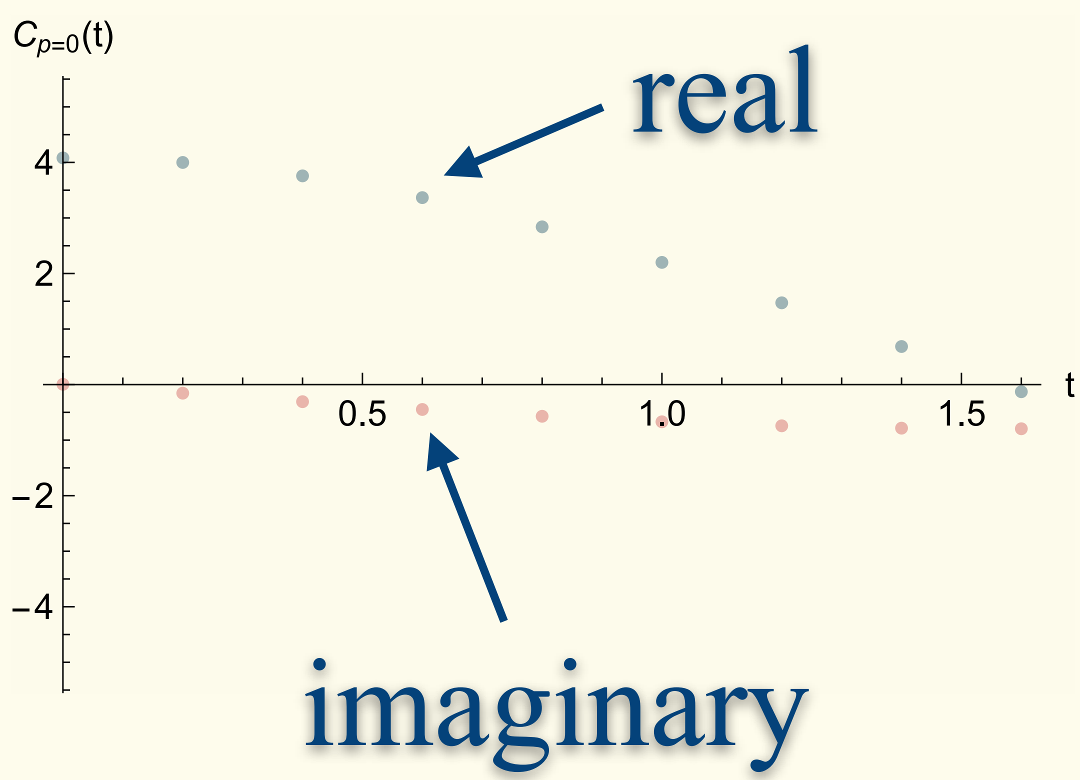
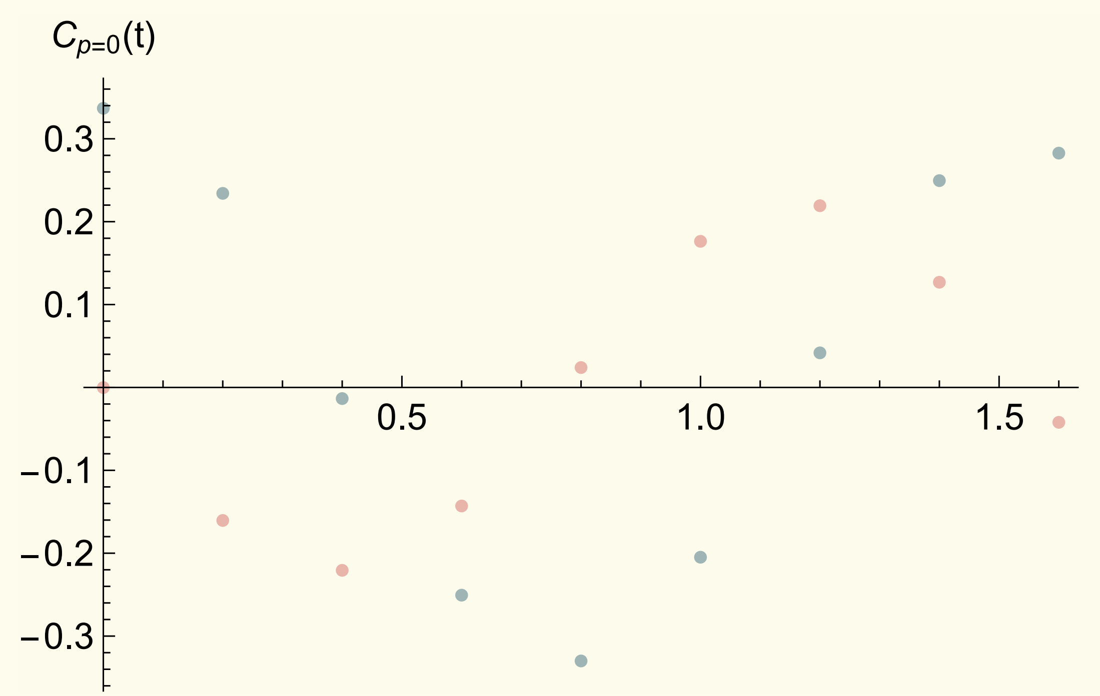


p=0



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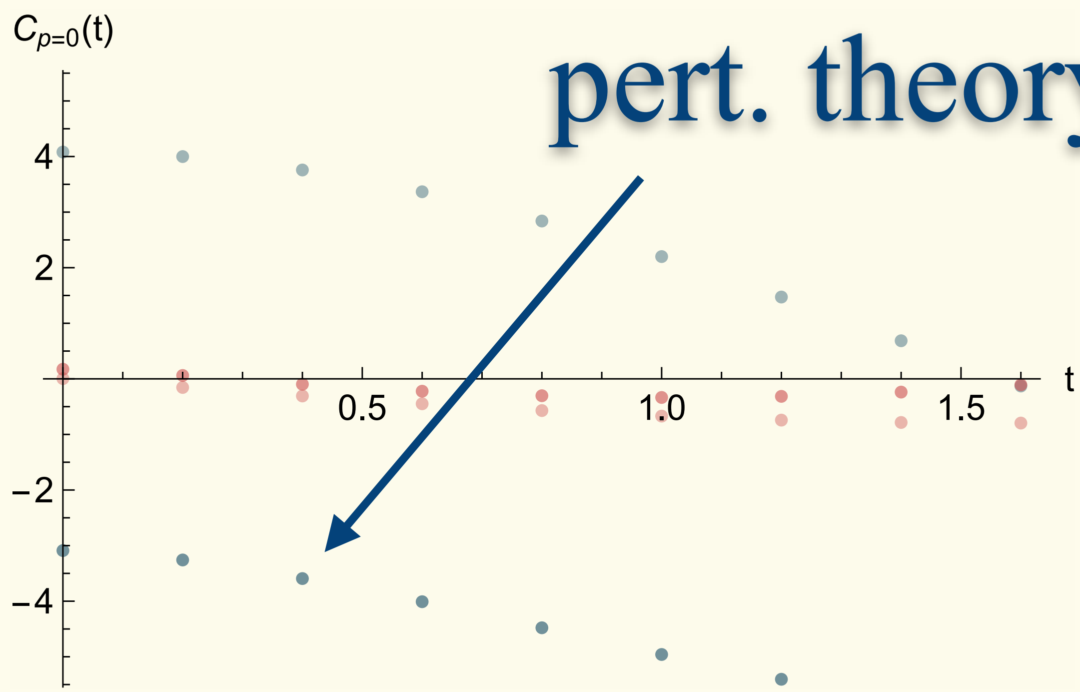
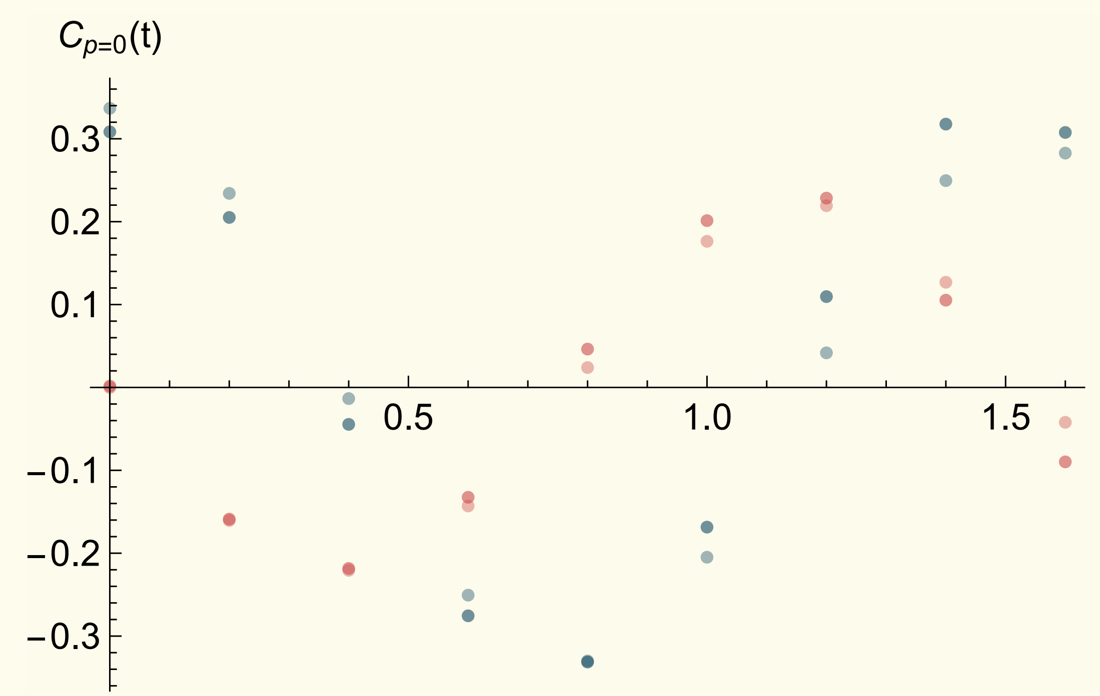


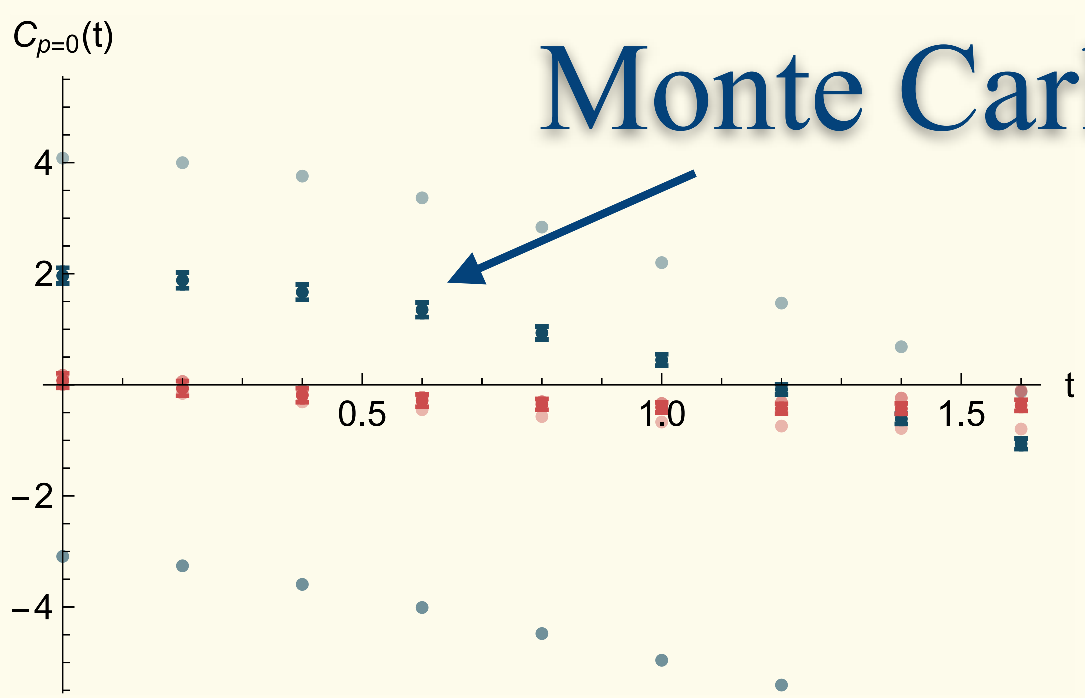
$p=0$



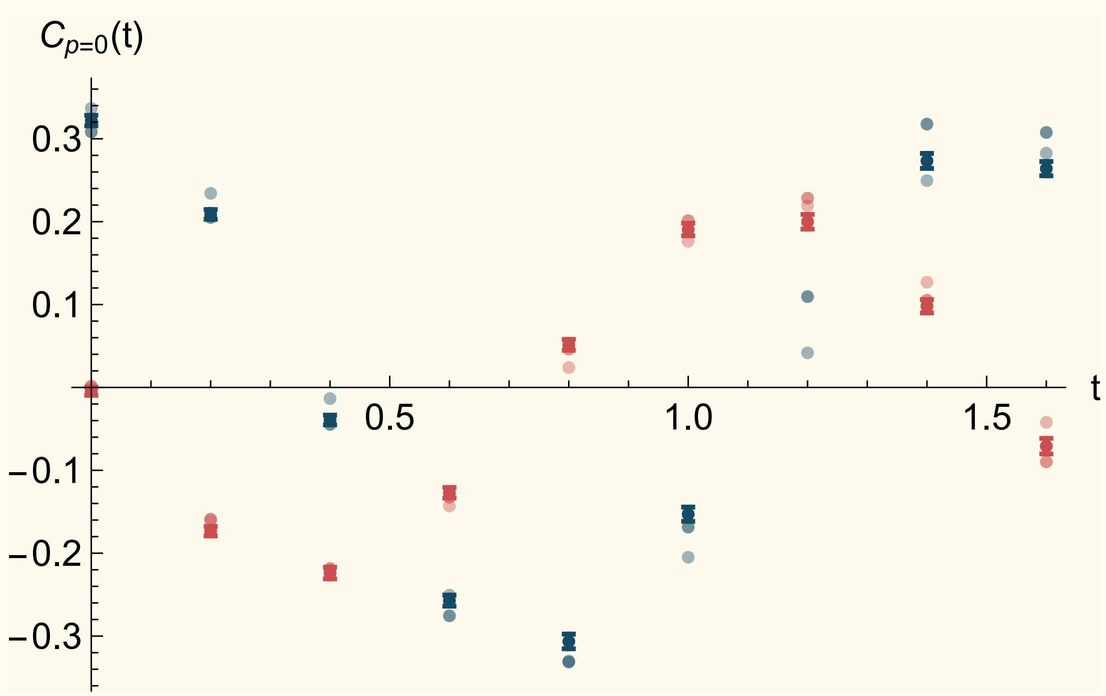
$p=2\pi/L$

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

strong coupling



p=0



p=2π/L

Application: Real Time Dynamics

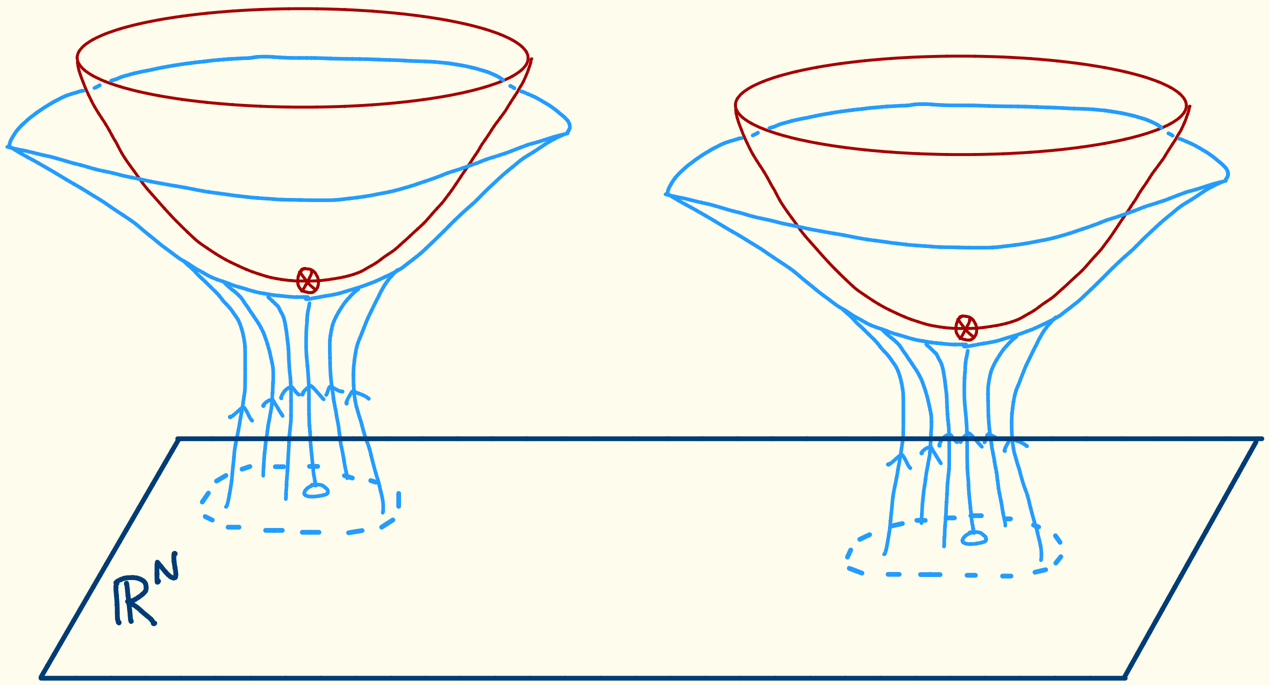
- Currently limited to small times : $t< 5/T$
- Cost increases sharply with t
- There has to be a catch:

simulation of a quantum computer performing the Schor algorithm

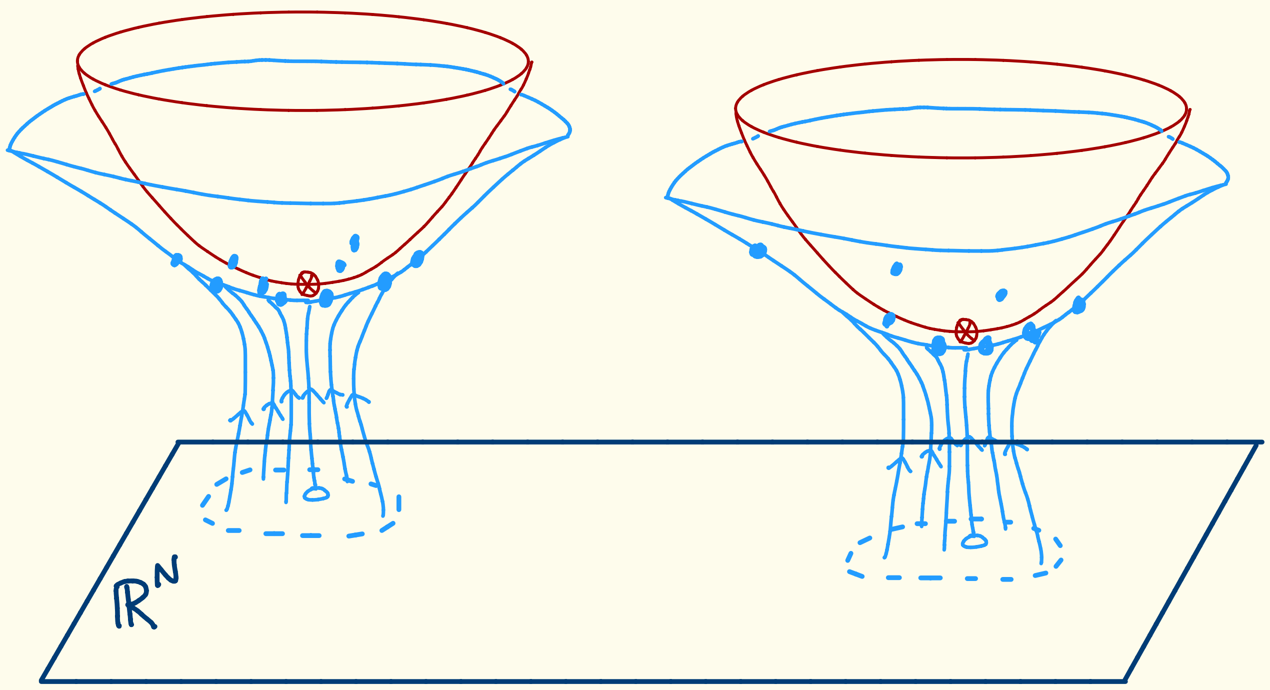
= nonsense

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

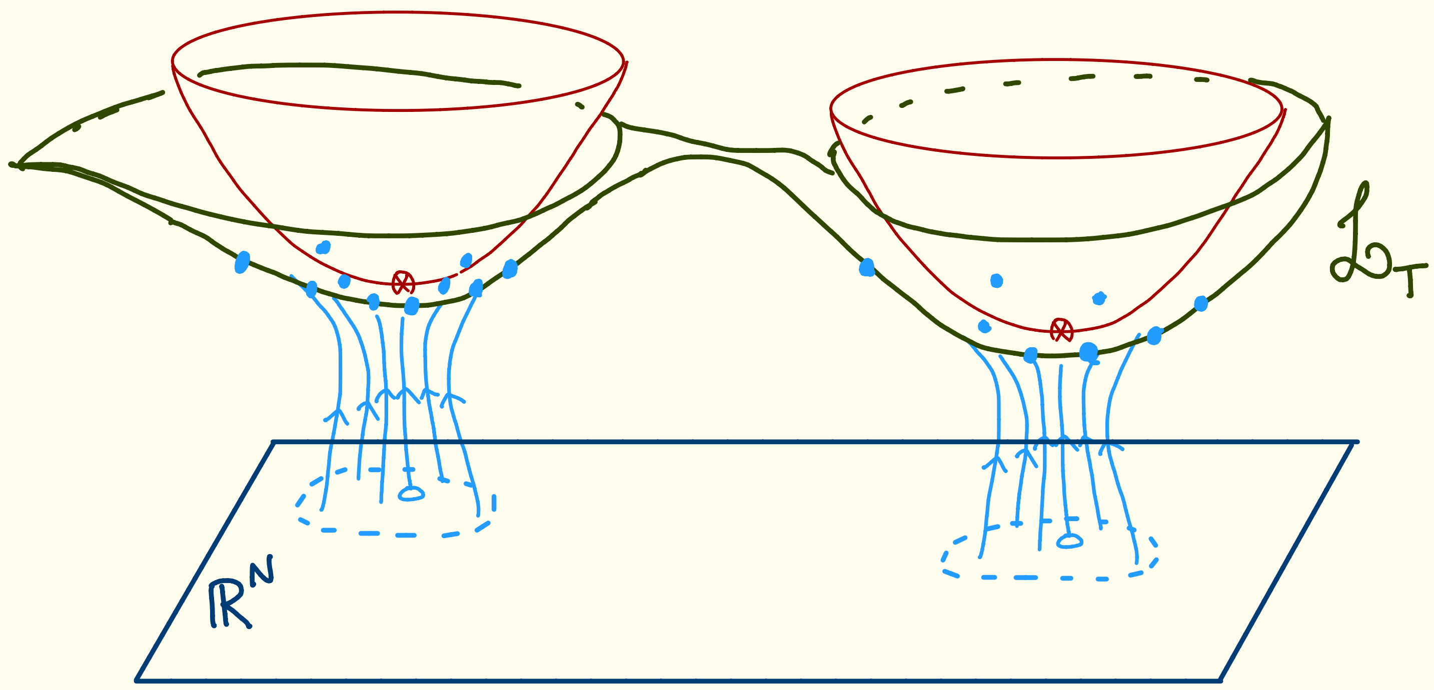
Bypassing the flow: machine learning



Bypassing the flow: machine learning



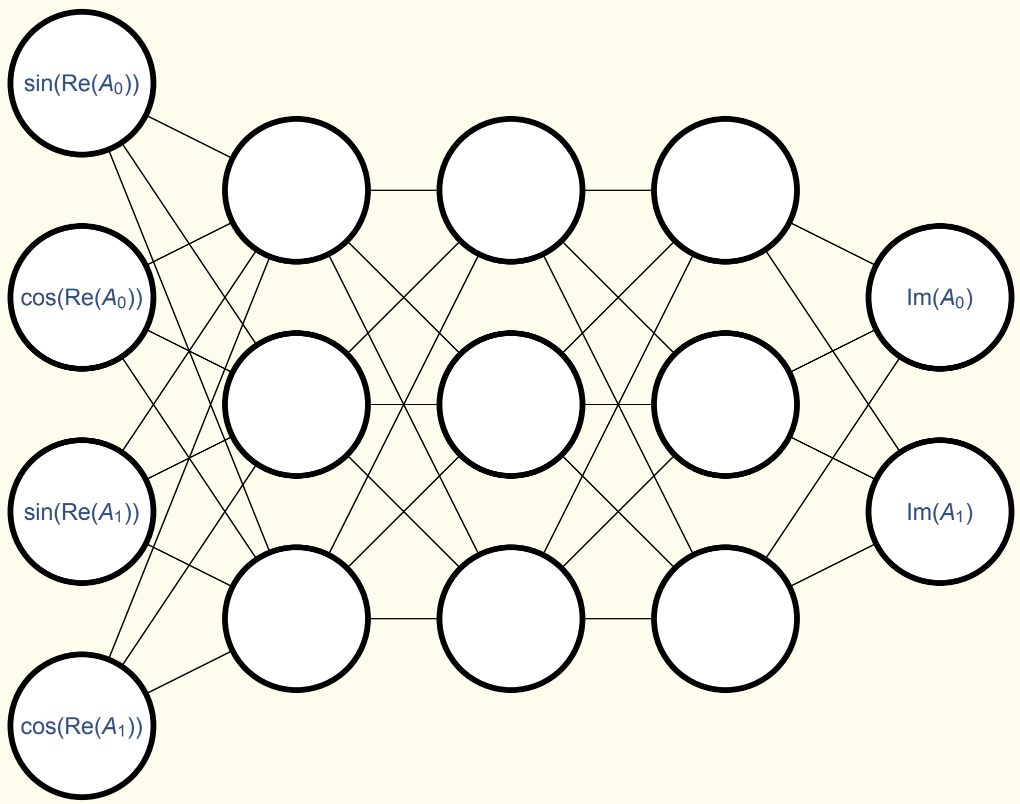
Bypassing the flow: machine learning



$\mathcal{L}_T$=(rough?) interpolation of points of $\mathcal{M}_T$

Bypassing the flow: machine learning

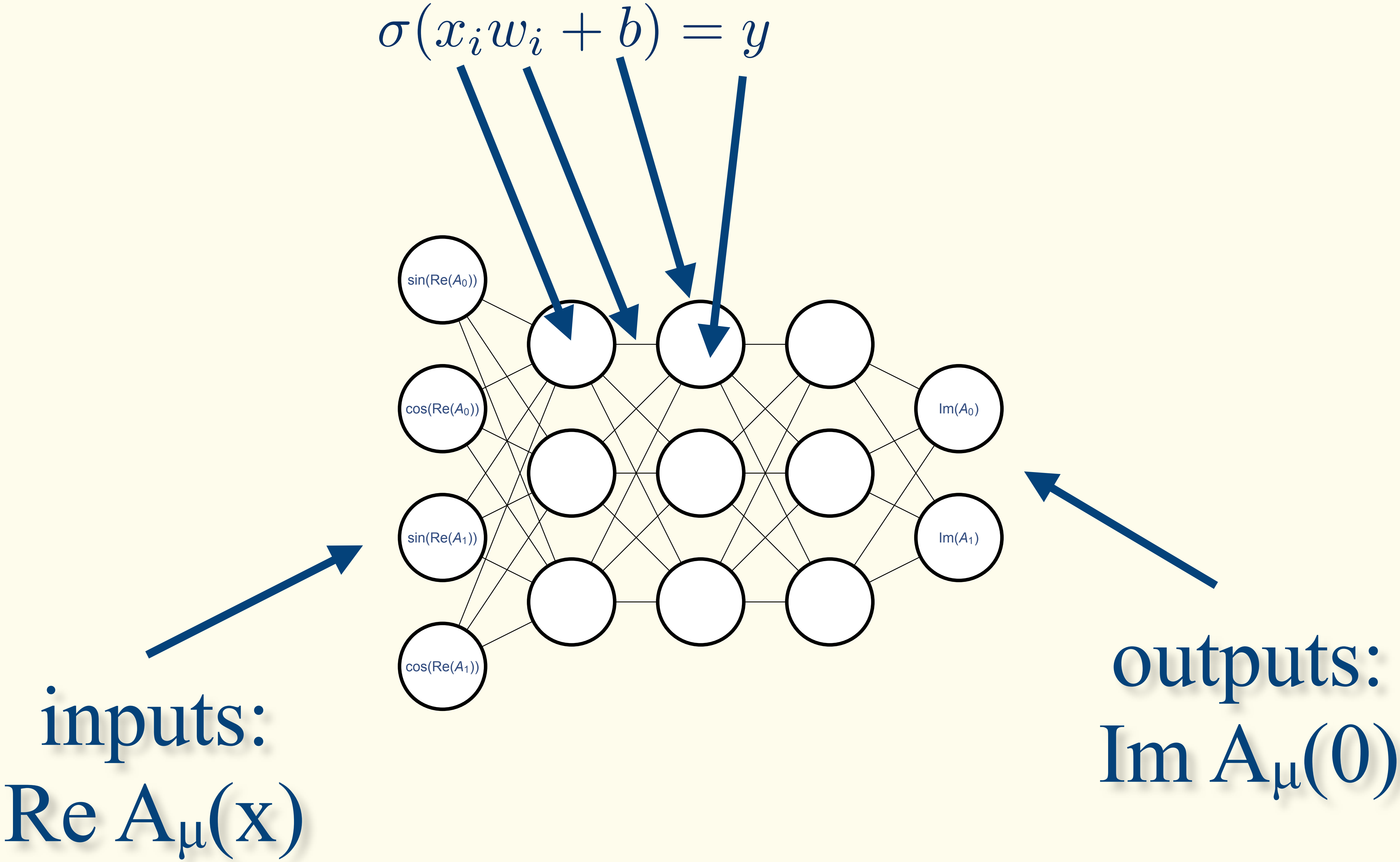
feed-forward neural net
(supervised training)



inputs:
Re $A_\mu(x)$

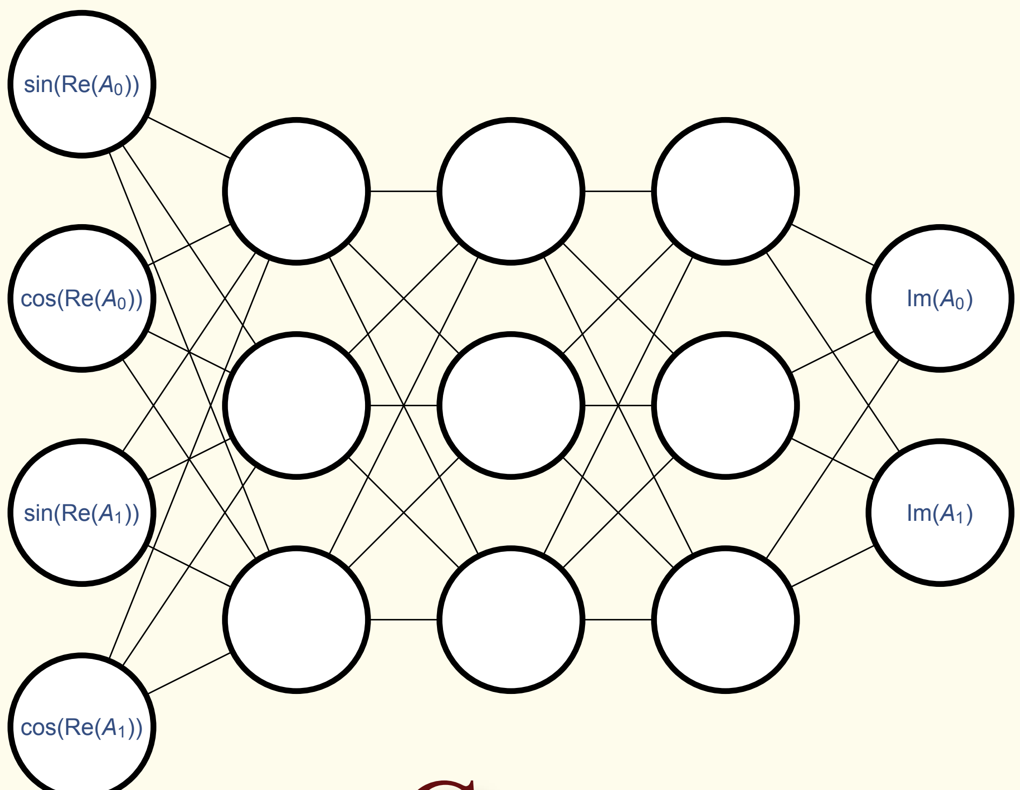
outputs:
Im $A_\mu(0)$

Bypassing the flow: machine learning



Bypassing the flow: machine learning

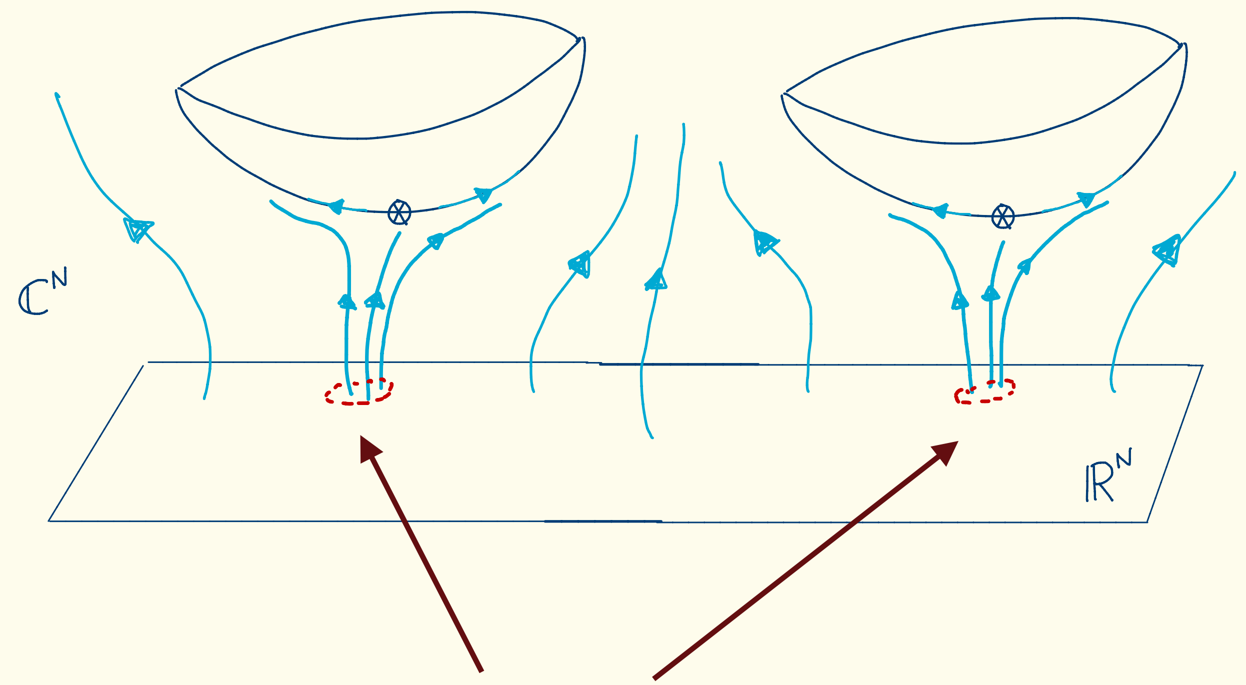
feed-forward neural net (supervised training)



Cost:

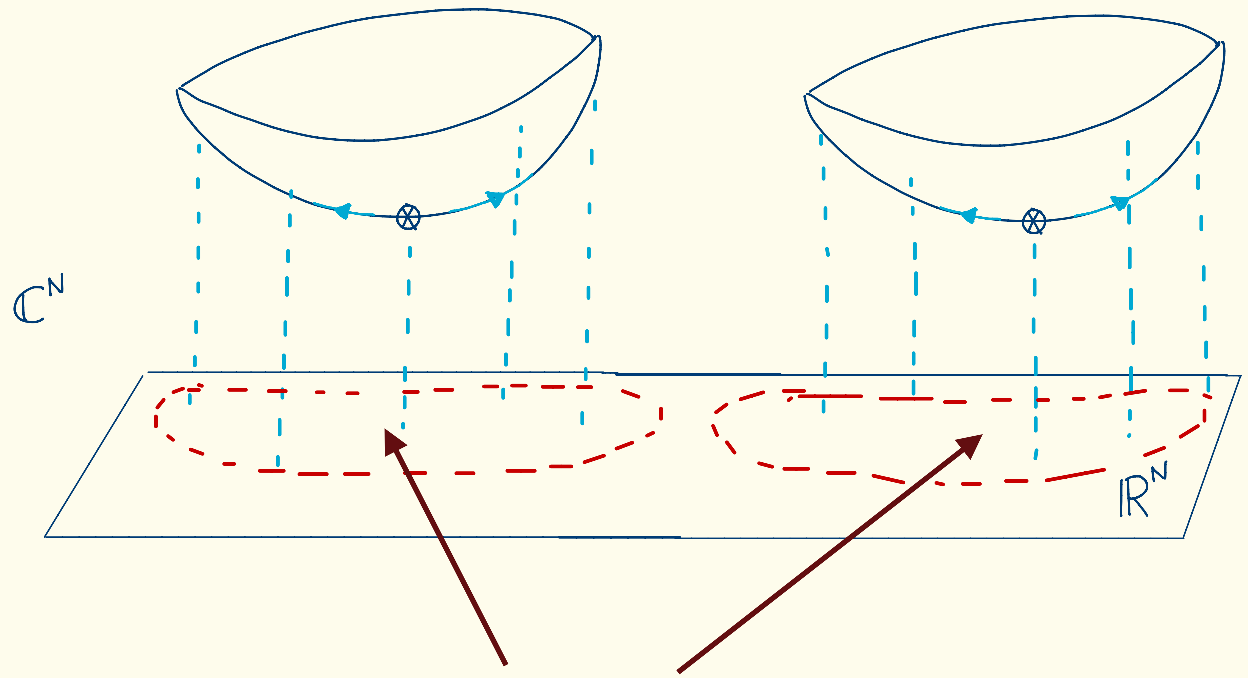
flowed configurations >> training >> sampling

Bypassing the flow: machine learning



isolated modes: trapping

Bypassing the flow: machine learning

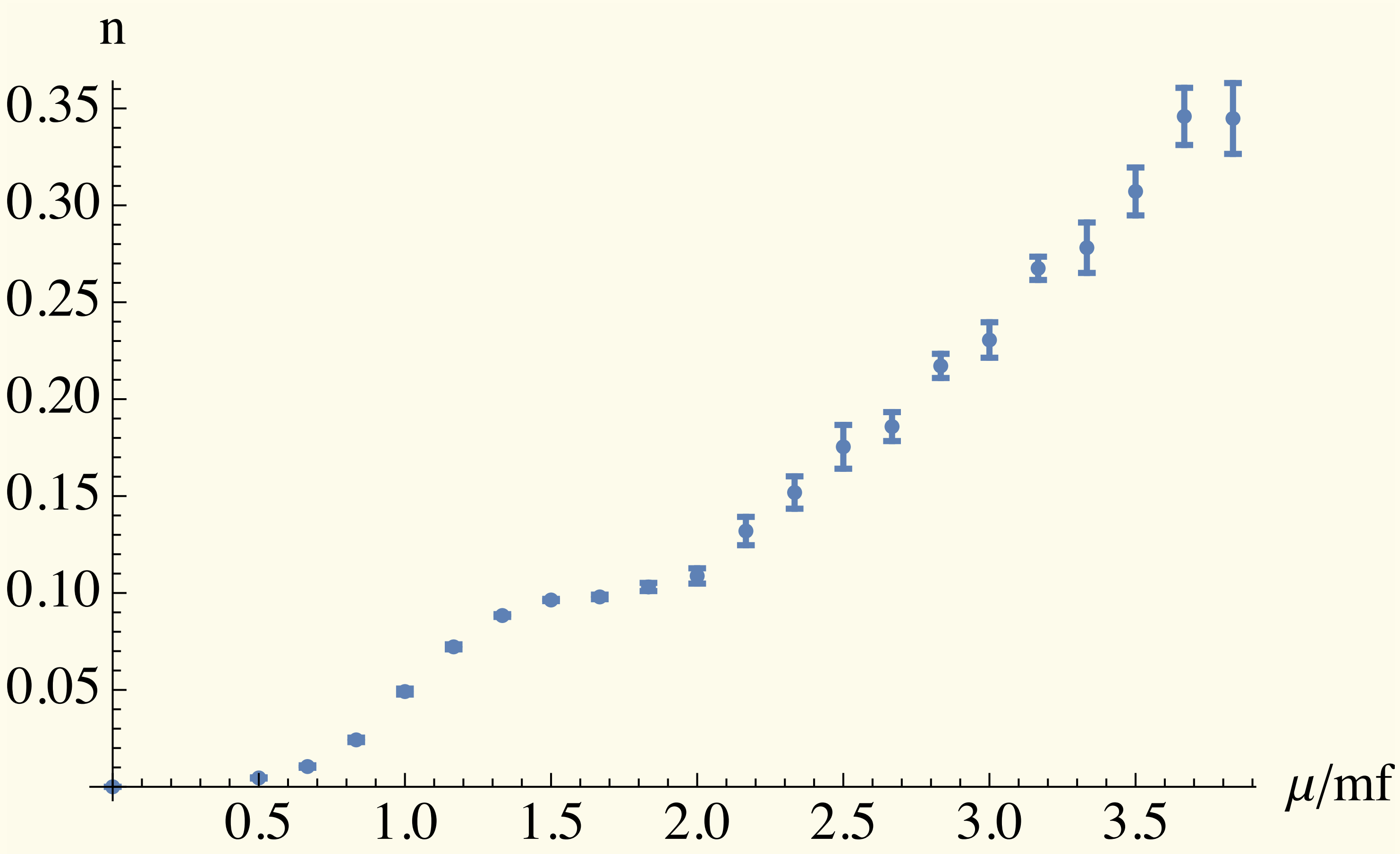


no trapping

continuous map between manifolds: $$\phi = \tilde{\phi}_R + t\ \phi_I$$

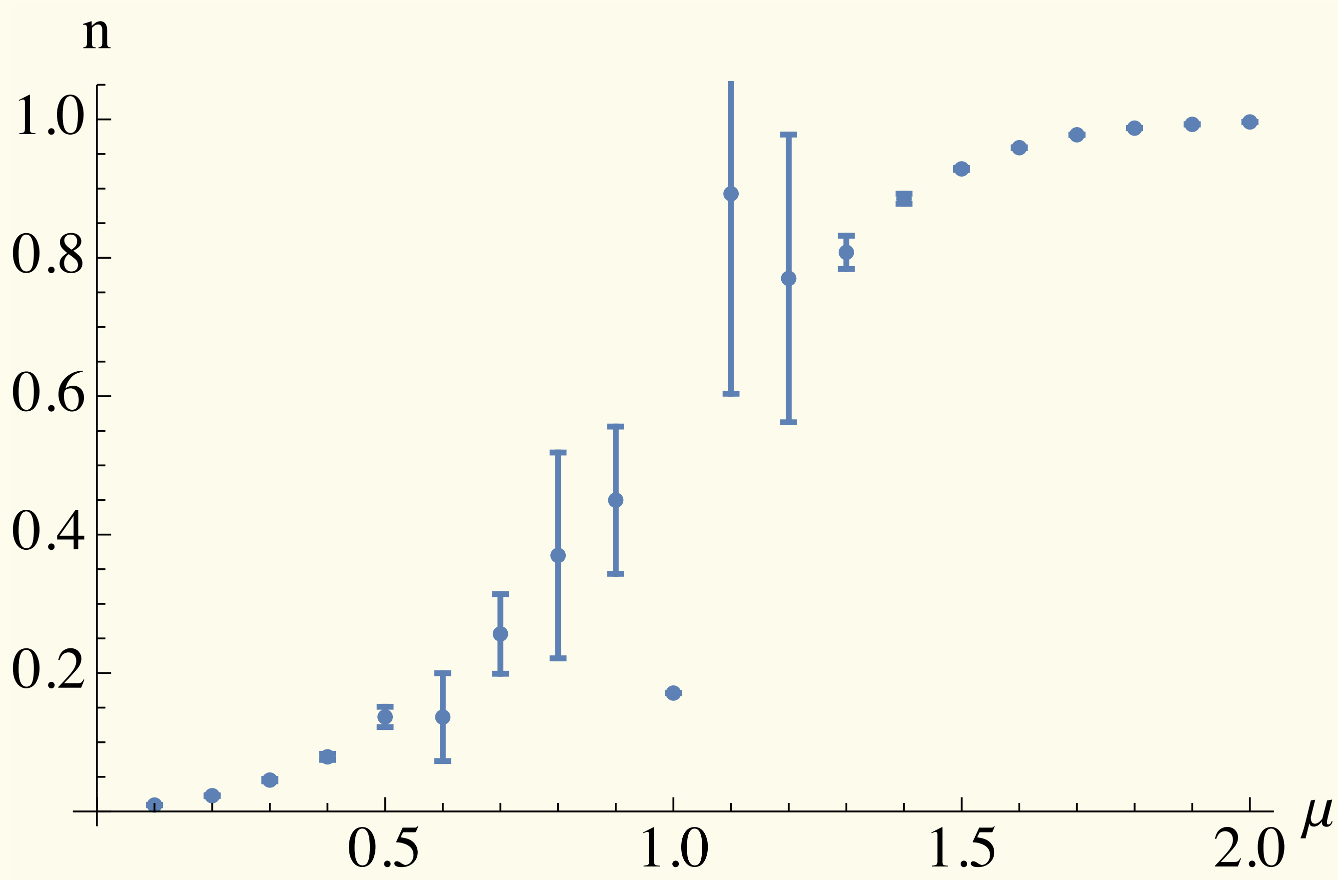
Bypassing the flow: machine learning

Wilson, 20 x10 lattice, $N_F=2$, $am_f=0.3$



Why stop there: let the network find a manifold with a "good" sign

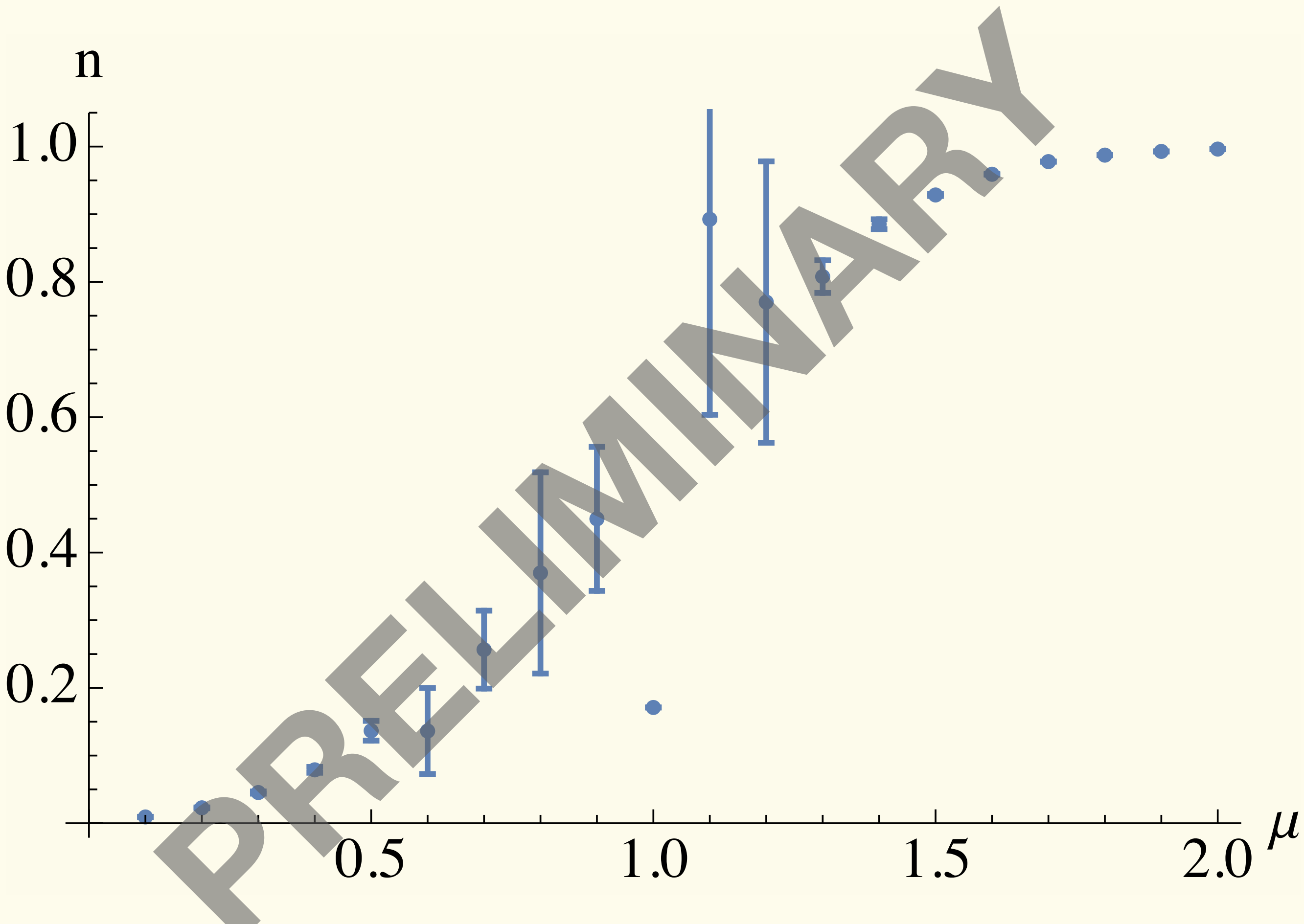
6^3 lattice



- It finds the shift to tangent plane in the 1st minute; then it finds a better "renormalized tangent plane"
- It doesn't get terribly better fast

Why stop there: let the network find a manifold with a "good" sign

6^3 lattice



- It finds the shift to tangent plane in the 1st minute; then it finds a better "renormalized" thimble
- It doesn't get terribly better fast

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, …