Complex paths beyond Lefschetz thimbles: real time dynamics and the sign problem

Andrei Alexandru

Paulo Bedaque, Gökçe Başar, Neill Warrington, Greg Ridgway
Henry Lamm, Scott Lawrence

Quark Confinement and
Hadron Spectrum
August 2018

THE GEORGE
WASHINGTON
UNIVERSITY
WASHINGTON, DC

The plan

- Importance sampling and sign problem
- Complexification and contour deformation
- Generalized thimble method
- Case studies: Massive Thirring model & real-time correlators
- New proposals: sign optimized manifolds and learnifolds

Motivation

- Physical models of interest require non-perturbative calculations that have a sign problem:
    - QCD at finite baryon density (RHIC, neutron star structure, etc)
    - Real time dynamics for strongly coupled QFT
    - Strongly correlated electrons (Hubbard model, etc.)
- While a generic solution to the sign problem is impossible, thimble methods are likely to work for a large class of problems.

QFT on the lattice

- The partition function is expressed as a path integral
- The fields are sampled on a grid; differential operators are replaced by finite difference ones

$$Z = \int \mathcal{D}\phi\, e^{-S[\phi]} \to Z_{\text{latt}} = \int_{\mathbb{R}^N} \prod_i \mathrm{d}\phi_i\, e^{-S[\phi]}$$

$$S_{\text{latt}} = \sum_n \left[\tilde{m}\phi_n^2 + \sum_\alpha \kappa_\alpha \phi_n \phi_{n+\hat{\alpha}} + \tilde{\lambda}\phi_n^4 \right]$$

- The partition function is a many-dimensional integral over **real** variables
- The integrand has **no singularity** for both bosonic and fermionic theories

Monte-Carlo sampling

- QFT correlators are statistical averages

$$\langle O \rangle = \frac{1}{Z} \int \mathcal{D}\phi \, e^{-S(\phi)} O(\phi)$$

- Estimate using importance sampling

$$\langle O \rangle \approx \frac{1}{N} \sum_{i=1}^{N} O(\phi_i) \qquad \{\phi_1, \ldots, \phi_N\} \text{ with } P(\phi) = \frac{1}{Z} e^{-S(\phi)}$$

- Stochastic errors decrease with sample size

$$\sigma_O = \sqrt{\langle O^2 \rangle - \langle O \rangle^2} \propto \frac{1}{\sqrt{N}}$$

Sign problem

- When the partition function is not real direct Monte-Carlo sampling is not possible
- The usual workaround involves *reweighting*

$$Z_0 = \int \mathcal{D}\phi \left| e^{-S(\phi)} \right| = \int \mathcal{D}\phi \, e^{-S_R(\phi)}$$

$$\langle O(\phi) \rangle_Z = \frac{\left\langle O(\phi) e^{-iS_I(\phi)} \right\rangle_{Z_0}}{\left\langle e^{-iS_I(\phi)} \right\rangle_{Z_0}}$$

- Sampling is done based on S_R; S_I is introduced in the observable: $\{\phi_1, \ldots, \phi_N\}$ with $P(\phi) \propto e^{-S_R(\phi)}$

$$\langle O \rangle \approx \frac{1}{N} \sum_{i=1}^{N} O(\phi_i) e^{-iS_I(\phi)} \Bigg/ \frac{1}{N} \sum_{i=1}^{N} e^{-iS_I(\phi)}$$

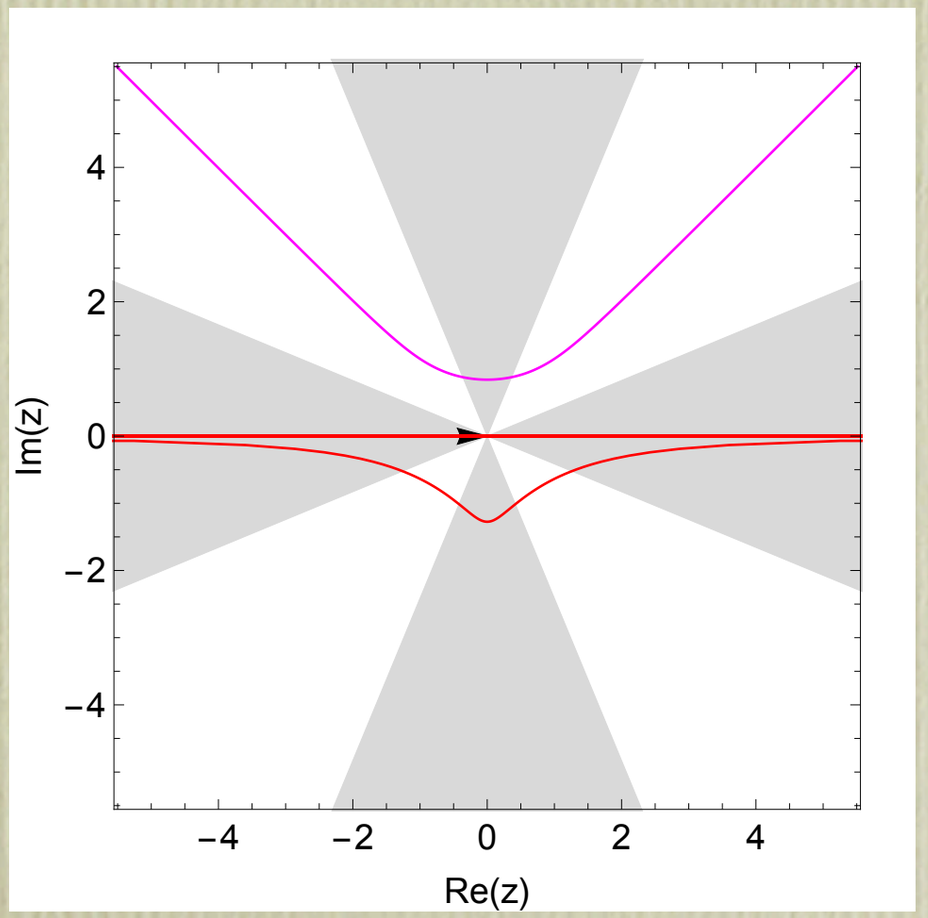
Sign problem

- A *sign problem* appears when the phase average is nearly zero (or zero): $e^{-iS_I(\phi_1)} + \ldots + e^{-iS_I(\phi_N)} \ll N$
- The cost of the calculation is inversely proportional to the phase average: $N \propto \left\langle e^{-iS_I(\phi)} \right\rangle^{-2}$
- For example in QCD

$$\left\langle e^{-iS_I} \right\rangle_{Z_0} = \frac{Z}{Z_0} = e^{-\beta V (f_{\text{baryon}} - f_{\text{isospin}})} \to 0 \text{ as } V \to \infty$$

- In QCD the calculation cost increases exponentially with the volume

Contour deformation



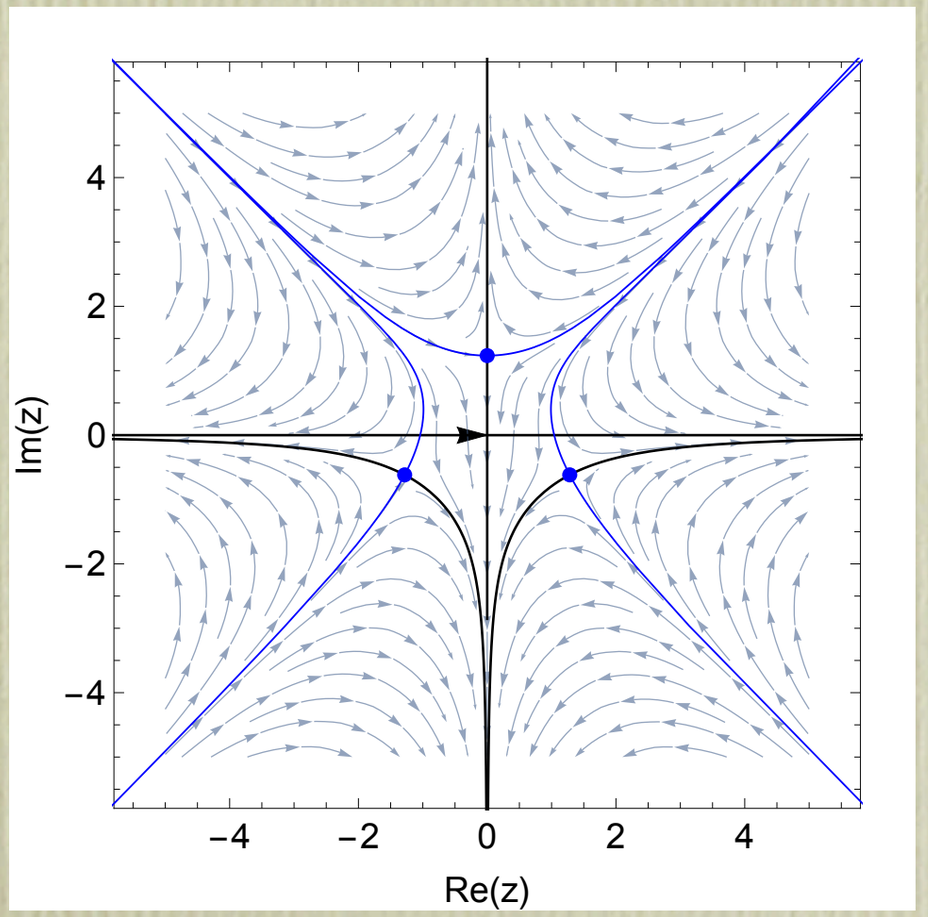
$$Z = \int_{-\infty}^{\infty} \mathrm{d}x\, e^{-S(x)}$$

$$S(x) = x^4 - x^2 + 10ix$$

$$Z = \int_{\mathcal{C}} \mathrm{d}z\, e^{-S(z)}$$

- Generalized Cauchy's theorem
- Deformation in the field variable space (lattice geometry unchanged)

Holomorphic gradient flow and Lefschetz thimbles



$$Z = \int_{-\infty}^{\infty} \mathrm{d}x\, e^{-S(x)}$$

$$\frac{dS}{dz} = 0 \quad \text{(critical points)}$$

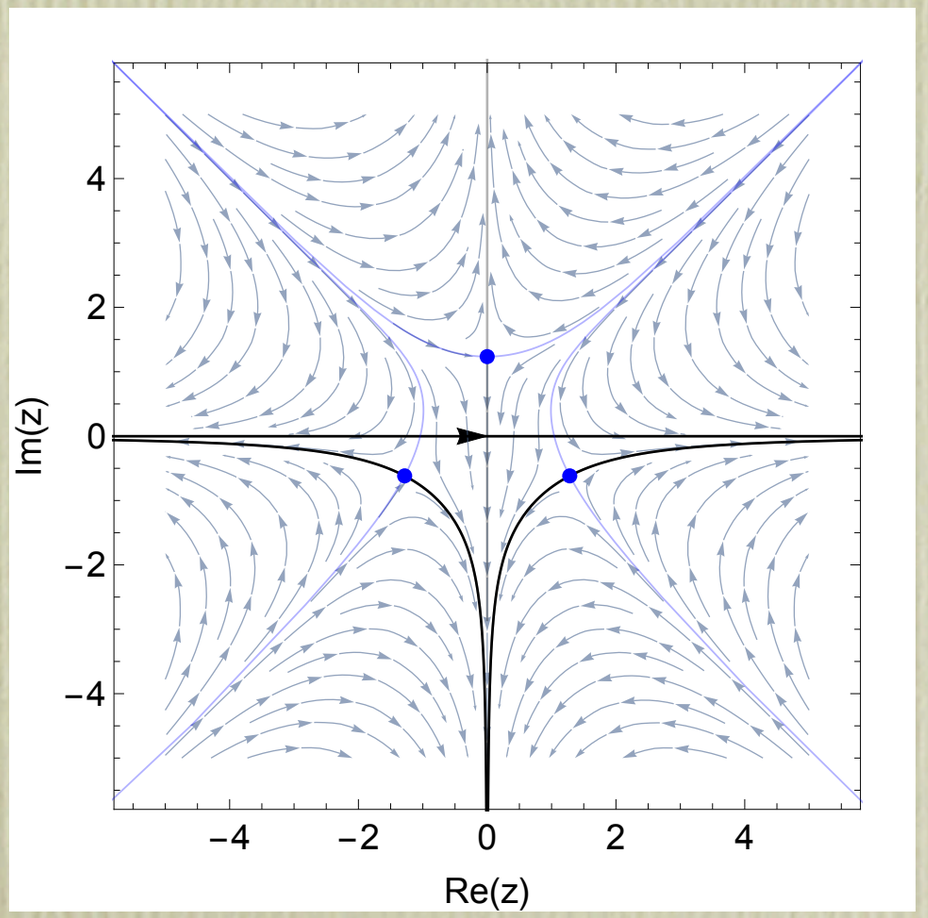
$$\frac{dz}{d\tau} = \overline{\frac{\partial S}{\partial z}}, \qquad z \equiv x + iy$$

$$\begin{cases} \dfrac{dx}{d\tau} = \dfrac{\partial S_R}{\partial x} = \dfrac{\partial S_I}{\partial y} \\ \dfrac{dy}{d\tau} = \dfrac{\partial S_R}{\partial y} = -\dfrac{\partial S_I}{\partial x} \end{cases}$$

Thimbles are generalizations of steepest descent/stationary phase paths.

M. Cristoforetti, F. Di Renzo, and L. Scorzato, *High density QCD on a Lefschetz thimble*, Phys. Rev. D86 (2012) 074506

Holomorphic gradient flow and Lefschetz thimbles



$$Z = \int_{-\infty}^{\infty} \mathrm{d}x\, e^{-S(x)}$$

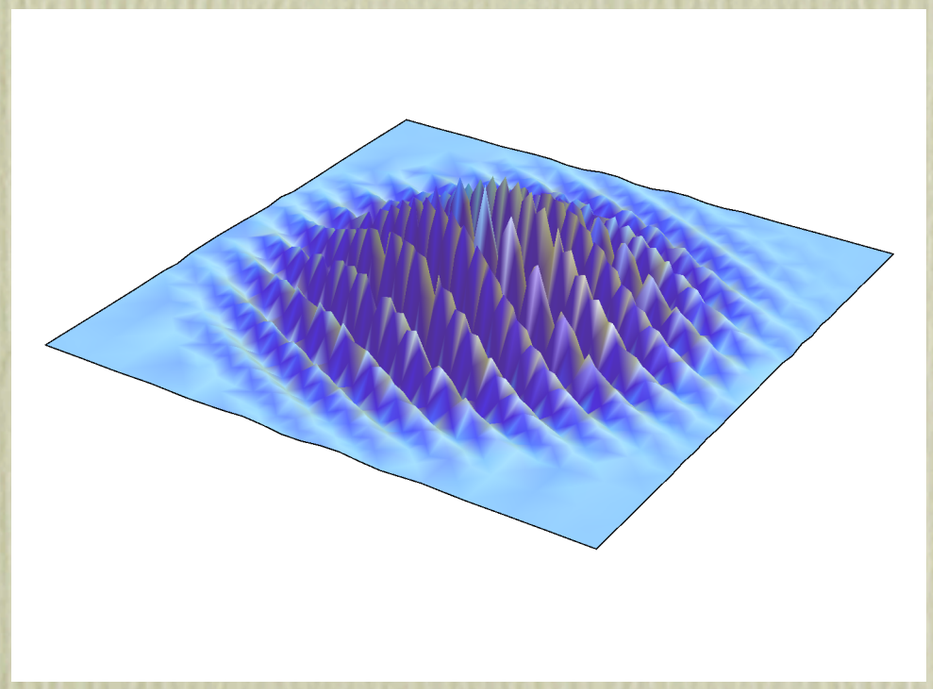
$$\frac{dS}{dz} = 0 \quad \text{(critical points)}$$

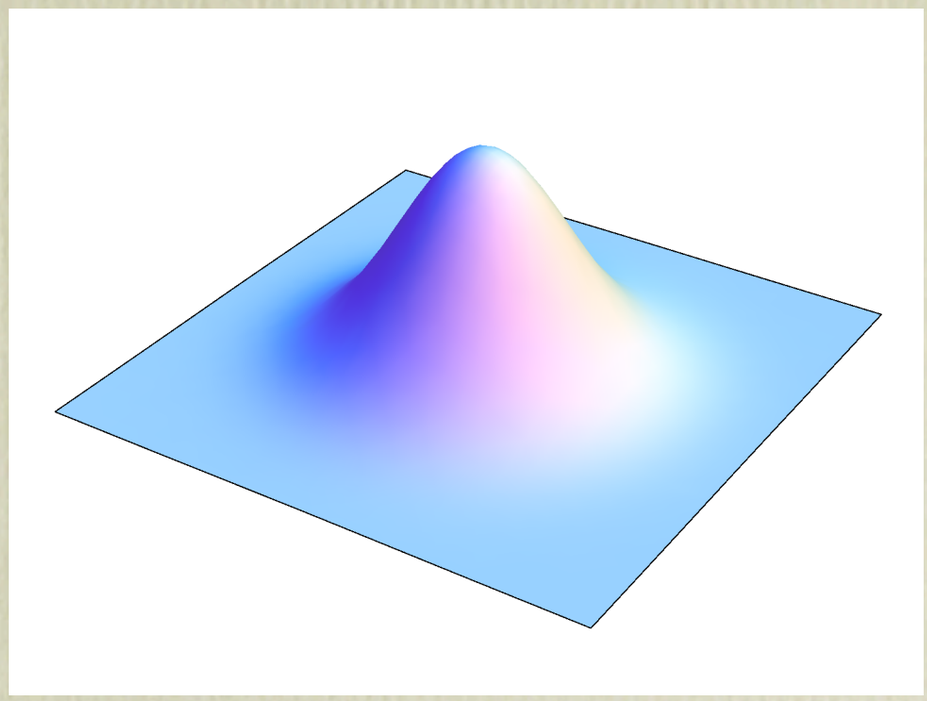
$$\frac{dz}{d\tau} = \overline{\frac{\partial S}{\partial z}}, \qquad z \equiv x + iy$$

$$\begin{cases} \frac{dx}{d\tau} = \frac{\partial S_R}{\partial x} = \frac{\partial S_I}{\partial y} \\ \frac{dy}{d\tau} = \frac{\partial S_R}{\partial y} = -\frac{\partial S_I}{\partial x} \end{cases}$$

$$Z = \sum_{\sigma} n_\sigma \int_{J_\sigma} dz\, e^{-S(z)}$$

Lefschetz thimble



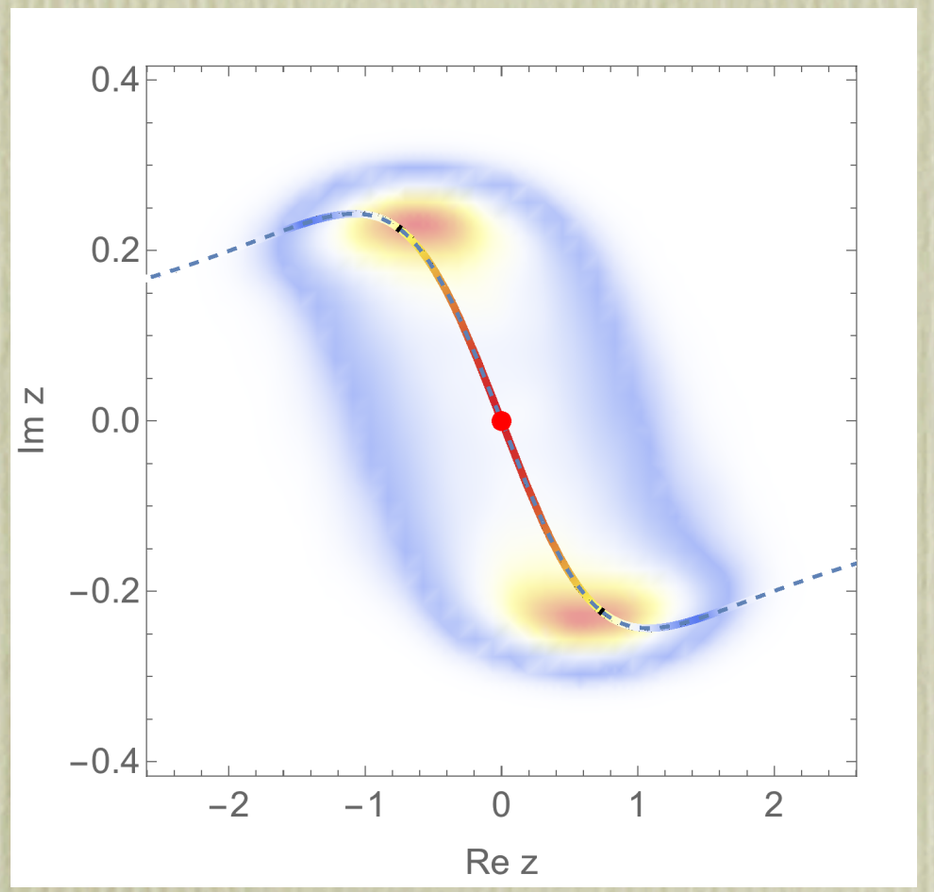


$e^{-S(x_1,x_2)}$ (real plane)

$e^{-S(z_1,z_2)}$ (gaussian thimble)

$$S(x_1, x_2) = x_1^2 + x_2^2 + 10ix_1 + 20ix_2 + ix_1x_2/3$$

Complex Langevin vs contour deformation



$$S(z) = \frac{1}{2}(1+i)z^2 + \frac{1}{4}z^4$$

Gert Aarts, arXiv:1308.4811

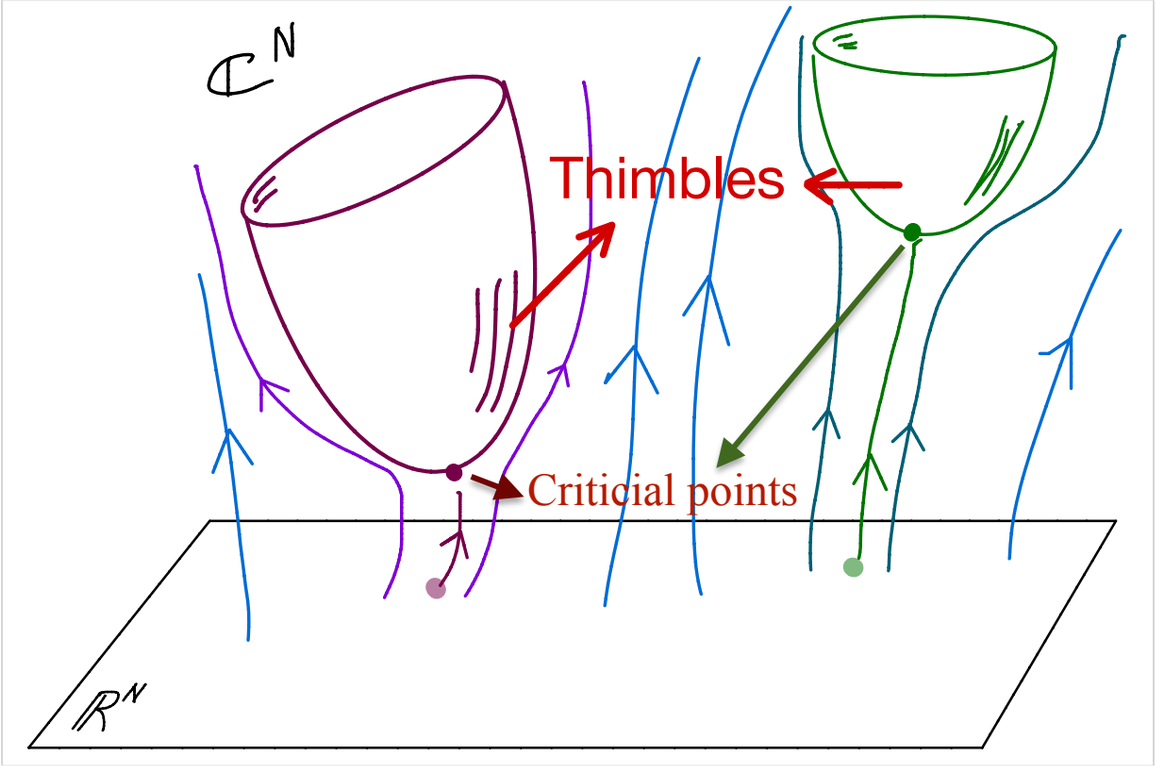
- Complex Langevin follows the stochastic differential equation

$$\dot{z} = -\partial_z S(z) + \eta$$

- The process moves freely in the complex plane with possible runaways

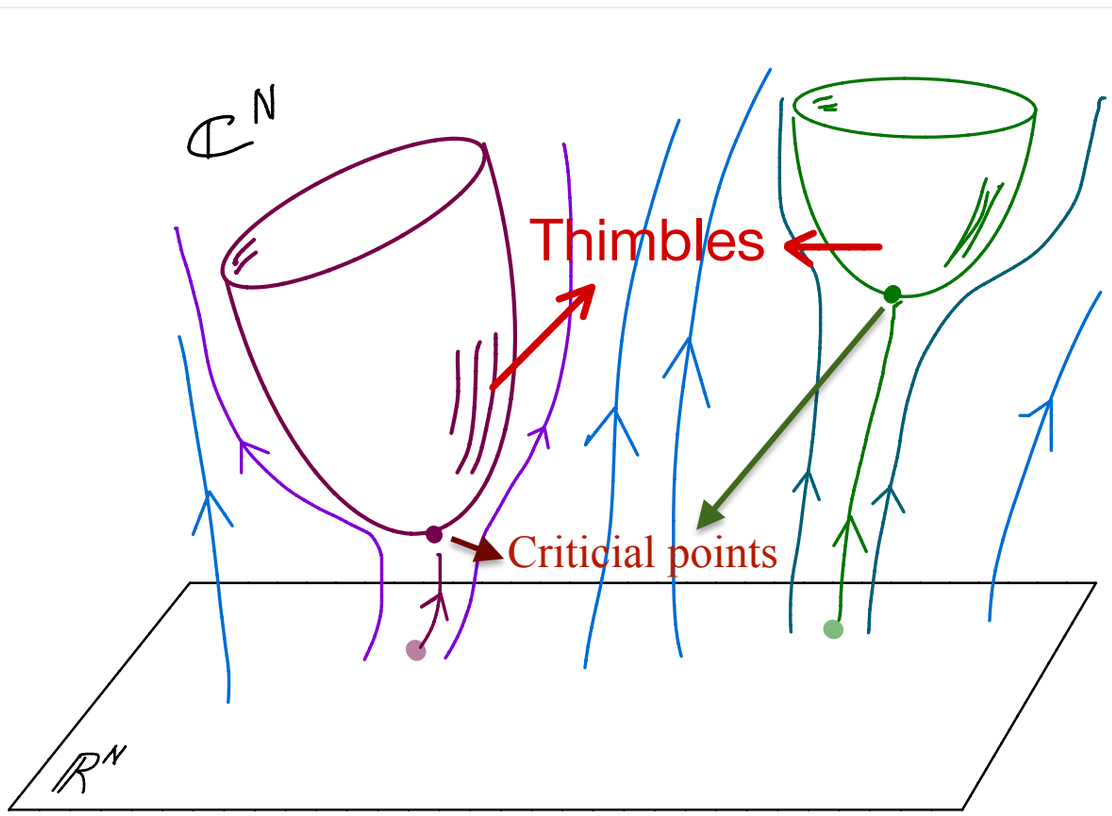
- Complex integration is constrained on a manifold of similar dimension with the original integration contour

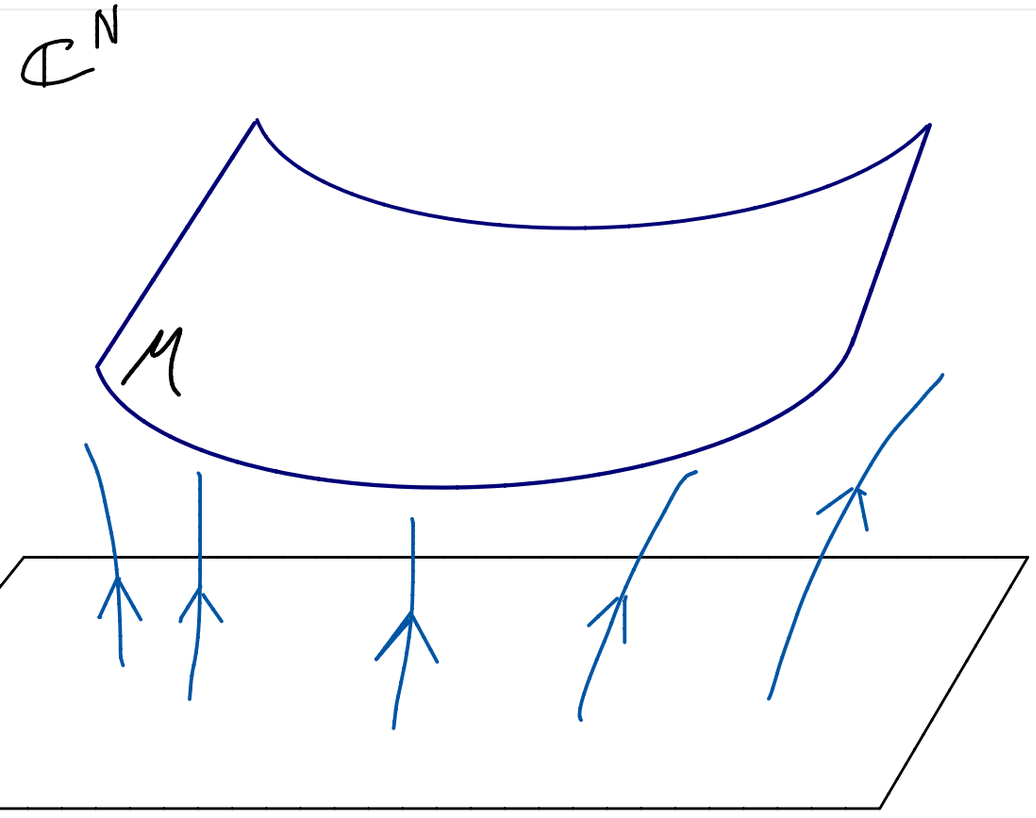
Generalized thimble method



- Most systems require multiple thimble
- Thimble decomposition is hard
- Use the manifolds generated by the holomorphic flow

Manifolds generated by holomorphic gradient flow



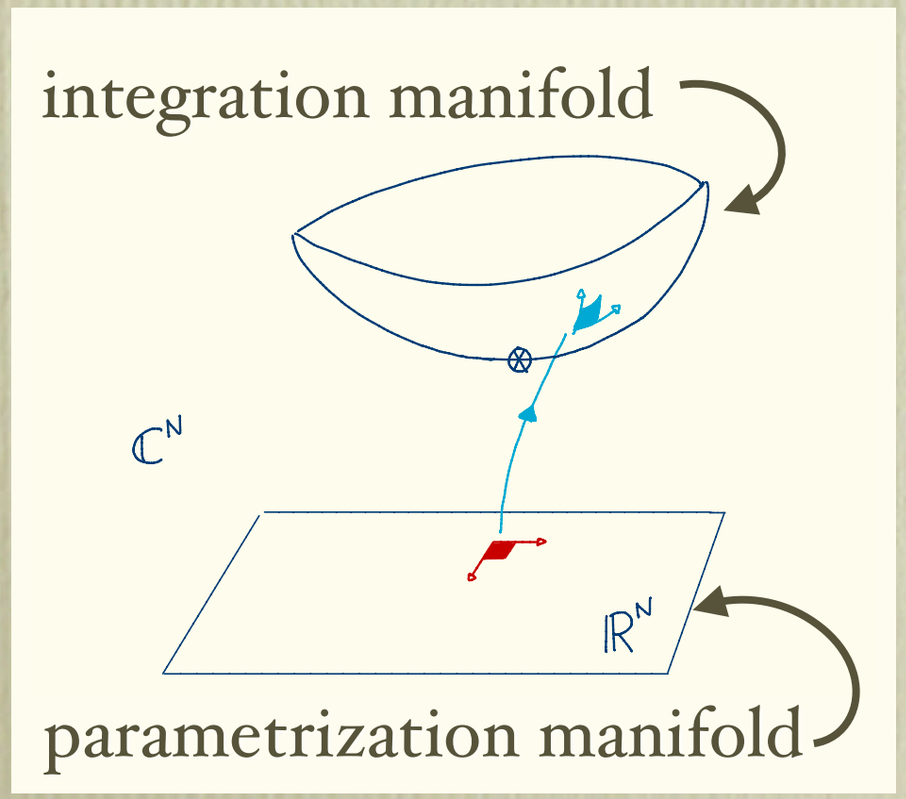


$$T_{\rm flow} \to \infty \quad \Rightarrow \quad \mathcal{M} \to \text{sum over thimbles}$$

Basic idea

$$Z = \int_{\mathcal{M}} \mathrm{d}^N z\, e^{-S(z)} = \int_{\mathbb{R}^N} \mathrm{d}^N x \underbrace{\left\| \frac{\partial z_i}{\partial x_j} \right\|}_{\det J(x)} e^{-S(z(x))}$$

$$\langle \mathcal{O}(z) \rangle = \frac{1}{Z} \int_{\mathbb{R}^N} \mathrm{d}^N x \underbrace{\left| \det J e^{-S(z(x))} \right|}_{e^{-S_{\mathrm{eff}}(x)}} \Phi(x) \mathcal{O}(z(x)) = \frac{\langle \mathcal{O}(z(x)) \Phi(x) \rangle_{S_{\mathrm{eff}}}}{\langle \Phi(x) \rangle_{S_{\mathrm{eff}}}}$$

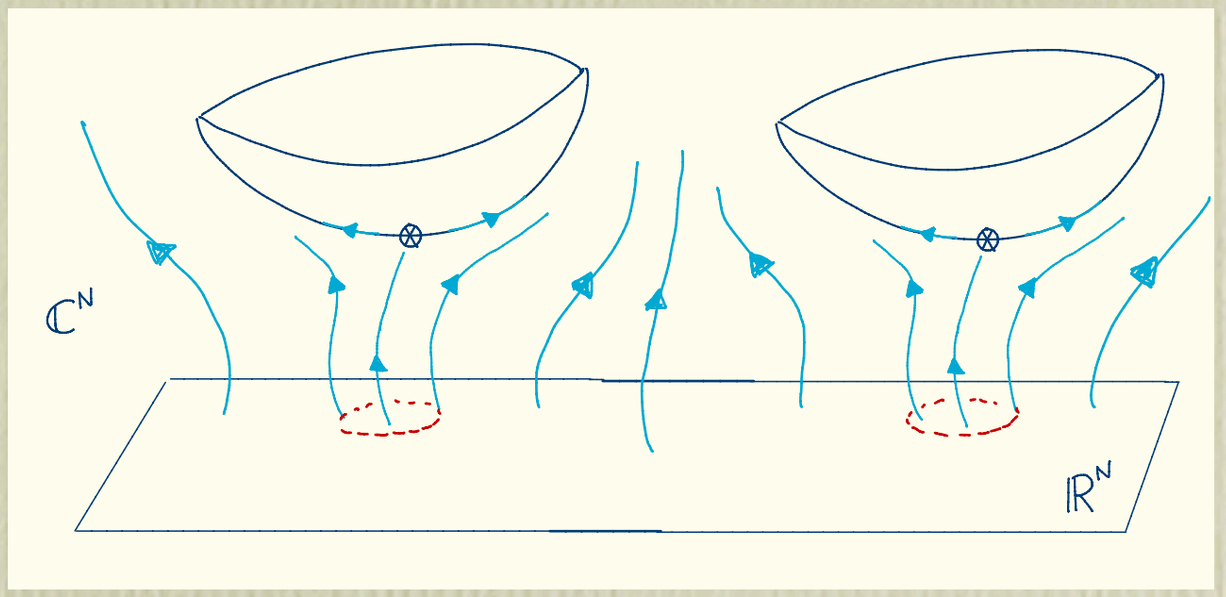


$$S_{\mathrm{eff}}(x) = S_R(z(x)) - \ln |\det J(x)|$$

$$\Phi(x) = e^{i[S_I(z(x)) - \mathrm{Im} \det J(x)]}$$

$$J_{ij} = \frac{\partial z_i}{\partial x_j}$$

Manifolds generated by holomorphic gradient flow



- Small regions are mapped (close) to thimbles and contribute significantly to the integral, S_I varies little.
- The other regions flow towards $S_R=\infty$ and contribute little to the integral.

Case study: massive Thirring model in 1+1D

$$\mathcal{L} = \bar{\psi}^a \left(\gamma^\mu \partial_\mu + m + \mu\gamma^0\right) \psi^a + \frac{g^2}{2N_f} (\bar{\psi}^a \gamma^\mu \psi^a)(\bar{\psi}^b \gamma_\mu \psi^b)$$

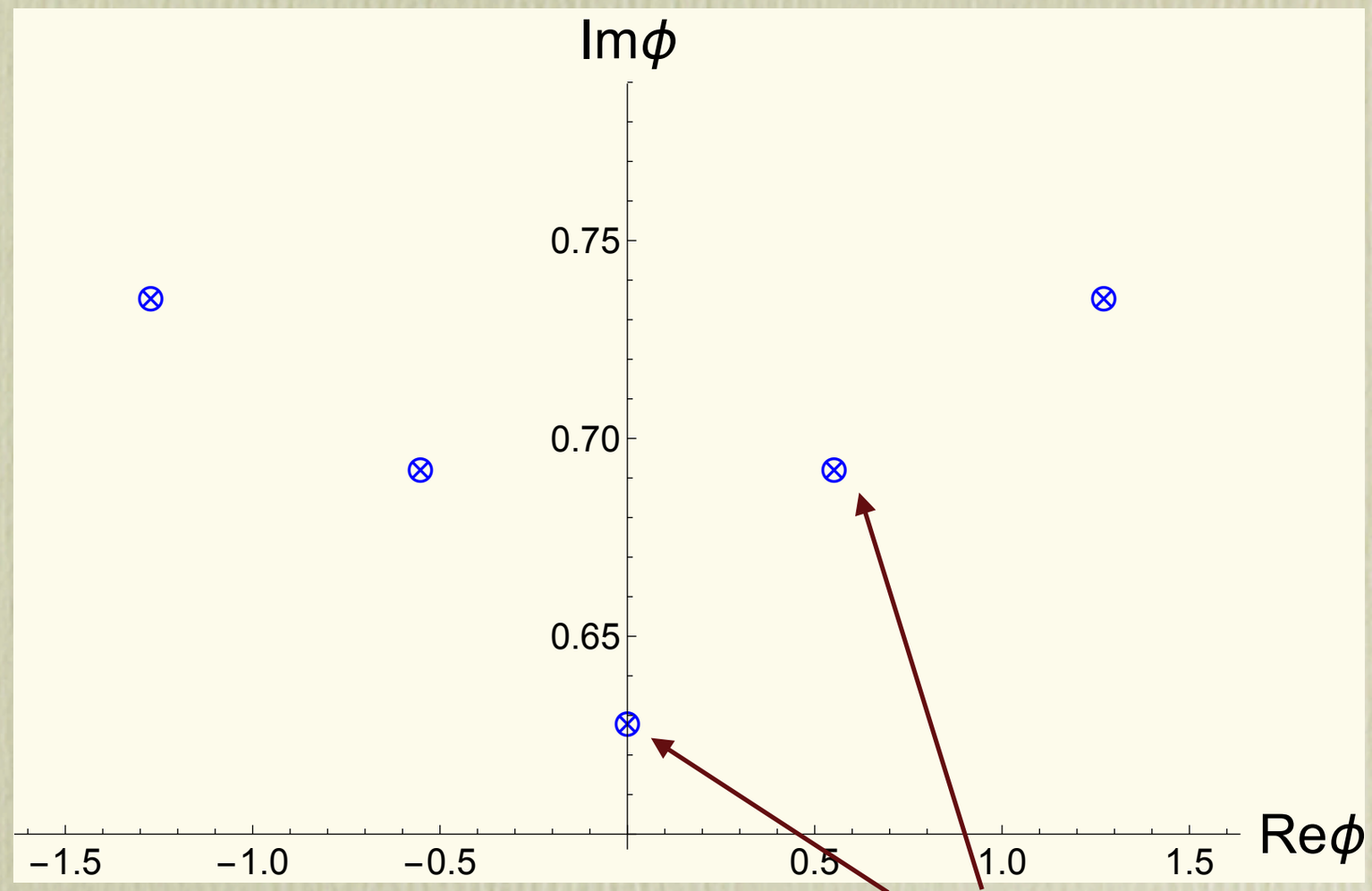
Auxiliary field A's

$$S = \int d^2x \ \left[\frac{N_F}{2g^2} A_\mu A_\mu + \bar{\psi}^\alpha (\not{\partial} + \mu\gamma_0 + i\not{A} + m)\psi^\alpha \right]$$

Discretization (compact A's)

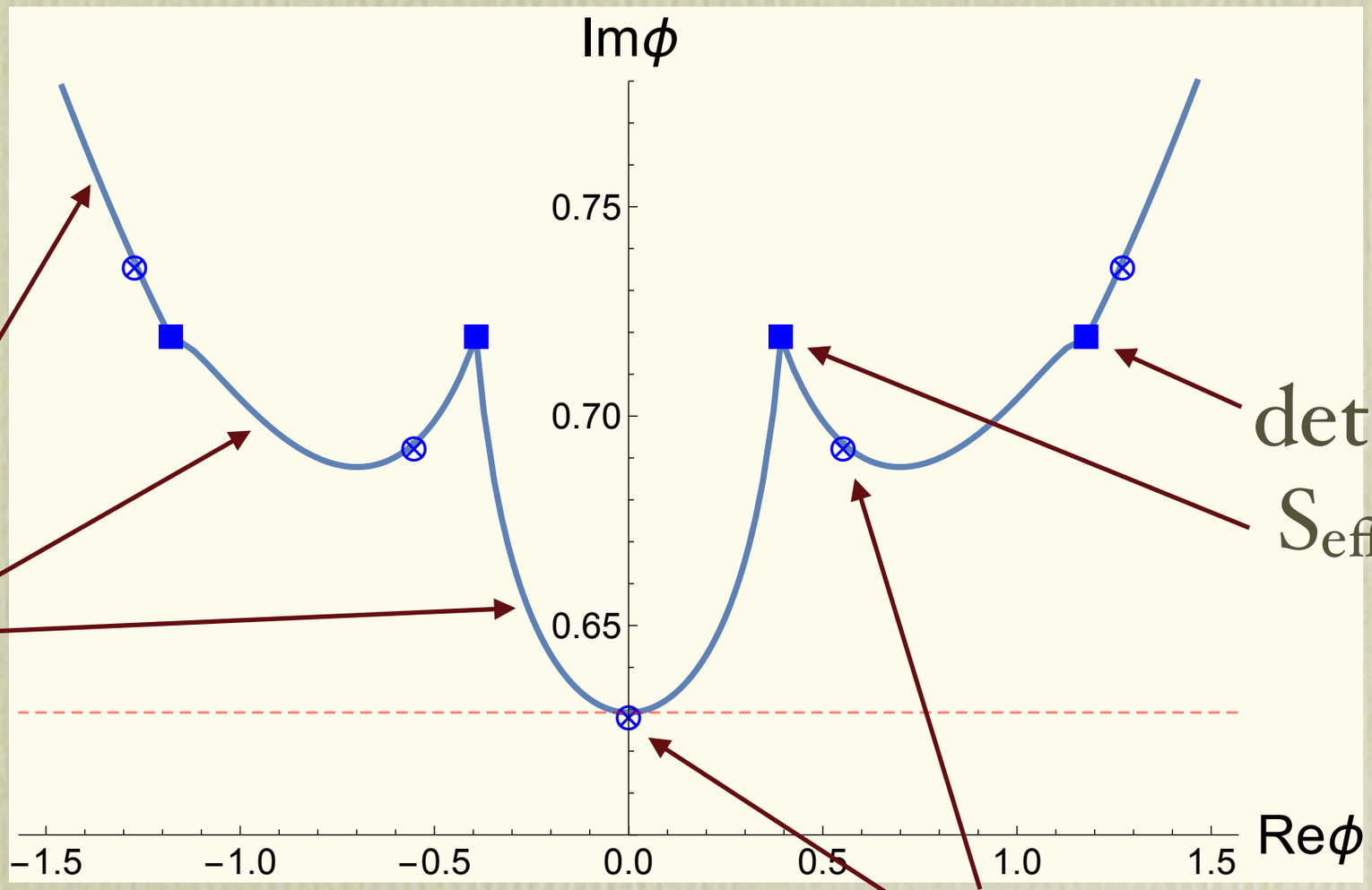
$$S = N_F \left(\frac{1}{g^2} \sum_{x,\nu} (1 - \cos A_\nu(x)) - \gamma \log\det D(A) \right)$$

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



critical points

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



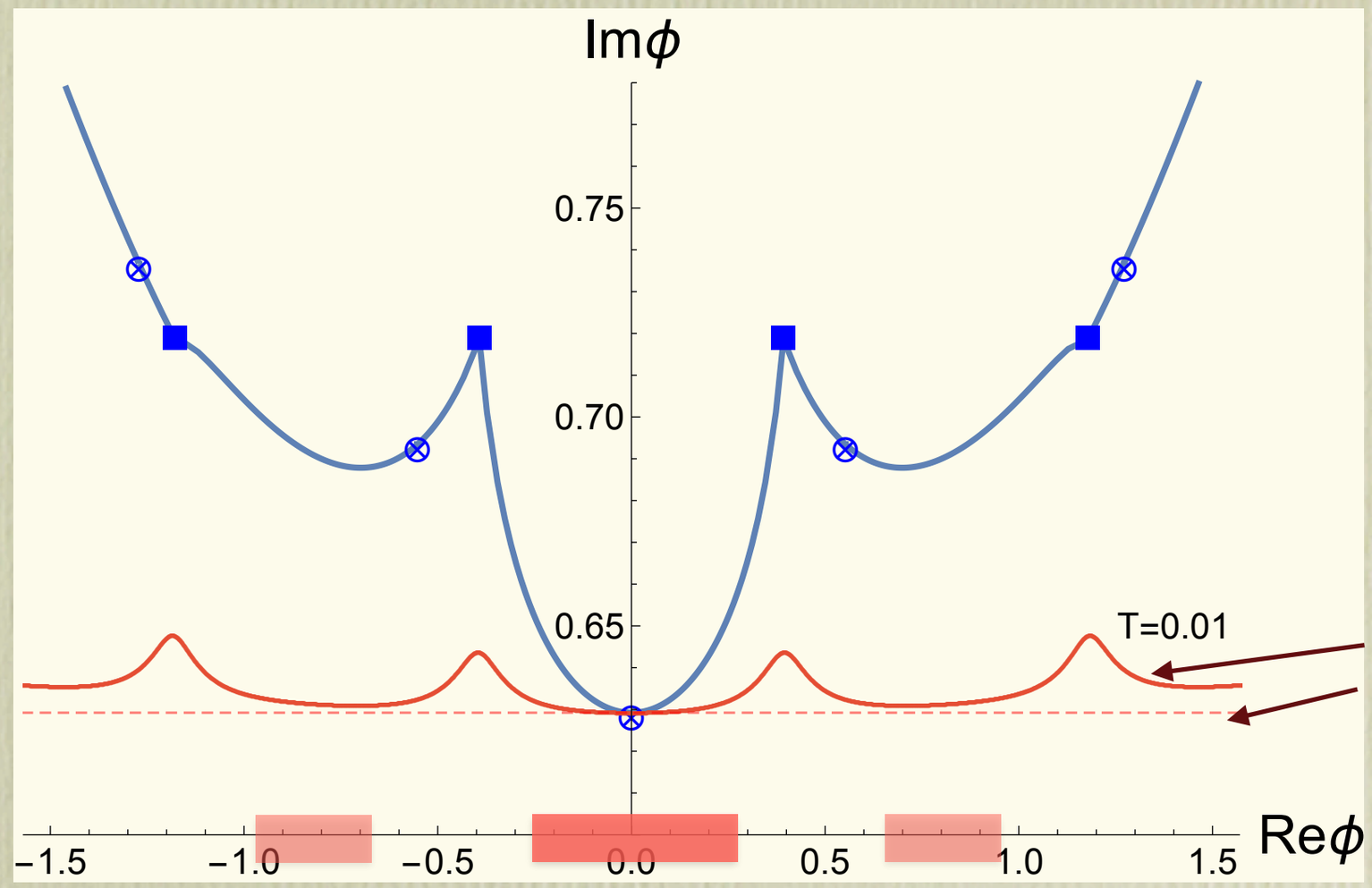
thimbles

detD=0,
$S_{eff} = \infty$

critical points

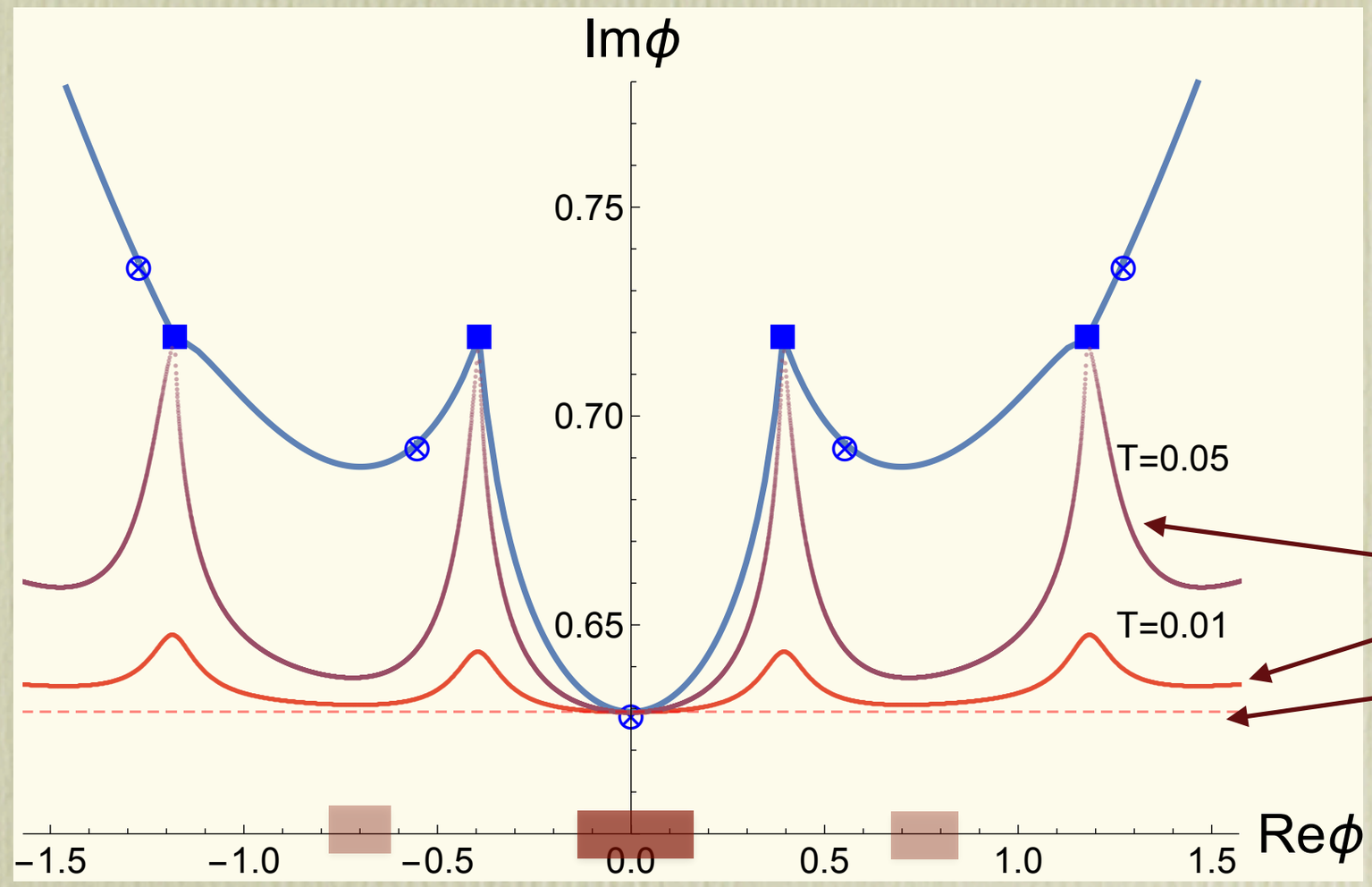
$$Z = \int \mathcal{D}A\, e^{-S_g(A)} \det D(A,\mu)$$

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



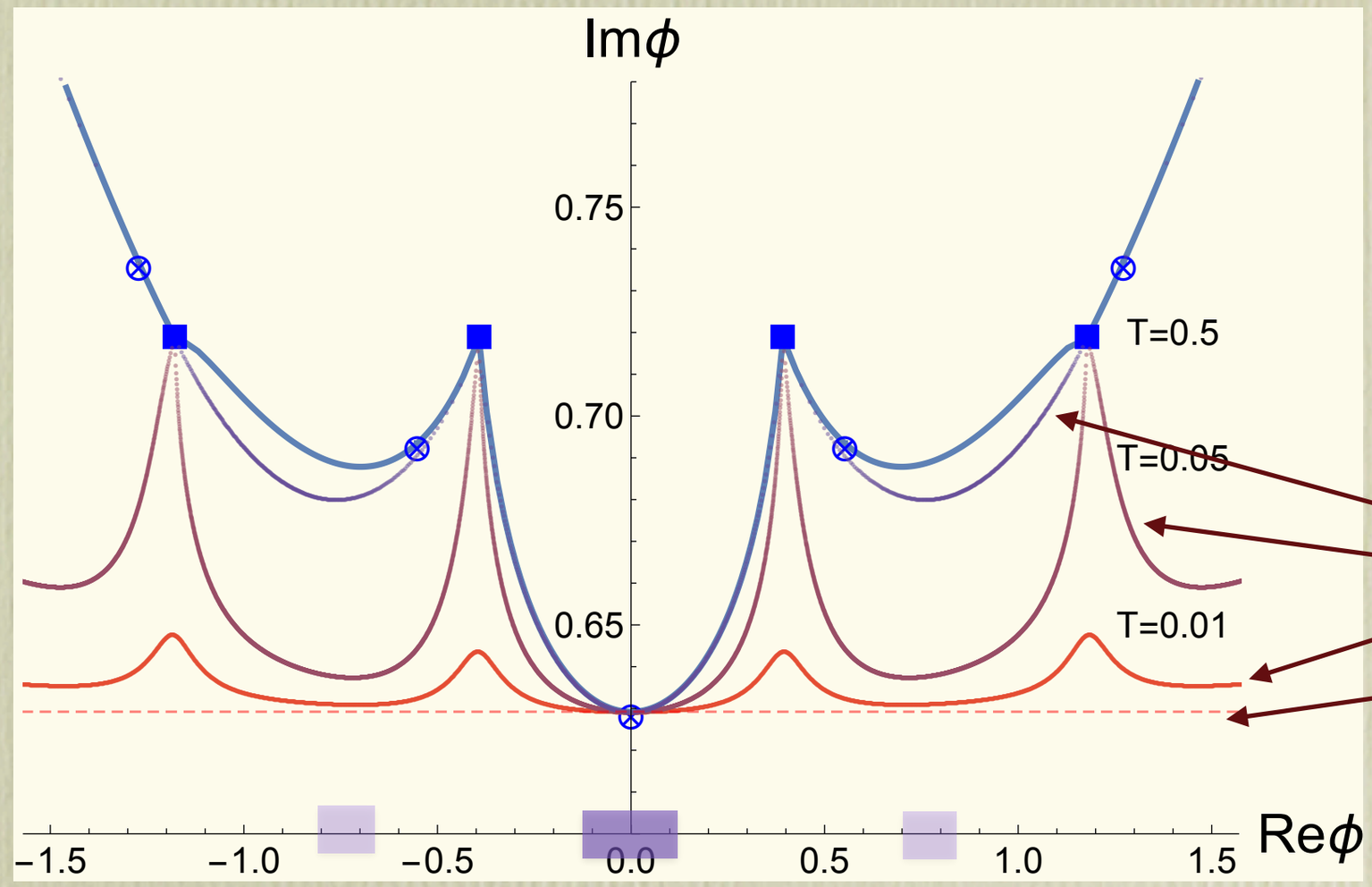
same homological class

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



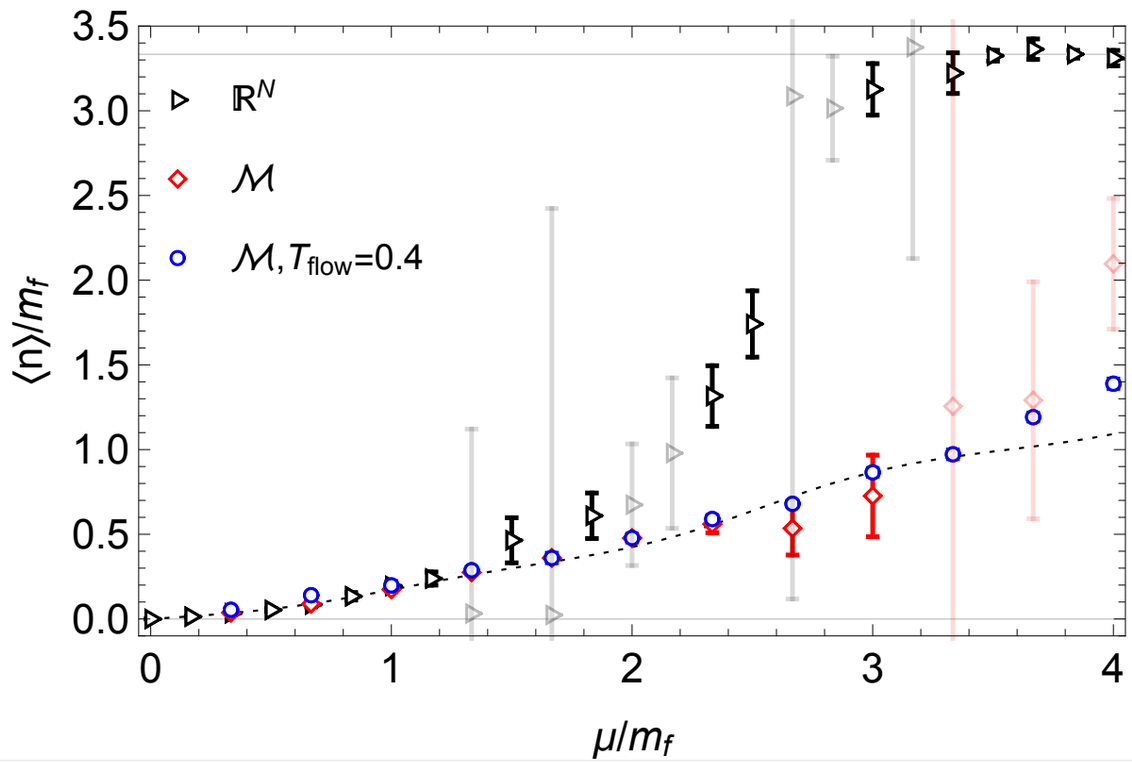
flowed tangent space

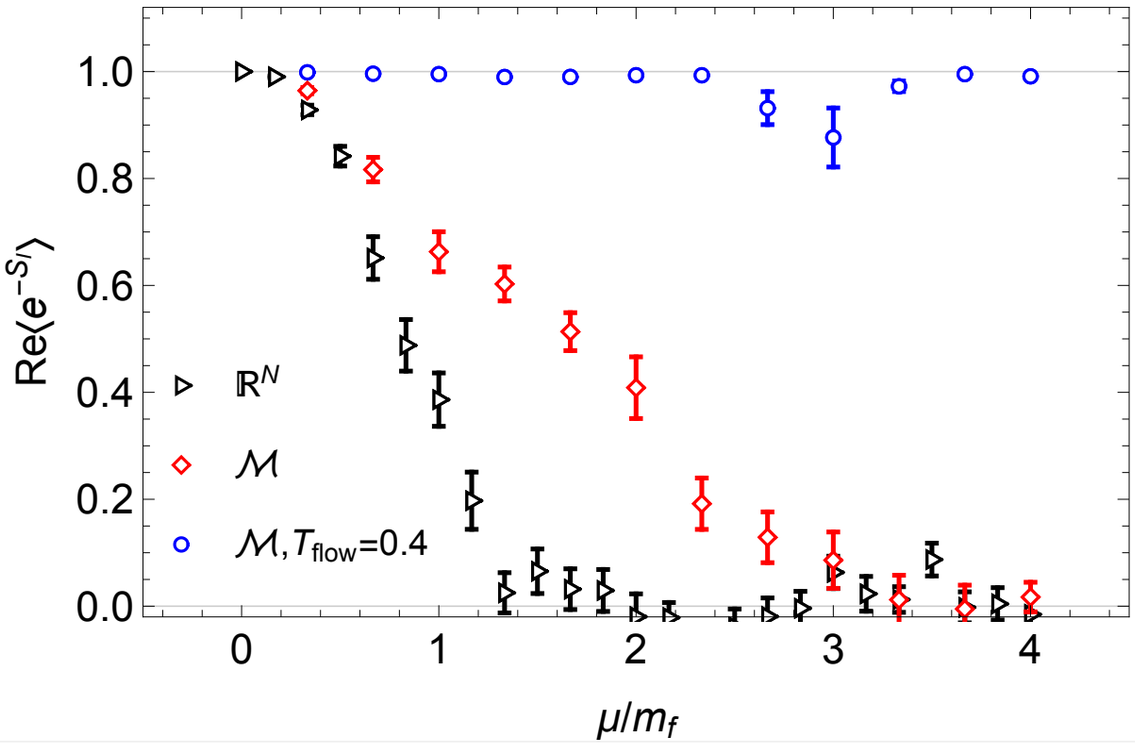
A projection of the thimbles: $\phi = \frac{1}{L^2}\sum_x A_0(x)$



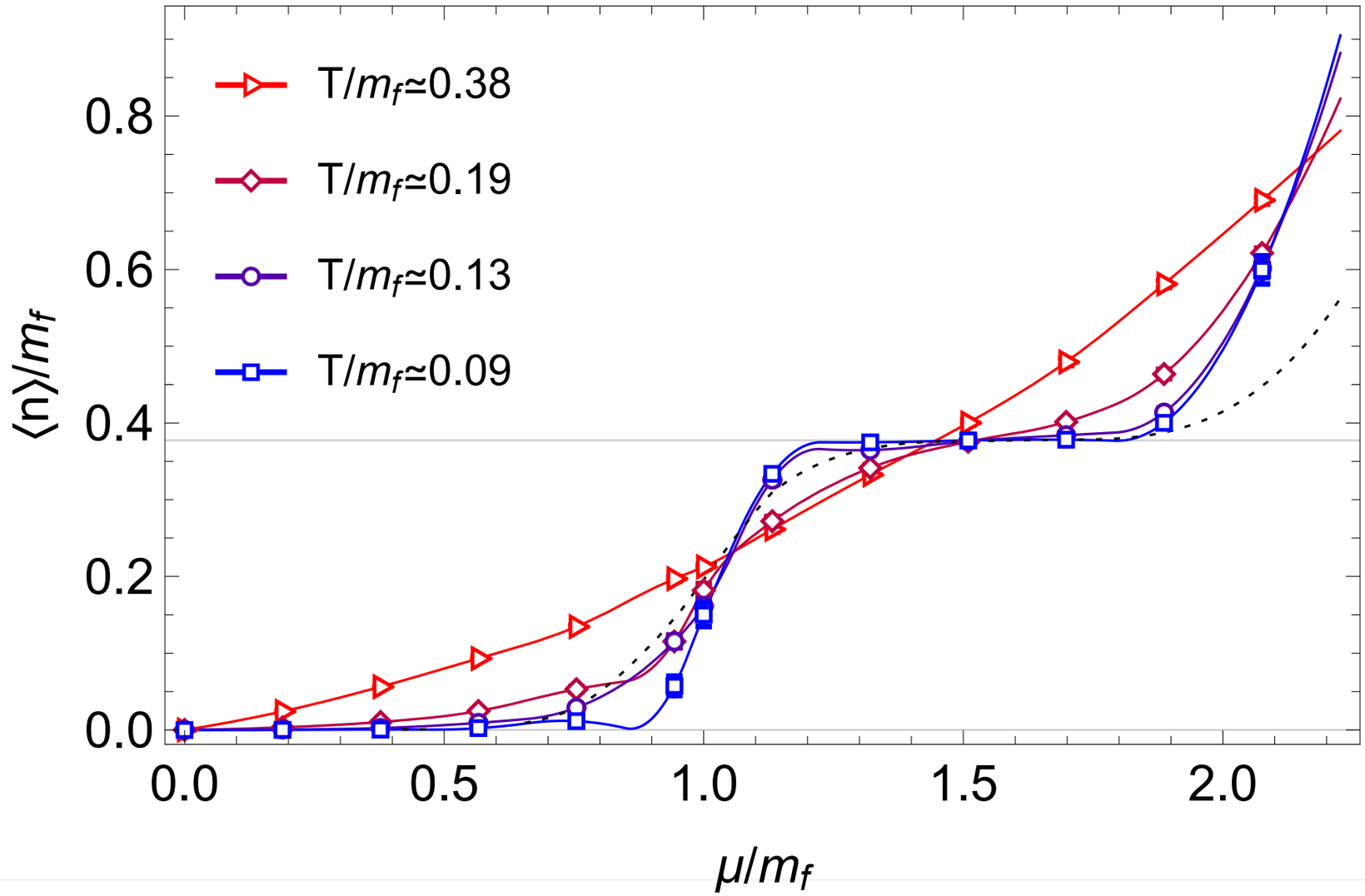
flowed tangent space

Sign problem





Silver blaze (cold limit)



Y. Tanizaki, Y. Hidaka, and T. Hayata, *Lefschetz-thimble approach to the Silver Blaze problem of one-site fermion model*, [arXiv:1610.00393].

Case study: real time physics

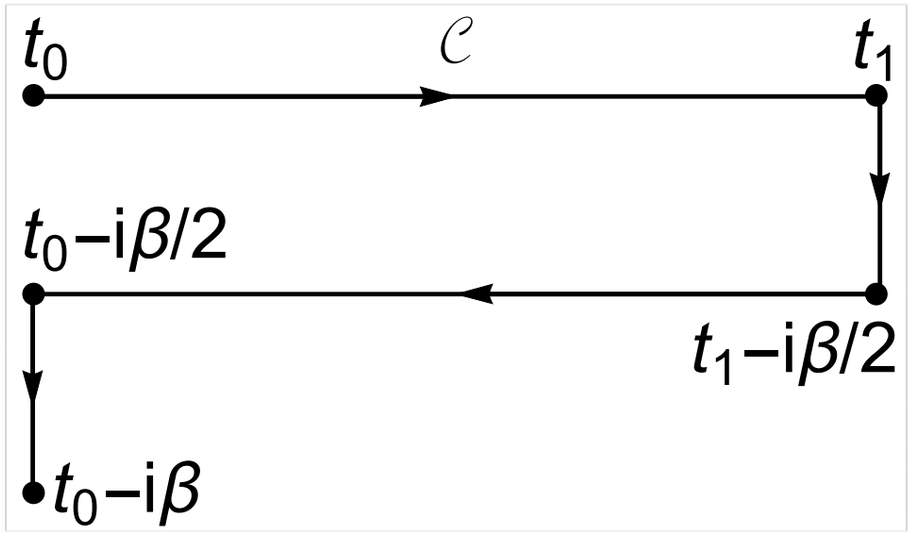
- Motivation: compute out-of-equilibrium correlators, transport coefficients non-perturbatively from first principles

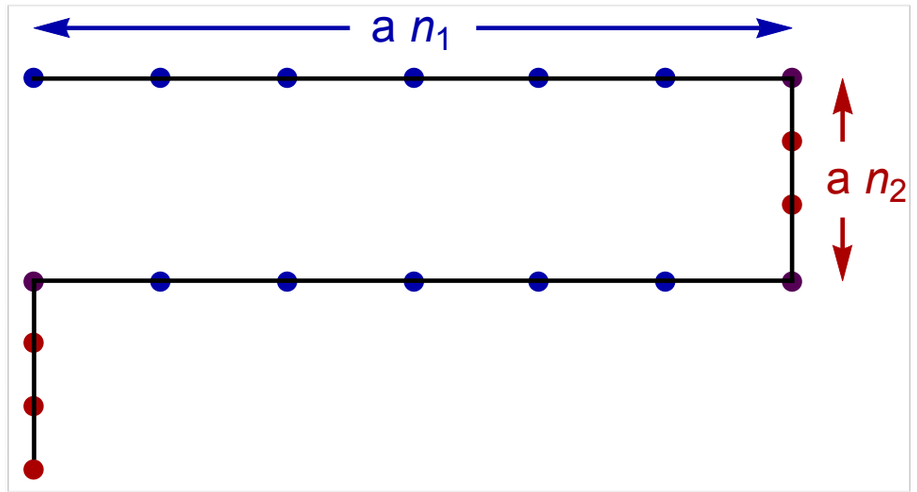
- Observables of interest are transport coefficient such as shear viscosity, conductivity, etc.

- At thermal equilibrium the observables are of the type

$$\langle \mathcal{O}_1(t)\mathcal{O}_2(t')\rangle = \mathrm{Tr}[\mathcal{O}_1(t)\mathcal{O}_2(t')\,\hat{\rho}], \quad \hat{\rho} = e^{-\beta H}$$

Real time physics

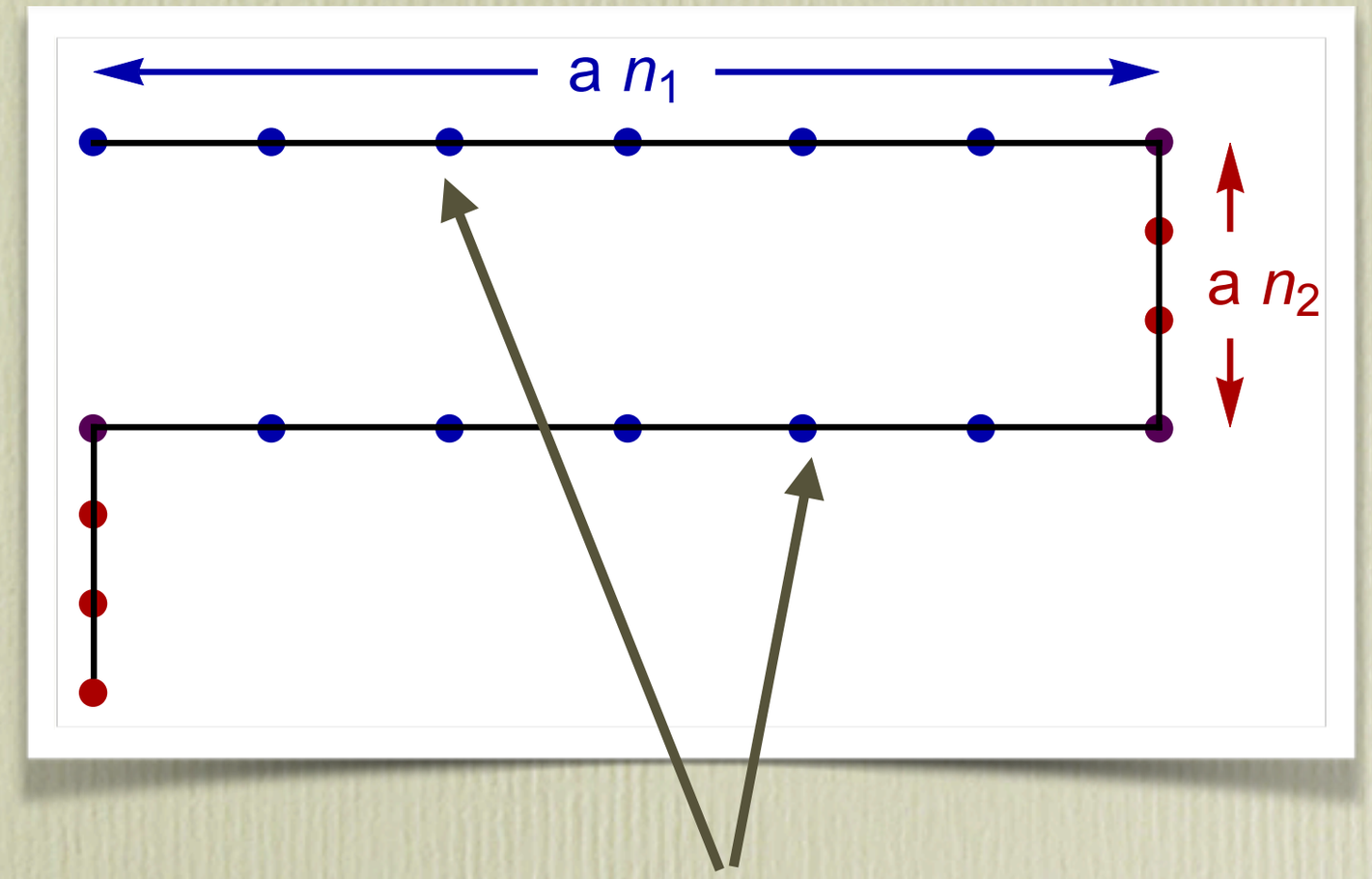




$$S_{SK}[\phi] = iS[\phi] = \int_{\mathcal{C}} dt\, L[\phi] \qquad \langle \mathcal{O}_1(t)\mathcal{O}_2(t')\rangle = \frac{1}{Z}\int \mathcal{D}\phi\, e^{-S[\phi]}\mathcal{O}_1(t)\mathcal{O}_2(t')$$

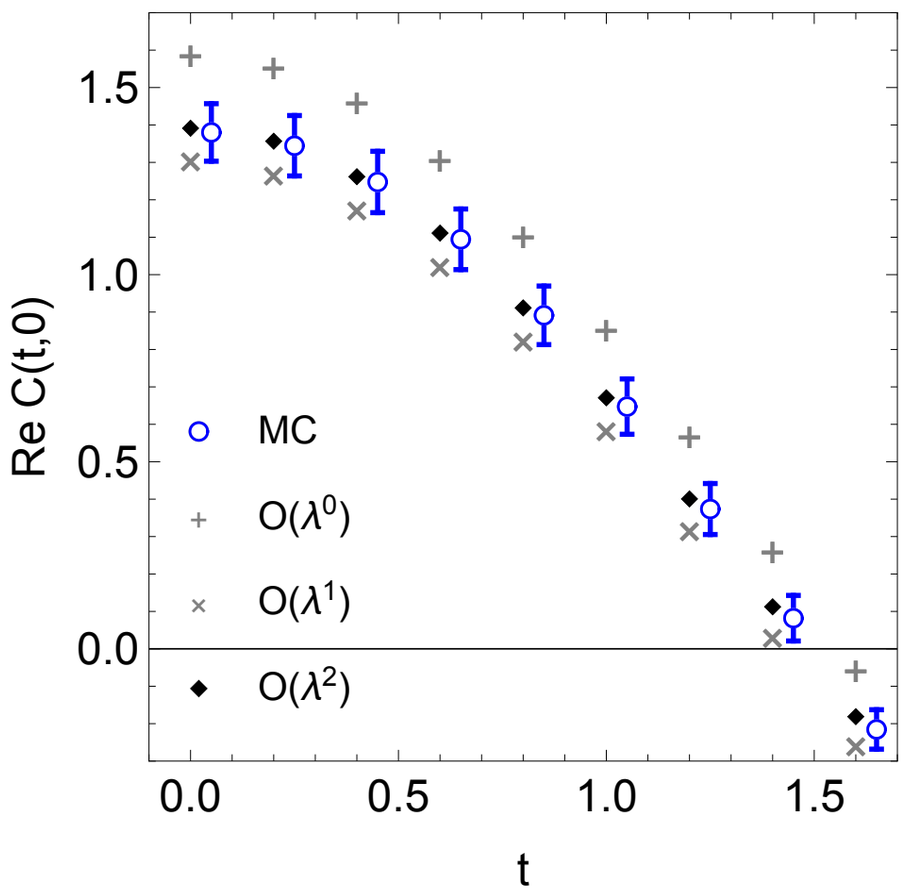
$$S[\phi] = \sum_{t,n} a_t a \left[\frac{(\phi_{t+1,n}-\phi_{t,n})^2}{2a_t^2} + \frac{1}{2}\left(\frac{(\phi_{t+1,n+1}-\phi_{t+1,n})^2}{2a^2} + \frac{(\phi_{t,n+1}-\phi_{t,n})^2}{2a^2} \right) \right.$$
$$\left. + \frac{1}{2}m^2 \frac{\phi_{t,n}^2+\phi_{t+1,n}^2}{2} + \frac{\lambda}{4!}\frac{\phi_{t+1,n}^4+\phi_{t,n}^4}{2} \right]$$

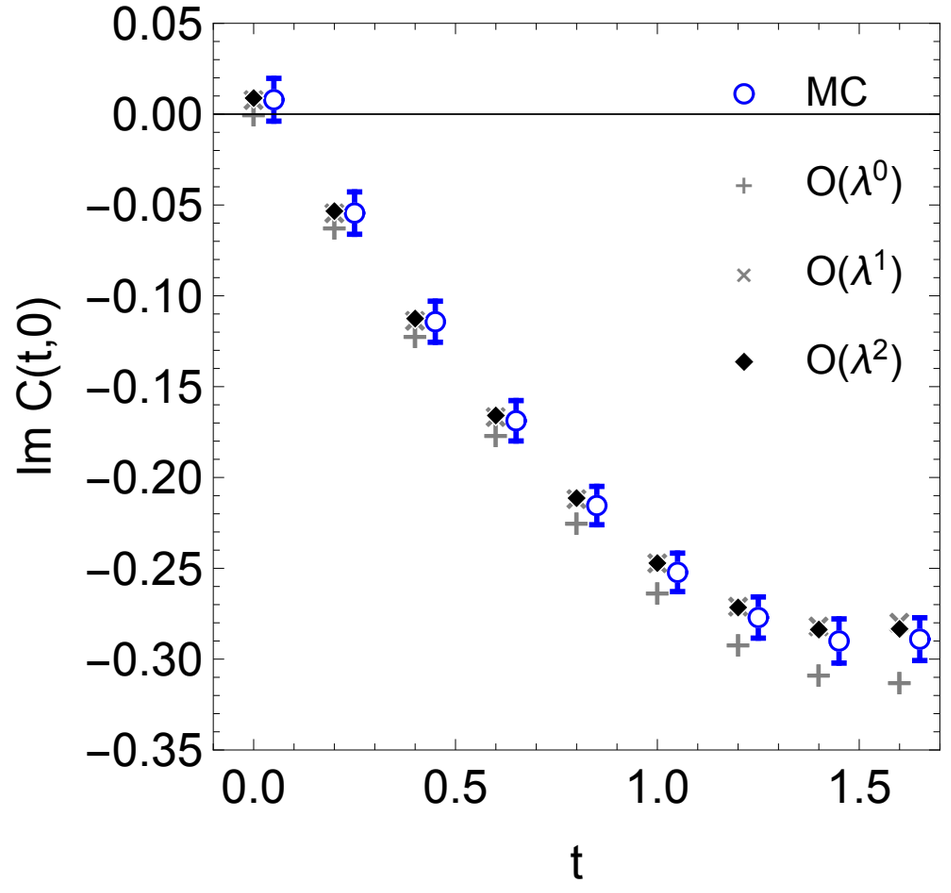
The worst sign problem



The field variables attached to real time legs contribute a purely imaginary factor to the action because $\exp(-aS_n) = \langle\phi_{n+1}|\exp(-iaH)|\phi_n\rangle$ produces a contribution to the action S_n that is purely imaginary.

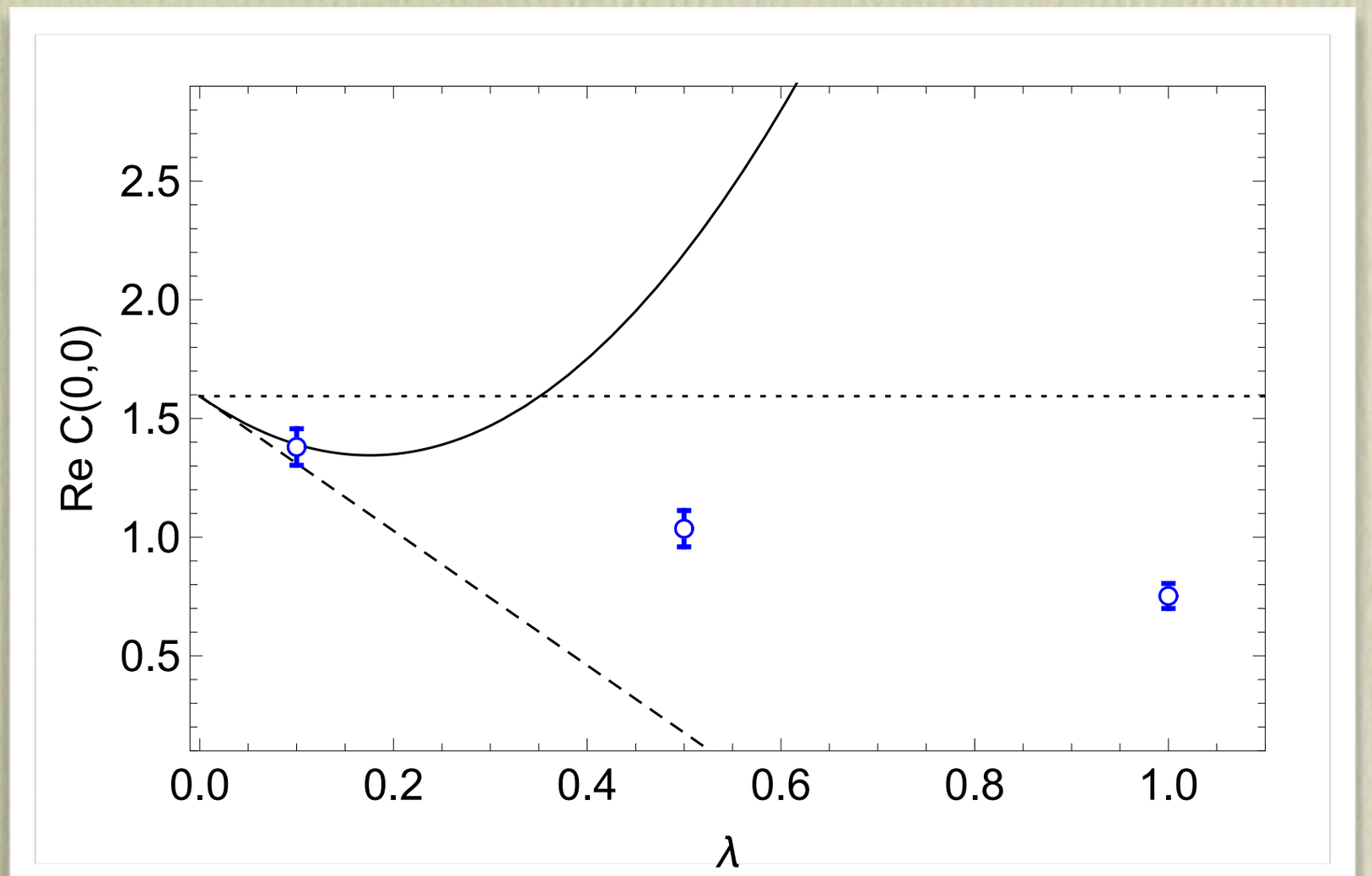
Real time physics (1+1D) weak coupling



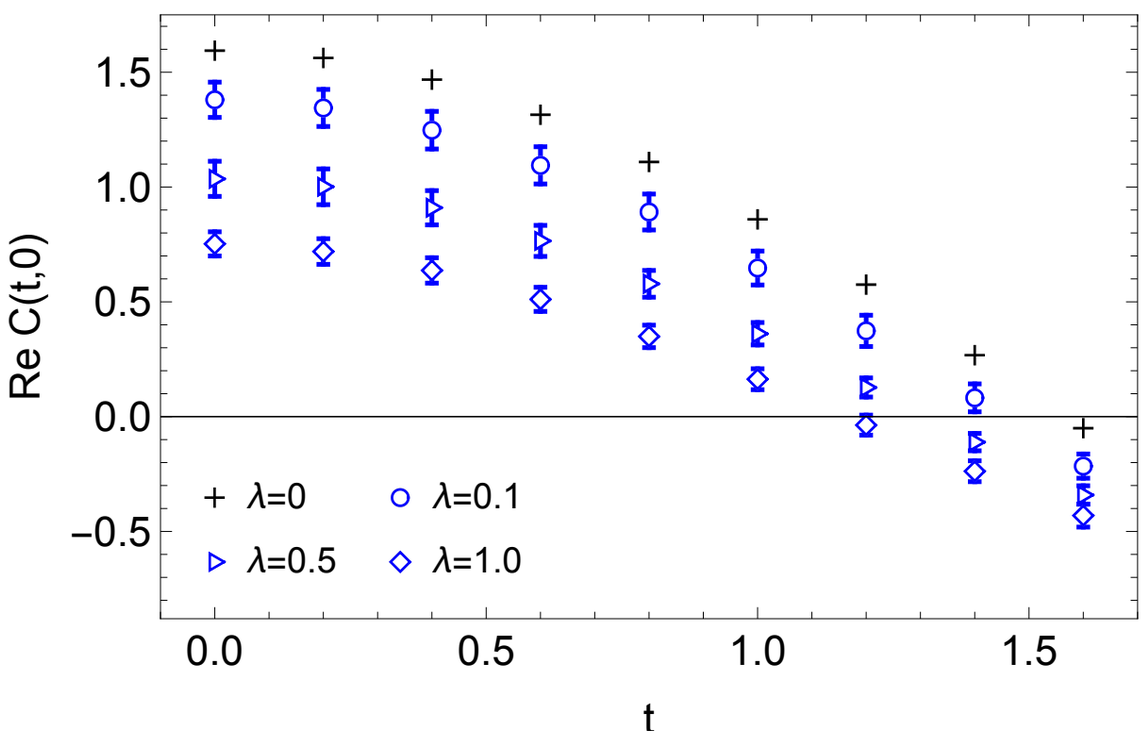


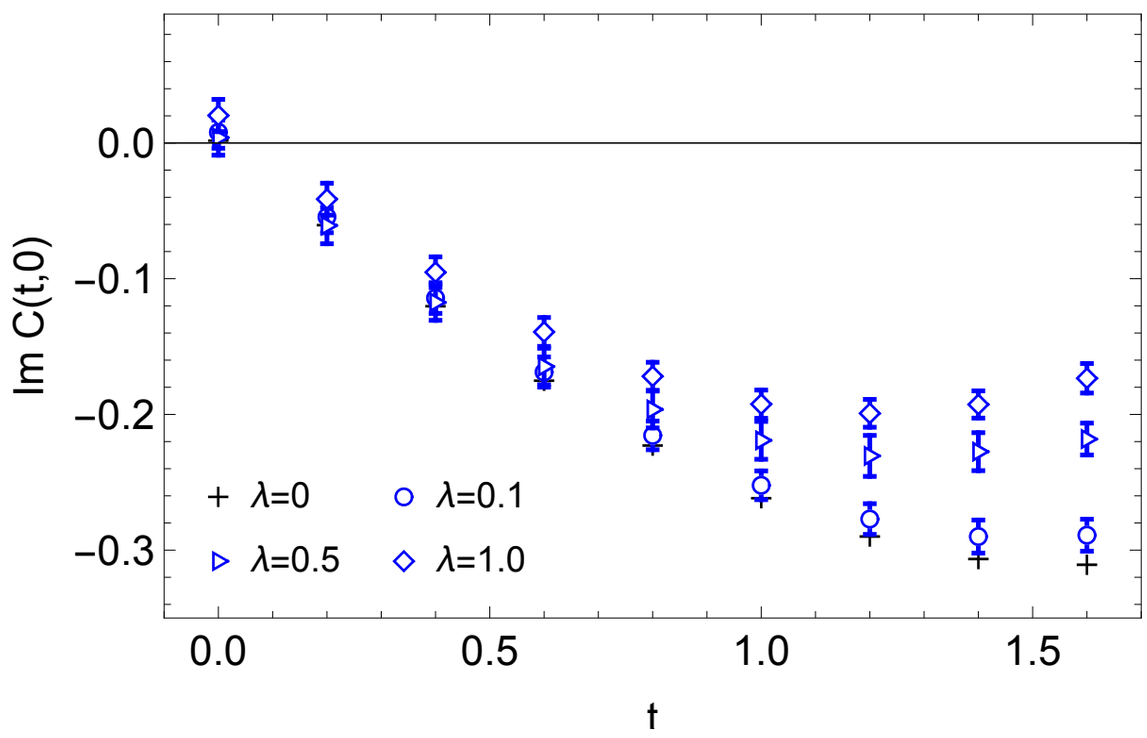
1+1D φ^4: $n_t=8$, $n_x=8$, $n_\beta=2$, $\lambda=0.1$

Real time physics (1+1D) perturbation theory



Real time physics (1+1D) strong coupling





1+1D φ^4: $n_t=8$, $n_x=8$, $n_\beta=2$, $\lambda=0.1,0.5,1.0$

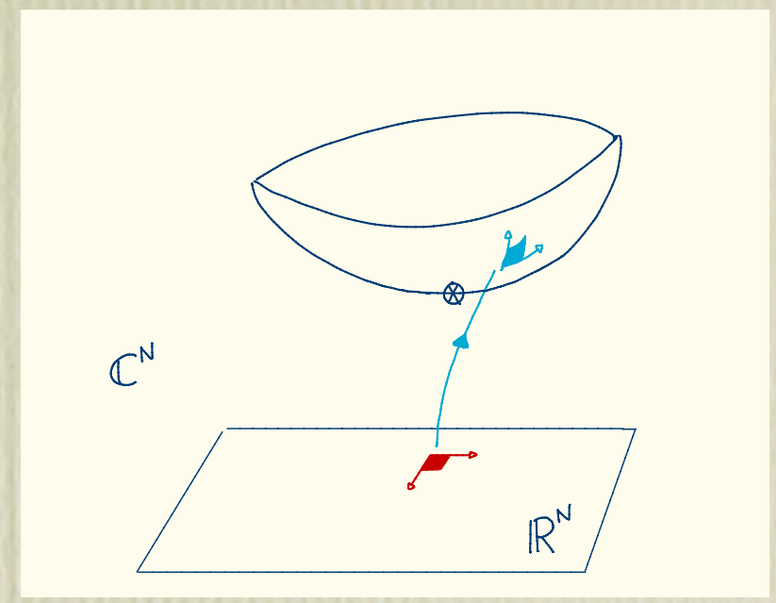
New directions

- On the flow manifolds sampling is done based on the effective action

$$S_{\text{eff}}(x) = S_R(z(x)) - \ln|\det J(x)|$$

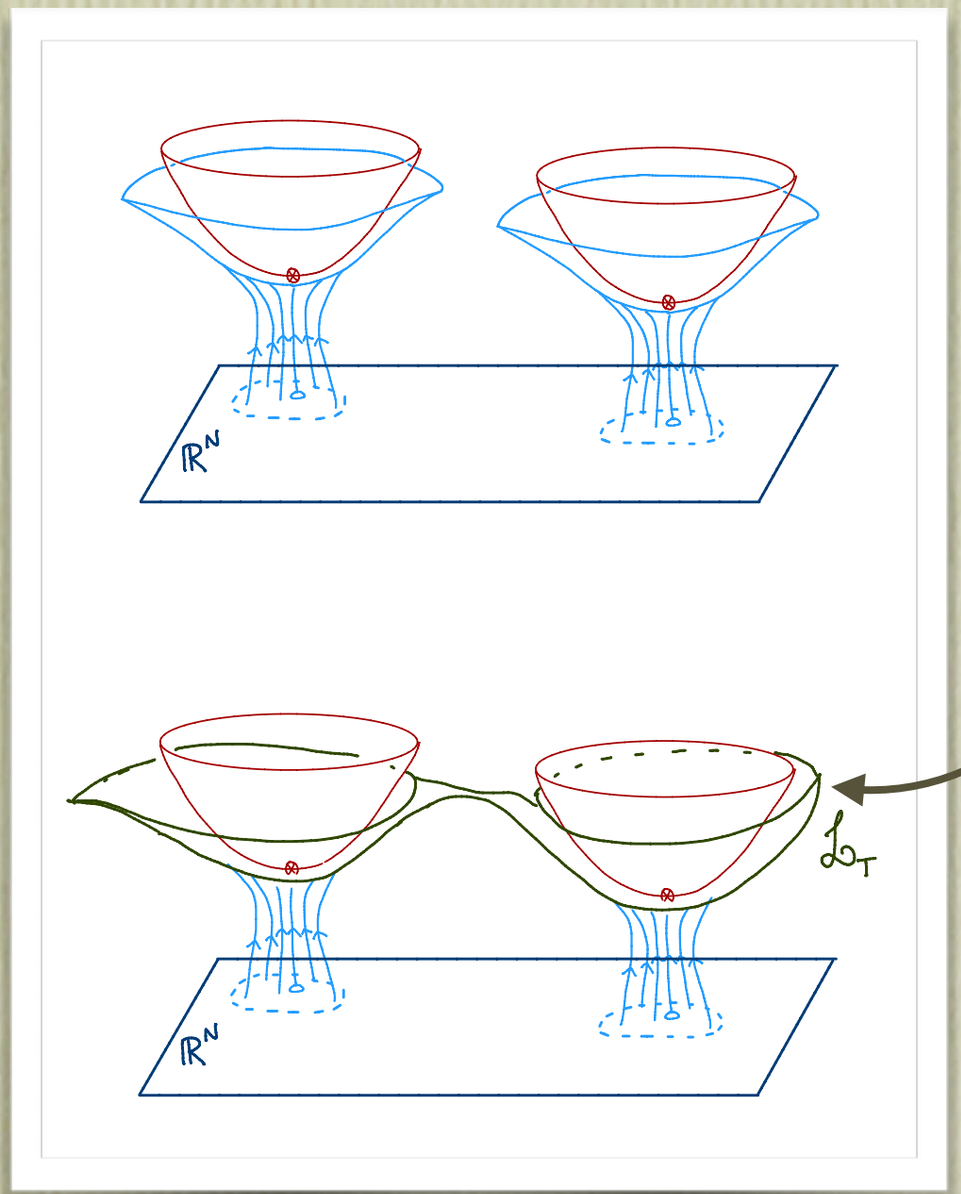
$$\frac{dz}{d\tau} = \overline{\frac{dS}{dz}}\,, \quad z(0) = x$$

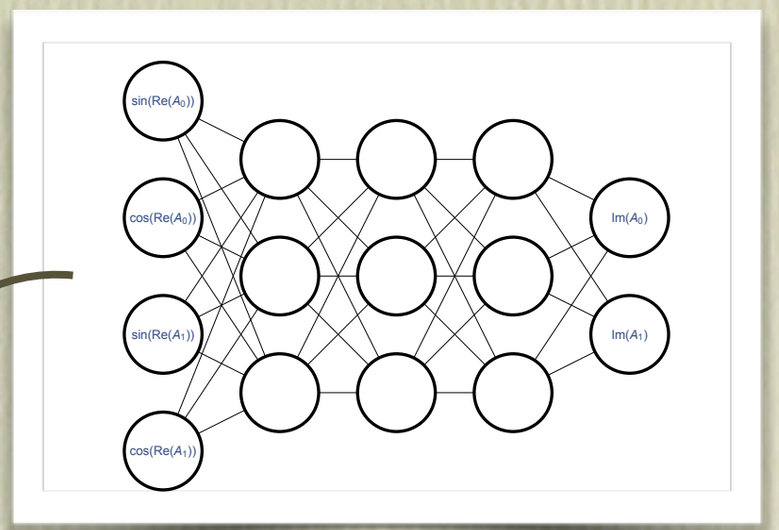
$$\frac{dJ}{d\tau} = \overline{H(z)J}\,, \quad J(0) = I \quad H(z)_{ij} = \frac{\partial^2 S}{\partial z_i \partial z_j}$$



- For each step integrate a set of differential equations to get z and J
- This is expensive, especially the calculation of J and det J
- To address this problem we used
  - improved sampling algorithms (avoid computing J or det J)
  - fast estimators for det J
  - **numerically cheaper integration manifolds**

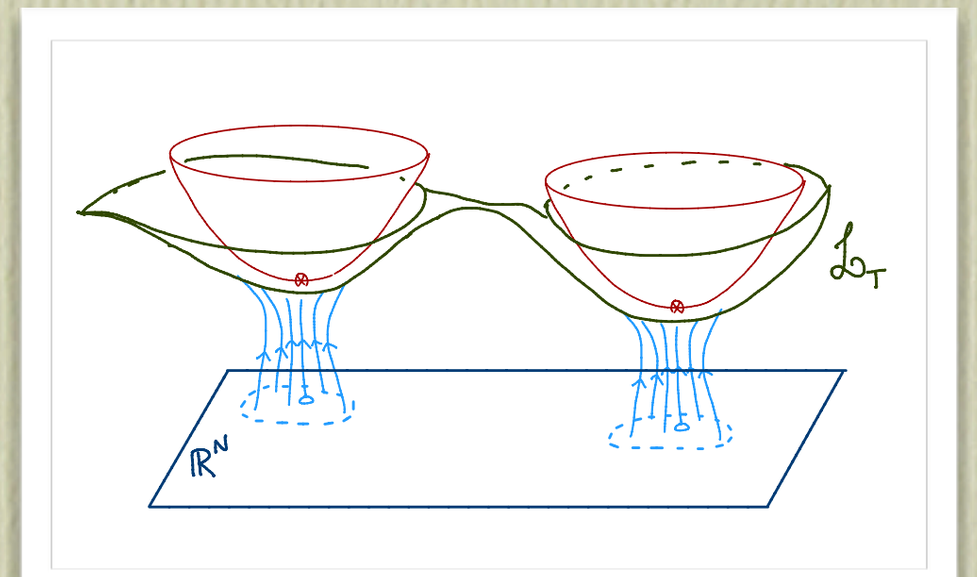
New directions — learnifold



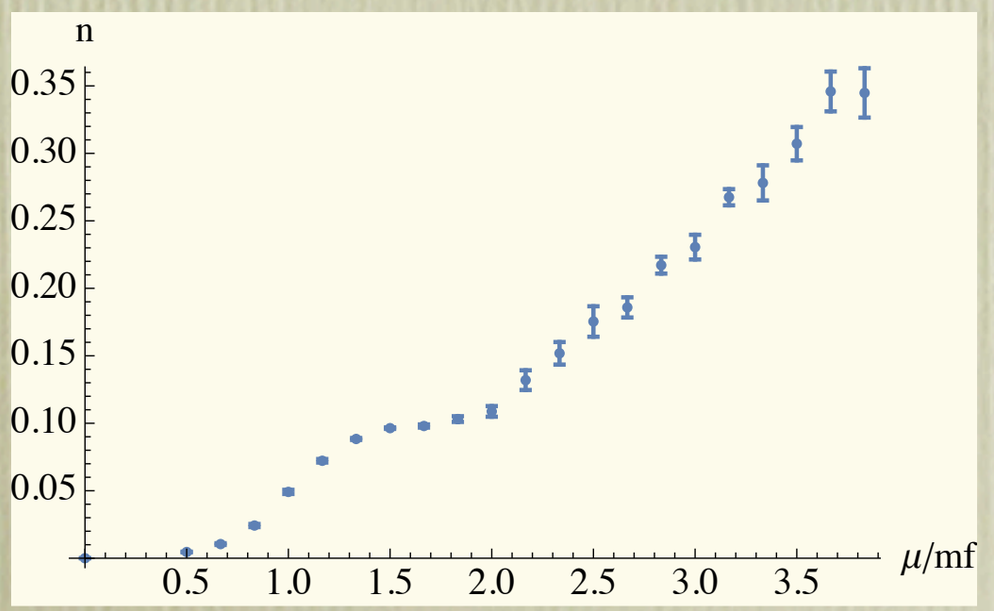


- Generate few configs on the integration manifold
- Use neural nets with appropriate symmetries to interpolate
- Integrate over the learnifold, the manifold defined by the trained neural net

New directions — learnifold



Wilson, 20×10 lattice, NF=2, am_f=0.3

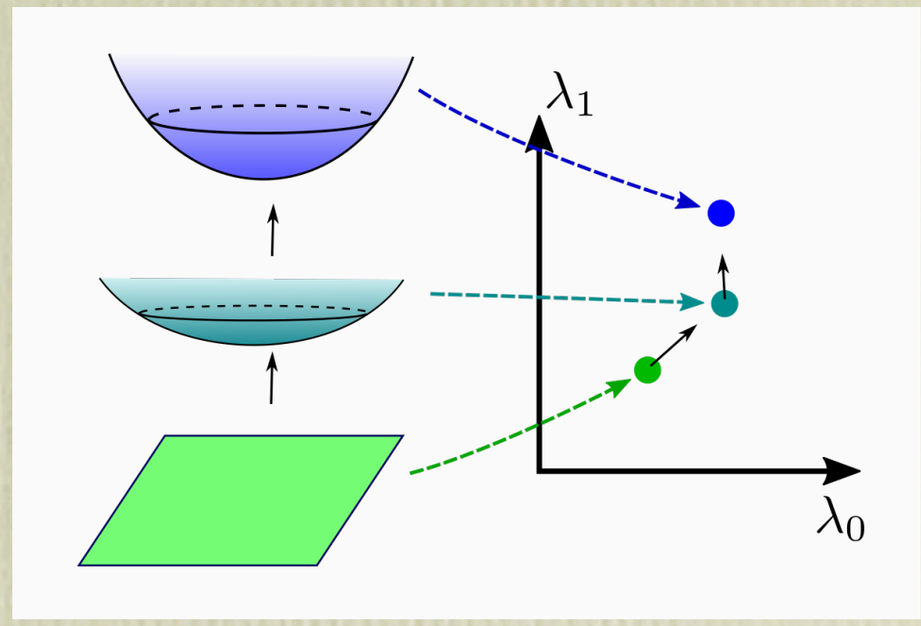


- We use a feed-forward network and train it using supervised learning
- The networks learns quickly about the constant shift, further improvements are slow
- Most of the cost is in generating the seed configurations with much less required for training
- Integrations over learnifold is fast and we were able to use it to explore larger parameter region for Thirring 1+1 model

Sign optimized manifolds

$$\langle\sigma\rangle = \frac{\int_{\mathcal{M}} dz\, e^{-S(z)}}{\int_{\mathcal{M}} dz\, e^{-S_R(z)}} = \frac{Z}{Z_{\rm pq}}$$

Since $\nabla_\lambda Z = 0$ the sign average can be optimized by minimizing the phase-quenched partition function



For a given ansatz $z = f_\lambda(x)$ we can maximize $\langle\sigma\rangle$ with respect to λ, using a stochastic gradient descent. For a well chosen ansatz, the estimate for the gradient can be computed quickly.

$$\nabla_\lambda \log\langle\sigma\rangle = \left\langle \nabla_\lambda S - \mathrm{Tr}\log J^{-1}\nabla_\lambda J \right\rangle_{\mathrm{Re}S_{\rm eff}}$$

Mori, Kashiwa & Ohnishi, arXiv:1705.05605 AA, Bedaque, Lamm & Lawrence, arXiv:1804.00697 Bursa & Kroyter, arXiv:1805.04941

Sign optimized manifolds

- For Thirring model in 2+1 dimensions, we use an ansatz motivated by the dense limit

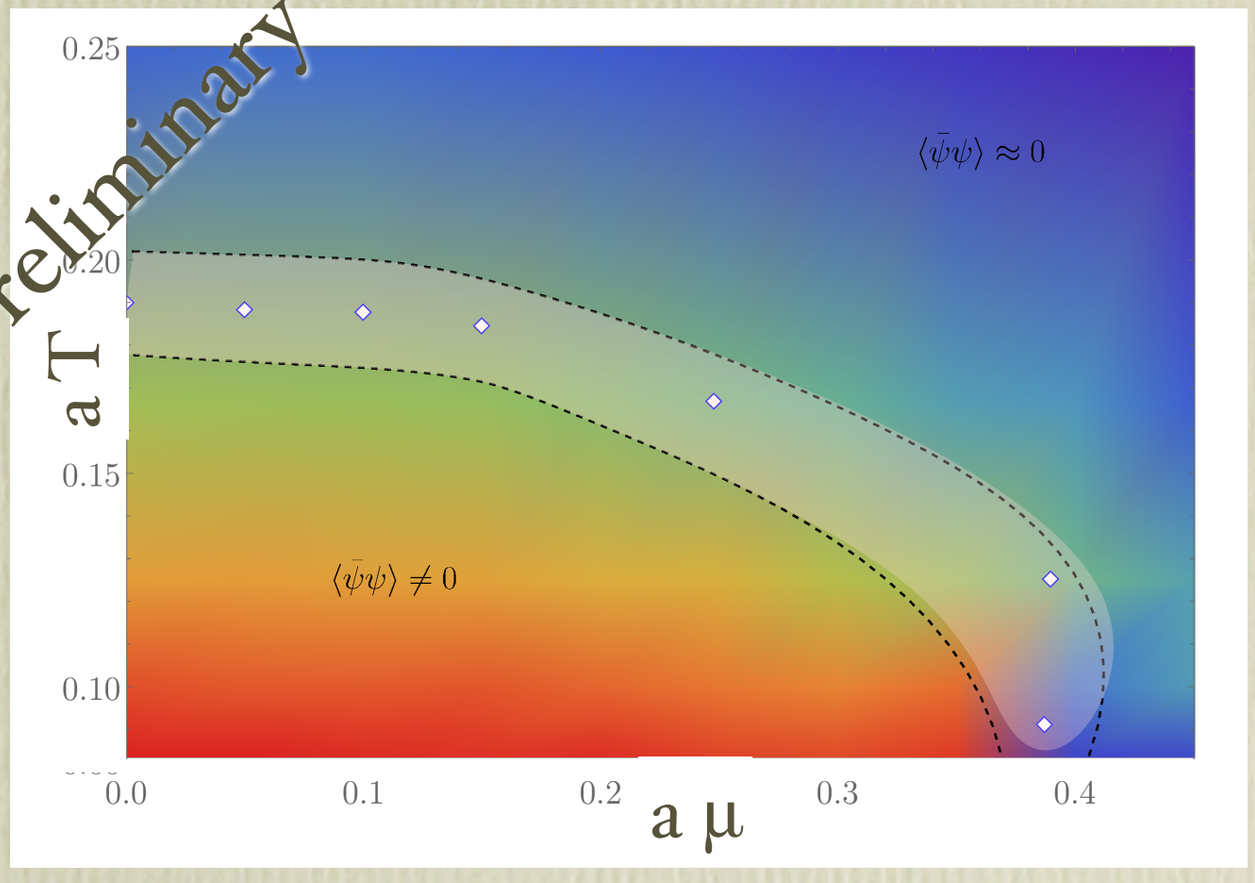
$$\begin{aligned} A_0(x) &\rightarrow A_0(x) + i f_\lambda[A_0(x)] \\ A_1(x) &\rightarrow A_1(x) \end{aligned}$$

$$f_\lambda(x) = \lambda_0 + \lambda_1 \cos x + \lambda_2 \cos 2x$$

- For this ansatz the Jacobian can be computed efficiently

$$\det J = \prod_x [1 + i f'(A_0(x))]$$

- We carry out the sign optimization for a set of temperatures and densities to investigate the phase diagram



Conclusions

- Complex manifold integration is a generic method for systems with sign problems: finite density QFTs, real time, etc.
- Field complexification serves as a knob to control the sign problem.
- Holomorphic gradient flow generates a continuous family of manifolds with improved sign average (with Lefschetz thimble decomposition a limiting case).
- Thimbles and holomorphic flow manifolds are only one option. There is a large degree of freedom in choosing complex deformations to address the numerical challenges specific to the system of interest (with new challenges and opportunities).

References

arXiv:1510.0325 arXiv:1512.0876 arXiv:1604.00956

arXiv:1605.08040 arXiv:1606.02742 arXiv:1609.01730

arXiv:1703.02414 arXiv:1703.06404 arXiv:1709.01971

arXiv:1804.00697 arXiv:1807.02027 arXiv:1808.xxxxx