Finite density simulations for strongly interacting field theories

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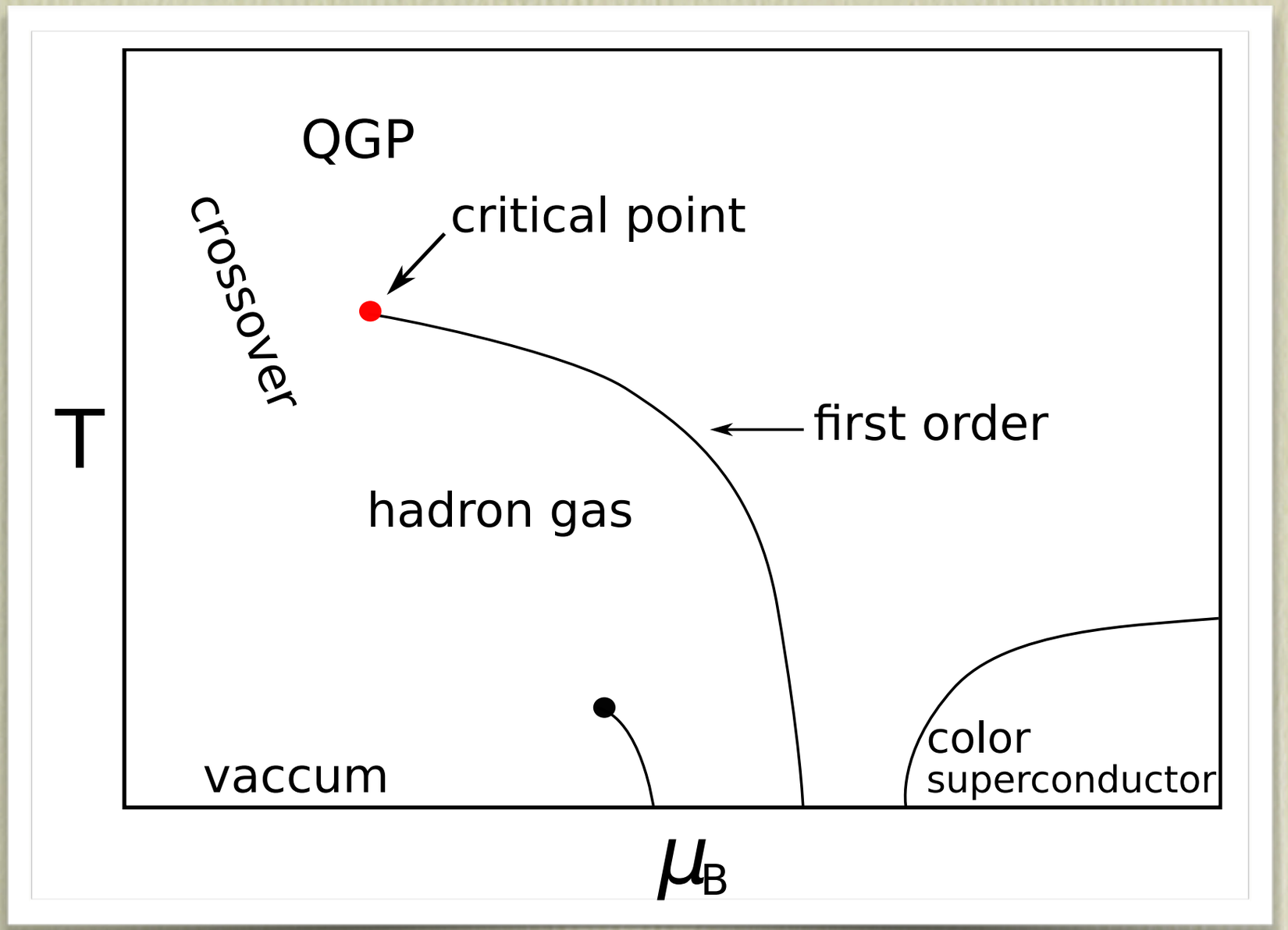
The plan

- Sign problem for QFTs at finite density
- Complexification and contour deformation
- Sampling method
- Case studies: real time correlators and Thirring model in 2+1 dimensions
- Outlook

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.)
- Complex path methods are likely to work for a large class of problems.

Motivation



$$Z_{GC}(T,V,\mu) = \int \mathcal{D}U e^{-S_g(U)} \det M(U,\mu)$$

complex

Thermal QFT

- The partition function

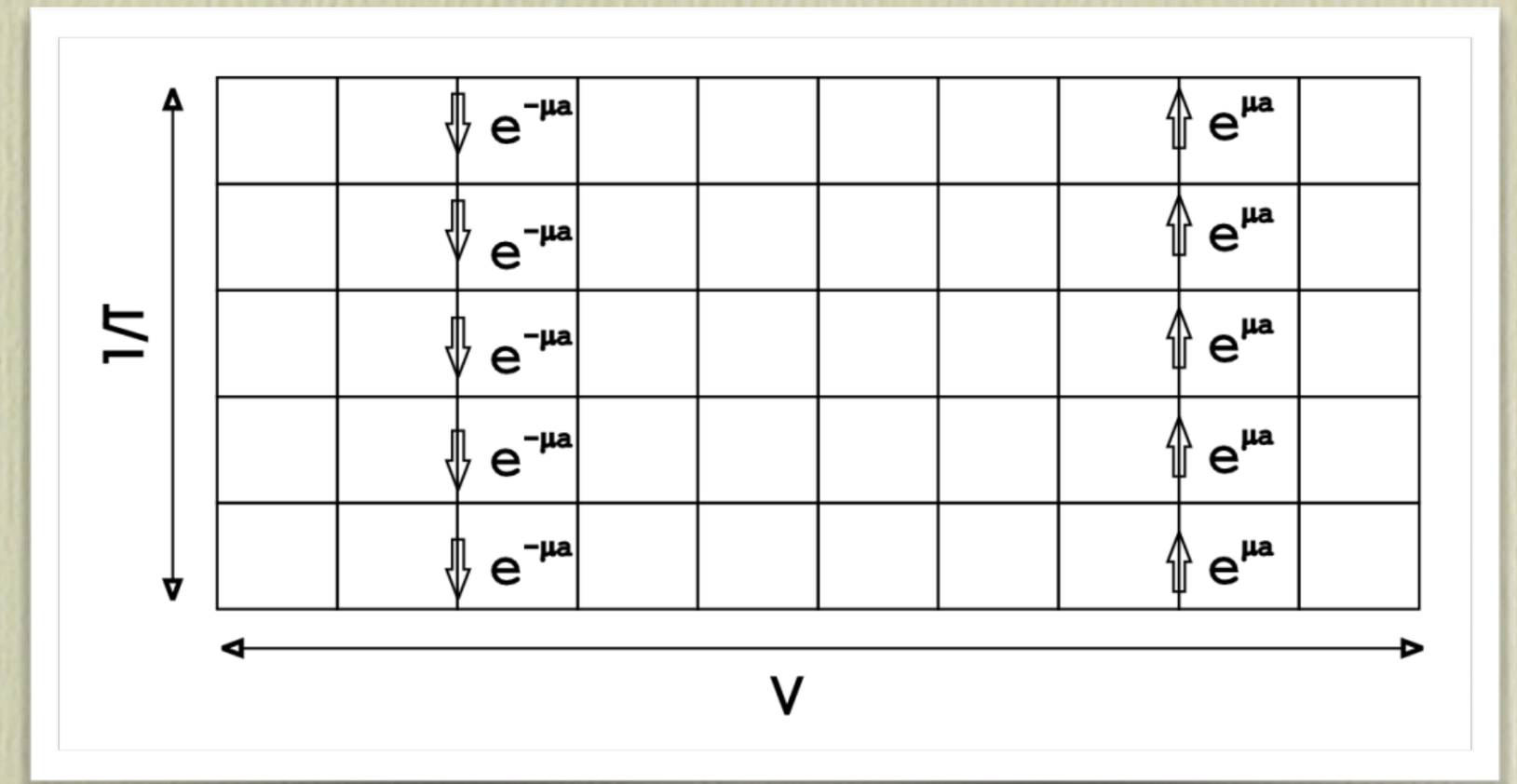
$$Z = \mathrm{Tr}\, e^{-\beta H} = \int \prod_{i=0}^{n-1} d\phi_i \, \langle \phi_0 \mid e^{-a_t H} \mid \phi_{n-1} \rangle \cdot \ldots \cdot \langle \phi_1 \mid e^{-a_t H} \mid \phi_0 \rangle$$

$$= \int \prod_{i=0}^{n-1} d\phi_i \, e^{-S_E(\phi)} \qquad \text{where } a_t = \beta/n$$

- The temperature is inversely proportional to the Euclidean "time" extent

- Volume is controlled by the size in the spatial direction and chemical potential by biasing the *hopping* in "time" direction

Grand canonical partition function



$$Z_{GC}(T,V,\mu) = \int \mathcal{D}U e^{-S_g(U)} \det M(U,\mu)^2$$

complex

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

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

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

QFT on the lattice

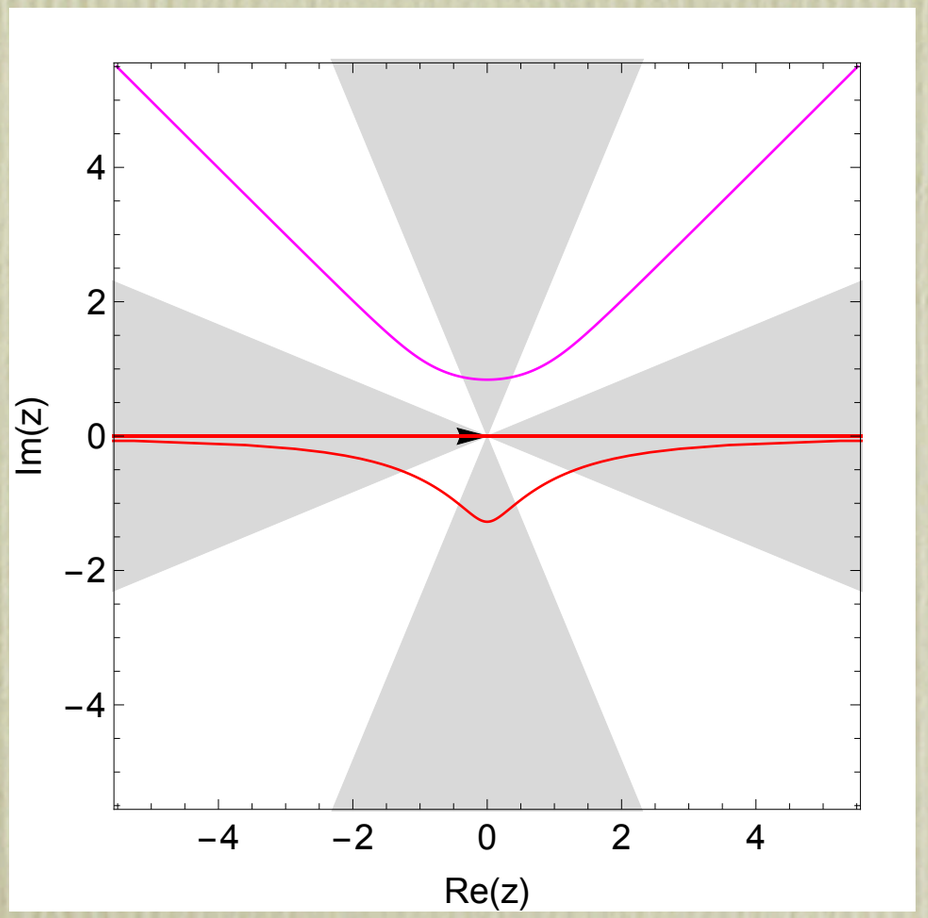
- The partition function is expressed as a path integral
- The fields are sampled on a grid; differential operators are replaced by finite difference ones

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

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

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

Contour deformation



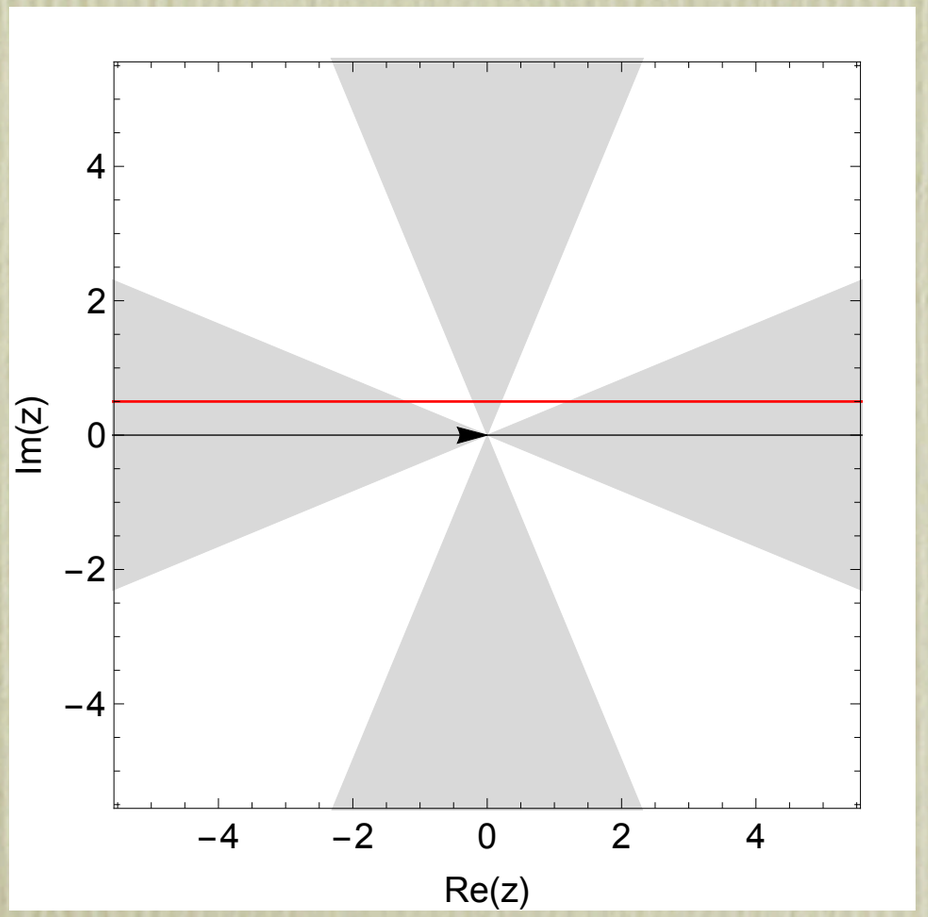
$$Z = \int_{-\infty}^{\infty} \mathrm{d}x\, e^{-S(x)}$$

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

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

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

Contour deformation



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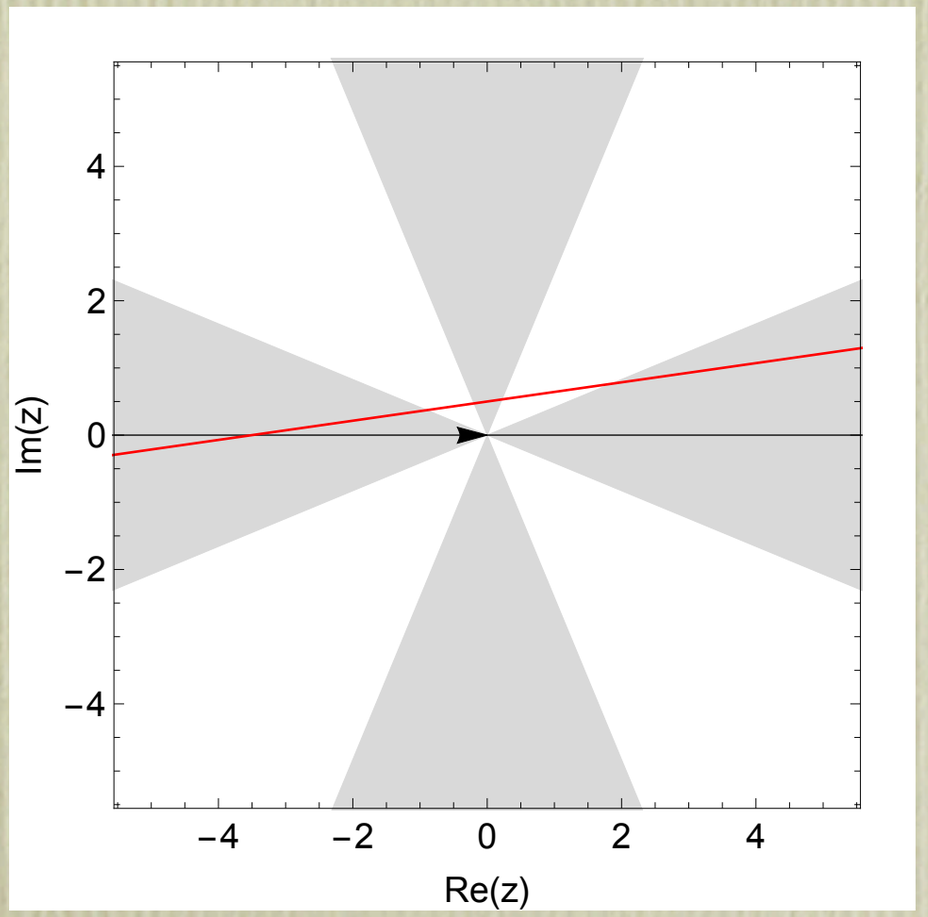

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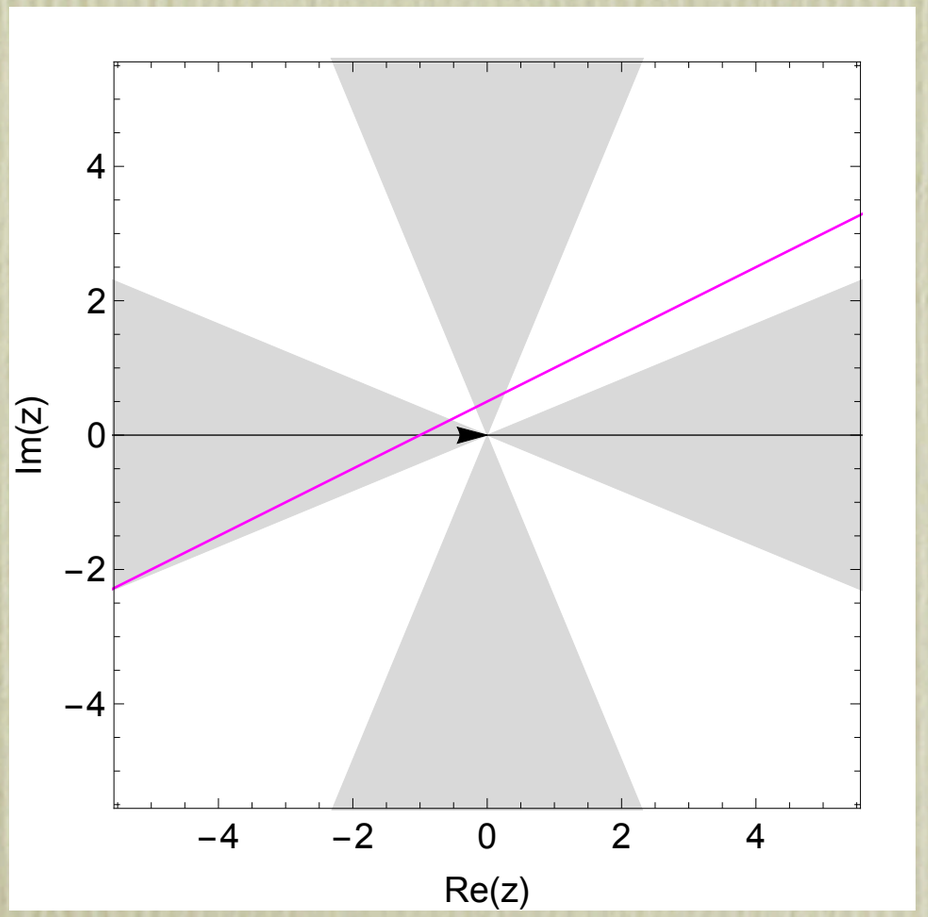

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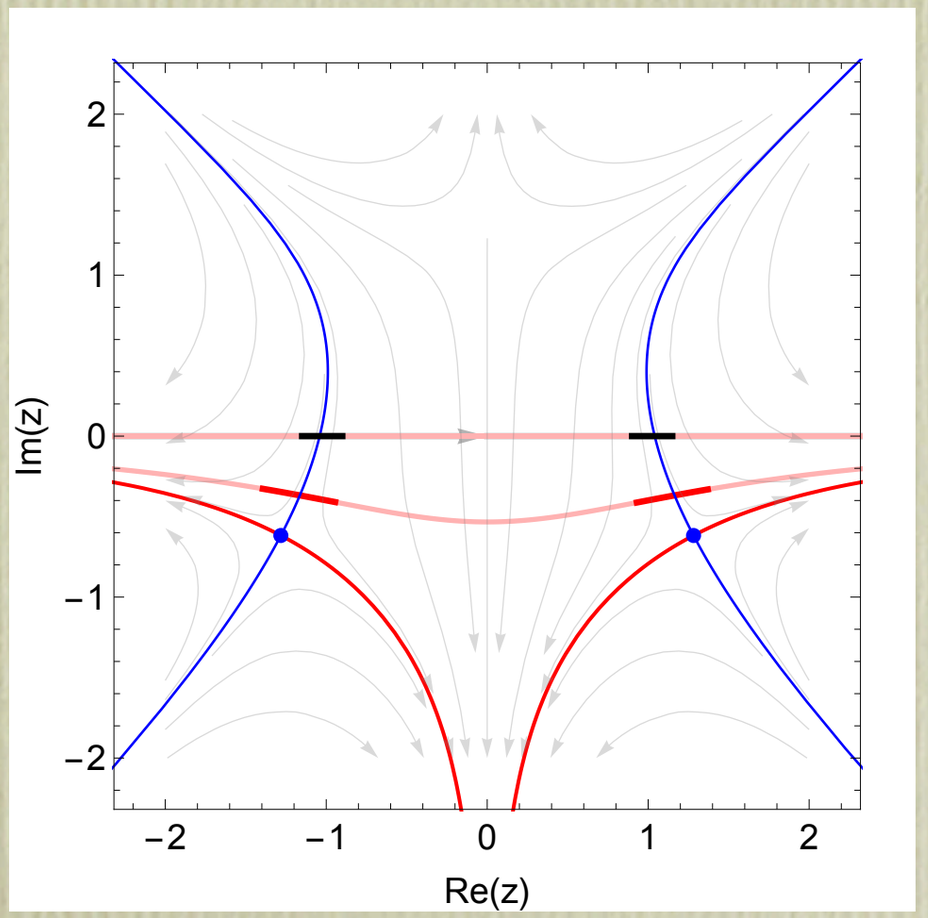
Holomorphic gradient flow and Lefschetz thimbles



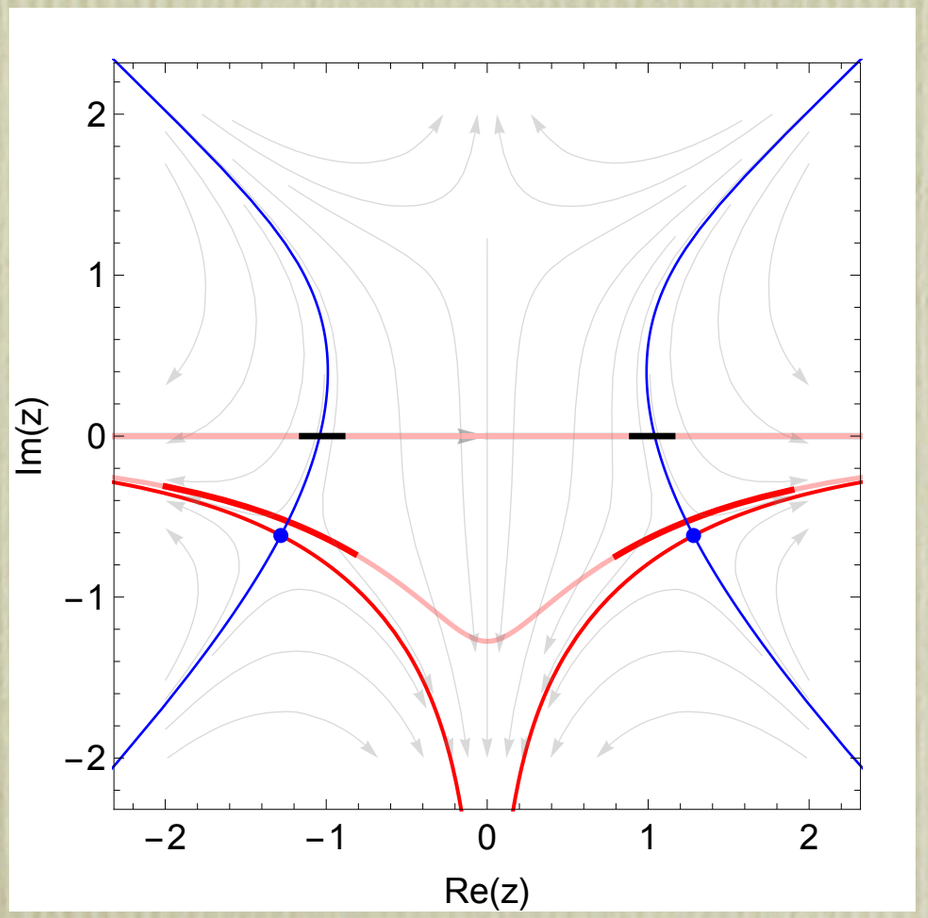
$$Z = \int_{-\infty}^{\infty} \mathrm{d}x\, e^{-S(x)}$$

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

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

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

Holomorphic gradient flow and Lefschetz thimbles



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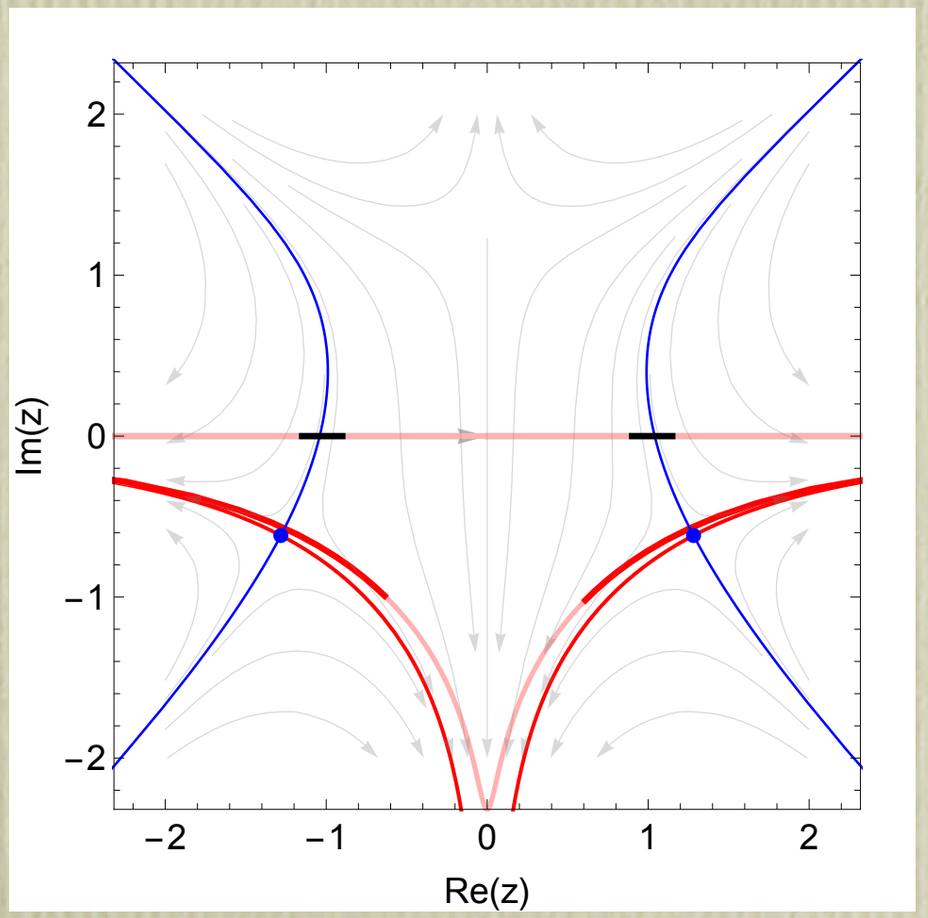

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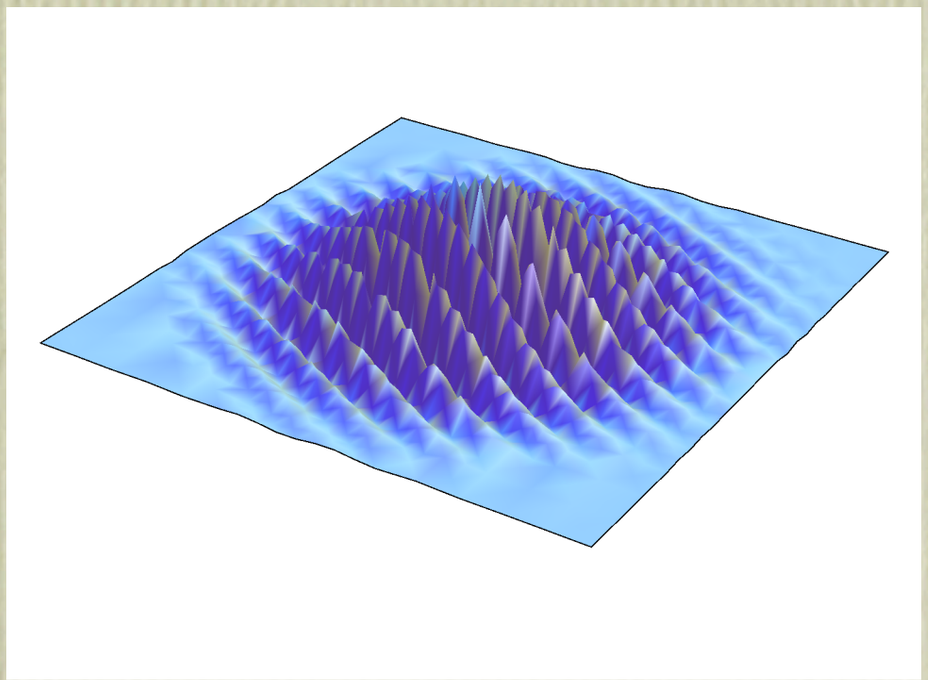
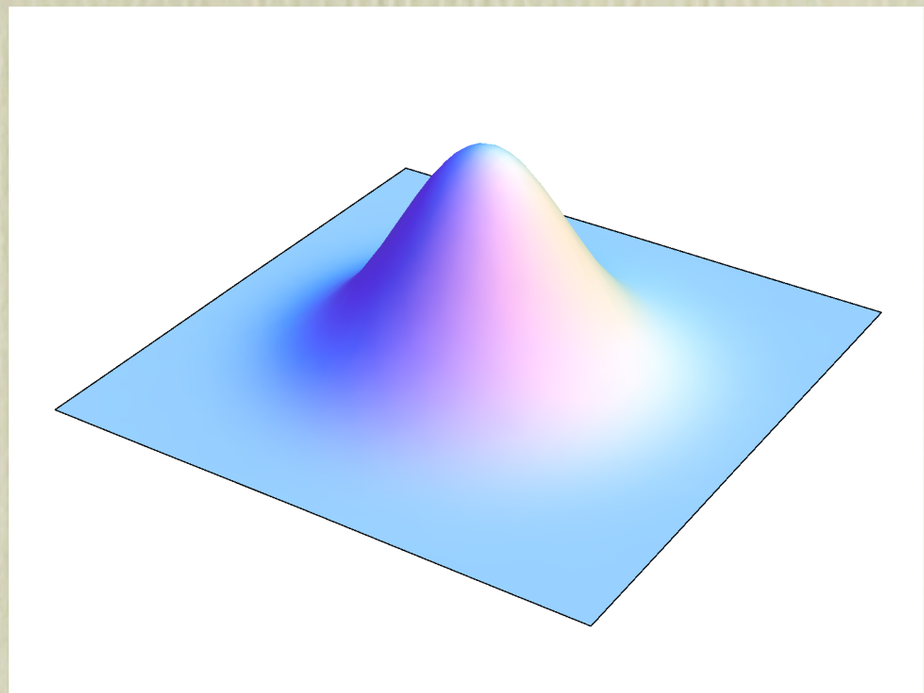
$$Z = \sum_{\sigma} n_\sigma \int_{J_\sigma} dz\, e^{-S(z)}$$

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

Lefschetz thimble



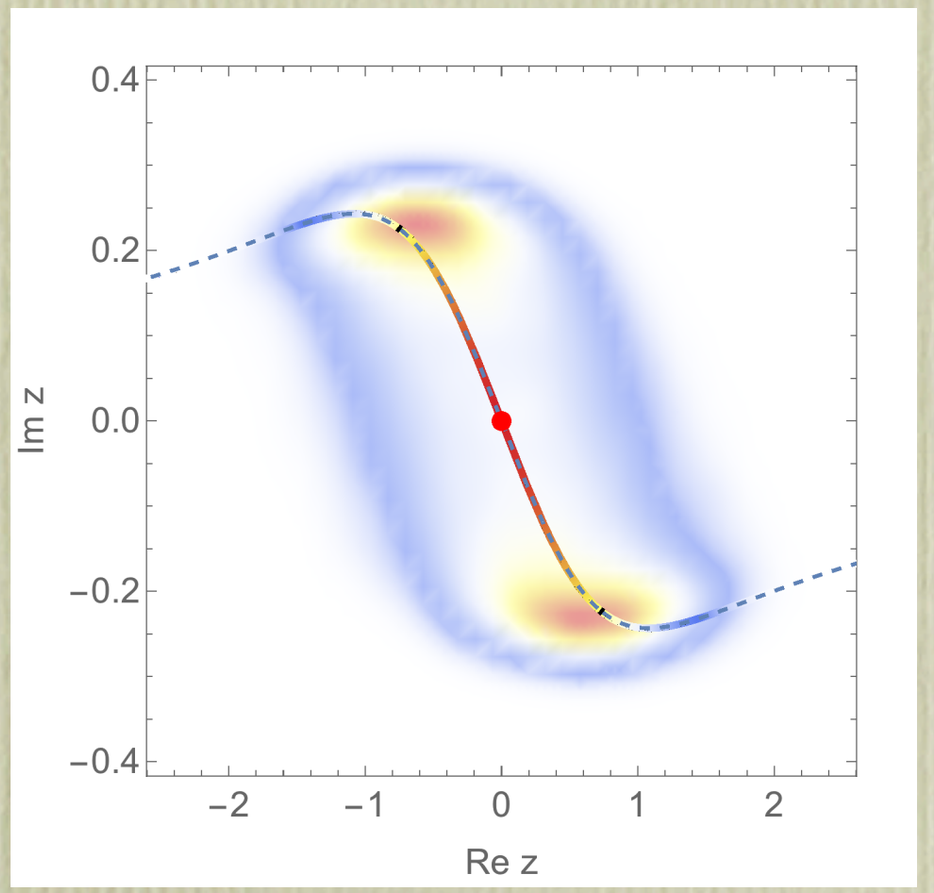
$e^{-S(x_1,x_2)}$ (real plane)



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

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

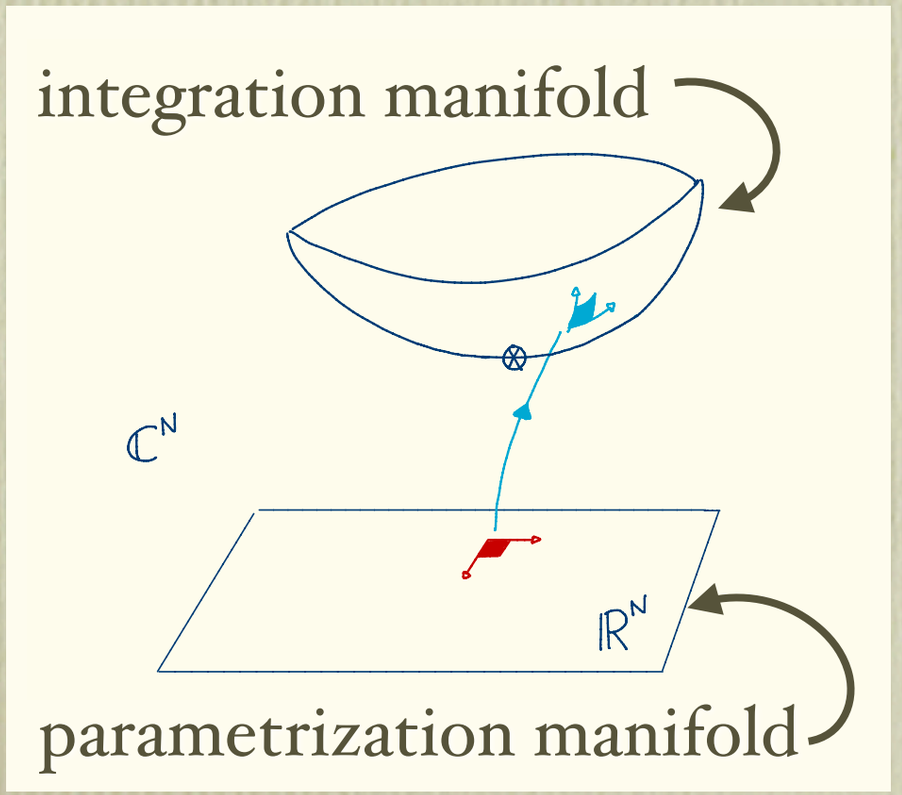
- The process moves freely in the complex plane with possible runaways

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

Basic idea

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

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



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

$$\Phi(x) = S_I(z(x)) - \mathrm{Im}\,\ln\det J(x)$$

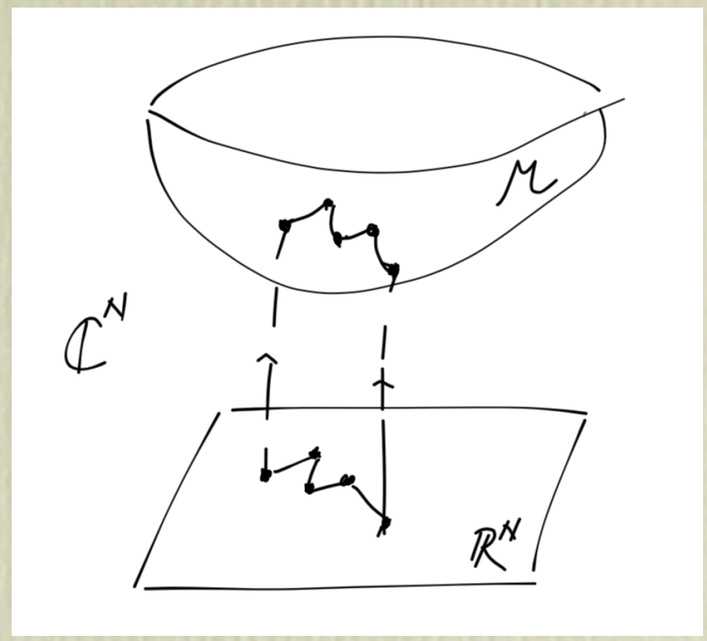
$$\langle O \rangle = \frac{\left\langle O(z(x)) e^{-i\Phi(x)} \right\rangle_0}{\left\langle e^{-i\Phi(x)} \right\rangle_0}$$

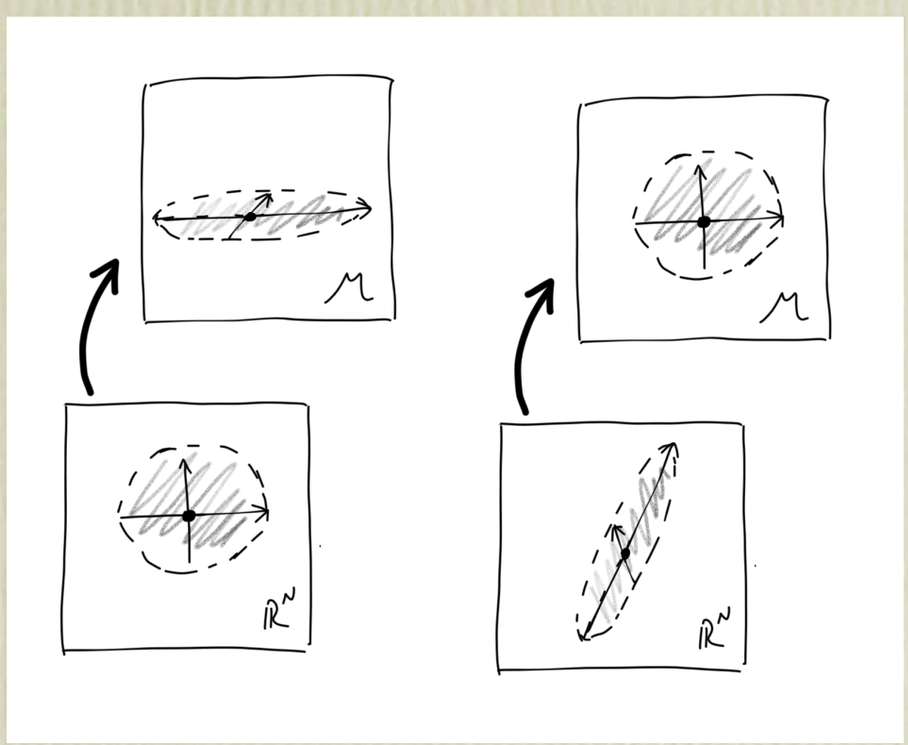
Importance sampling

- Propose new x (parametrization space)
- Compute z(x), J(x) using the map (flow, parametrization etc) and $S_{\text{eff}}(x)$

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

- z(x) map can be expensive, for example when defined by holomorphic flow.
- The Jacobian J(x) even more so. One possibility is to use fast estimators.
- anisotropic proposals (skew proposals with approximation of J^{-1})





AA, G. Basar, and P. Bedaque, *Monte Carlo algorithm for simulating fermions on Lefschetz thimbles*, Phys. Rev. D93 (2016), no. 1 014504

AA, G. Basar, P. F. Bedaque, G. W. Ridgway, and N. C. Warrington, *Fast estimator of Jacobians in the Monte Carlo integration on Lefschetz thimbles*, Phys. Rev. D93 (2016), no. 9 094514

Results

- finite density
  - 0+1 Thirring model (flow)
  - 1+1 Thirring model (flow, learnifold)
  - **2+1 Thirring model (sign-optimized manifold)**
  - 3+1 ϕ^4 Bose gas (flow)
  - 1+1 QED (flow)
- real time
  - **0+1 anharmonic oscillator (flow)**
  - 1+1 ϕ^4 Bose gas (flow)

Case study: real time physics

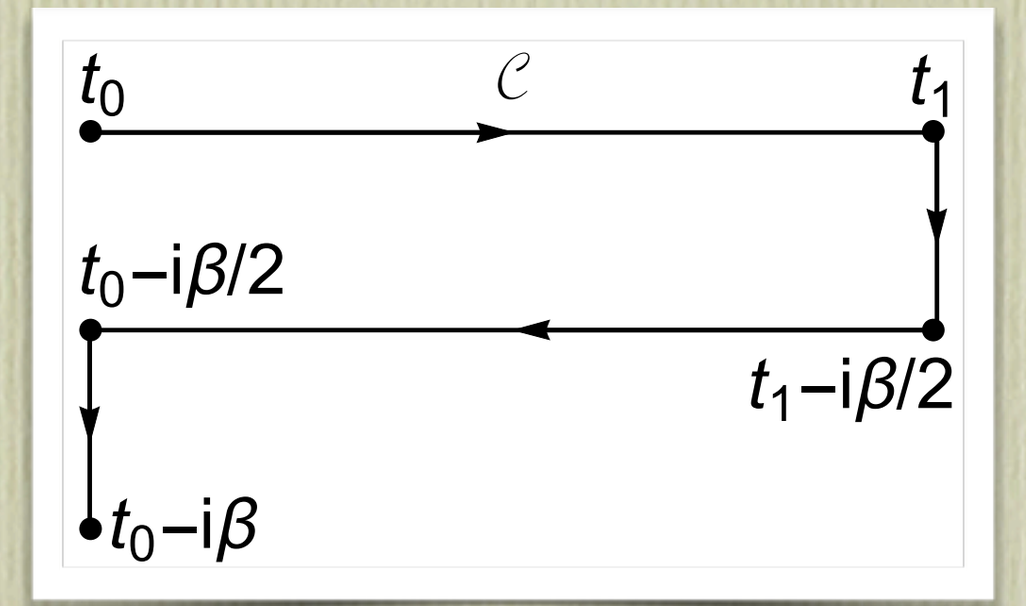
- Motivation: compute out-of-equilibrium correlators, transport coefficients non-perturbatively from first principles

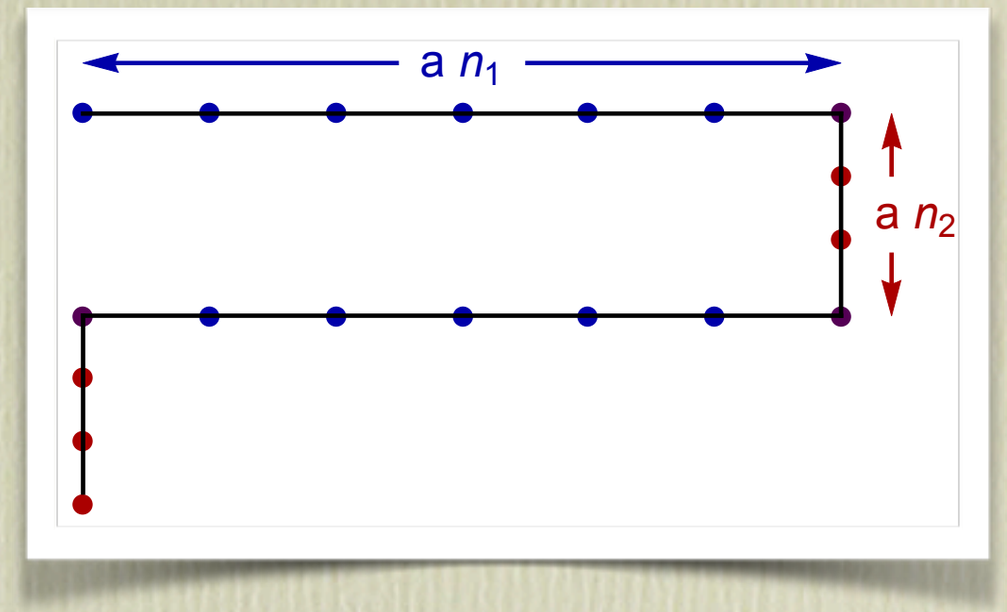
- Observables of interest are transport coefficient such as shear viscosity, conductivity, etc.

- At thermal equilibrium the observables are of the type

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

Real time physics

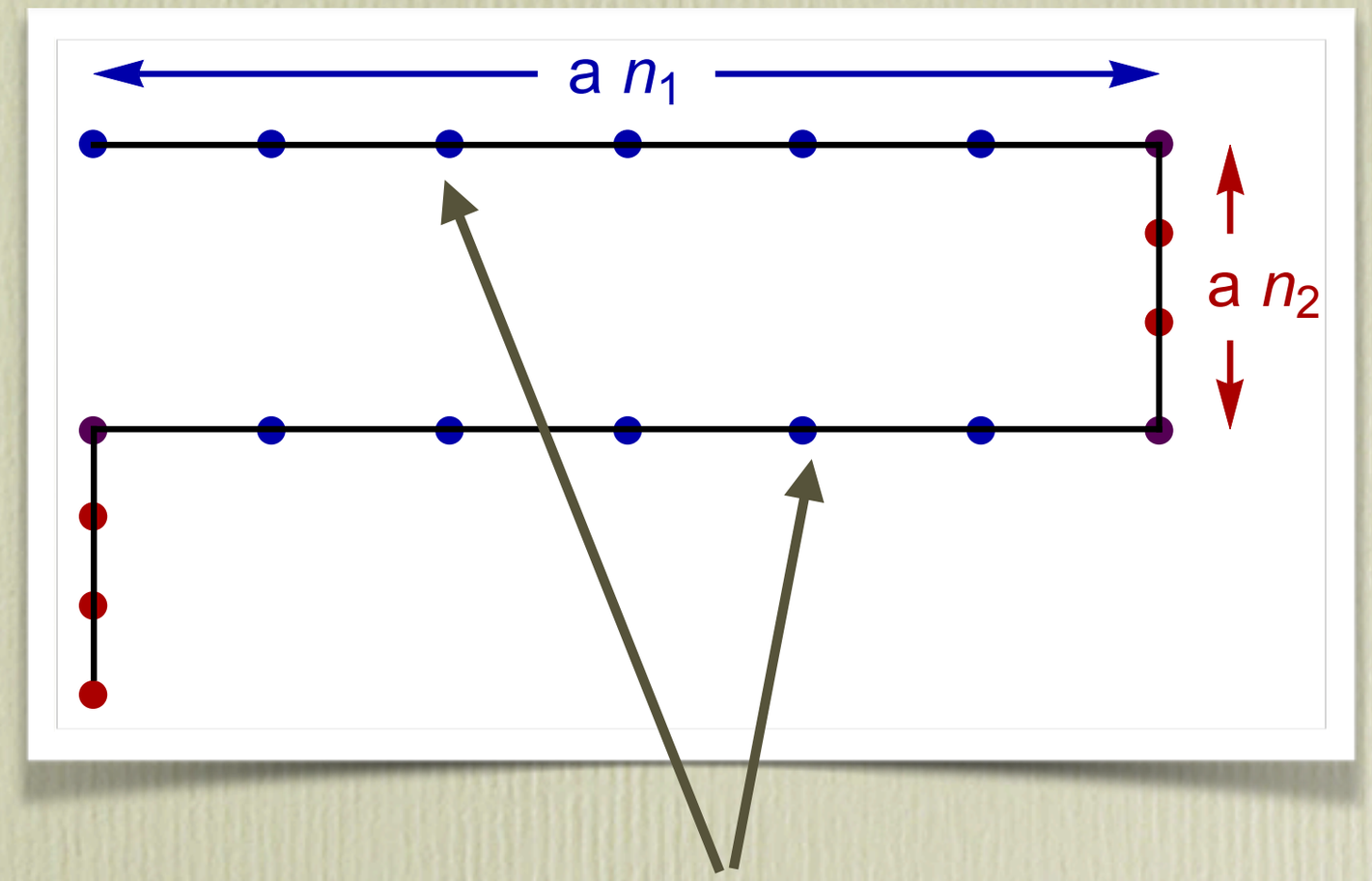




$$S_{SK}[\phi] = iS[\phi] = \int_{\mathcal{C}} dt\, L[\phi] \qquad \langle \mathcal{O}_1(t)\mathcal{O}_2(t')\rangle = \frac{1}{Z}\int \mathcal{D}\phi\, e^{-S[\phi]}\mathcal{O}_1(t)\mathcal{O}_2(t')$$

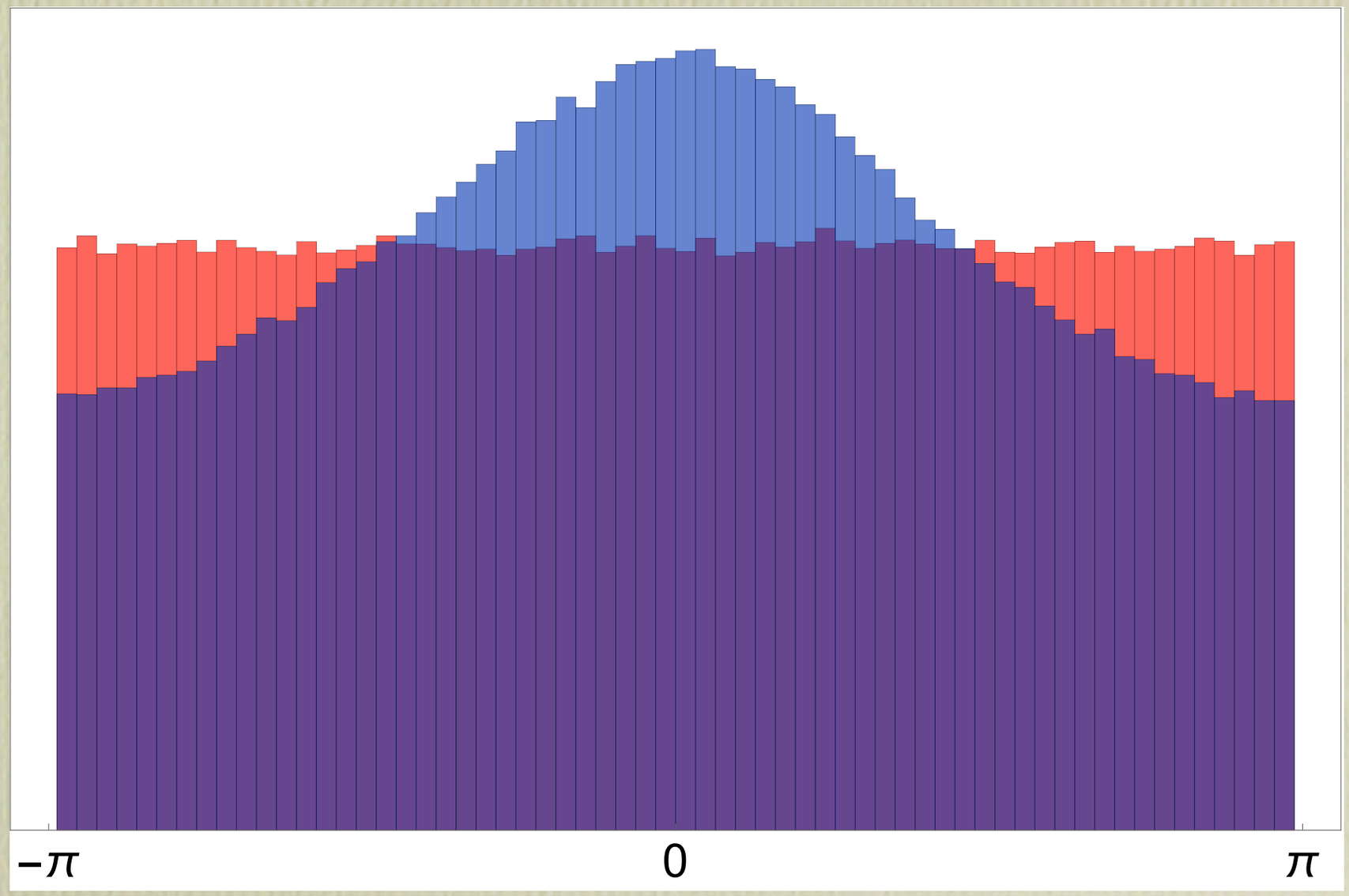
$$S[\phi] = \sum_{t,n} a_t a \left[\frac{(\phi_{t+1,n} - \phi_{t,n})^2}{2a_t^2} + \frac{1}{2}\left(\frac{(\phi_{t+1,n+1} - \phi_{t+1,n})^2}{2a^2} + \frac{(\phi_{t,n+1} - \phi_{t,n})^2}{2a^2} \right) \right.$$
$$\left. + \frac{1}{2}m^2 \frac{\phi_{t,n}^2 + \phi_{t+1,n}^2}{2} + \frac{\lambda}{4!}\frac{\phi_{t+1,n}^4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

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.

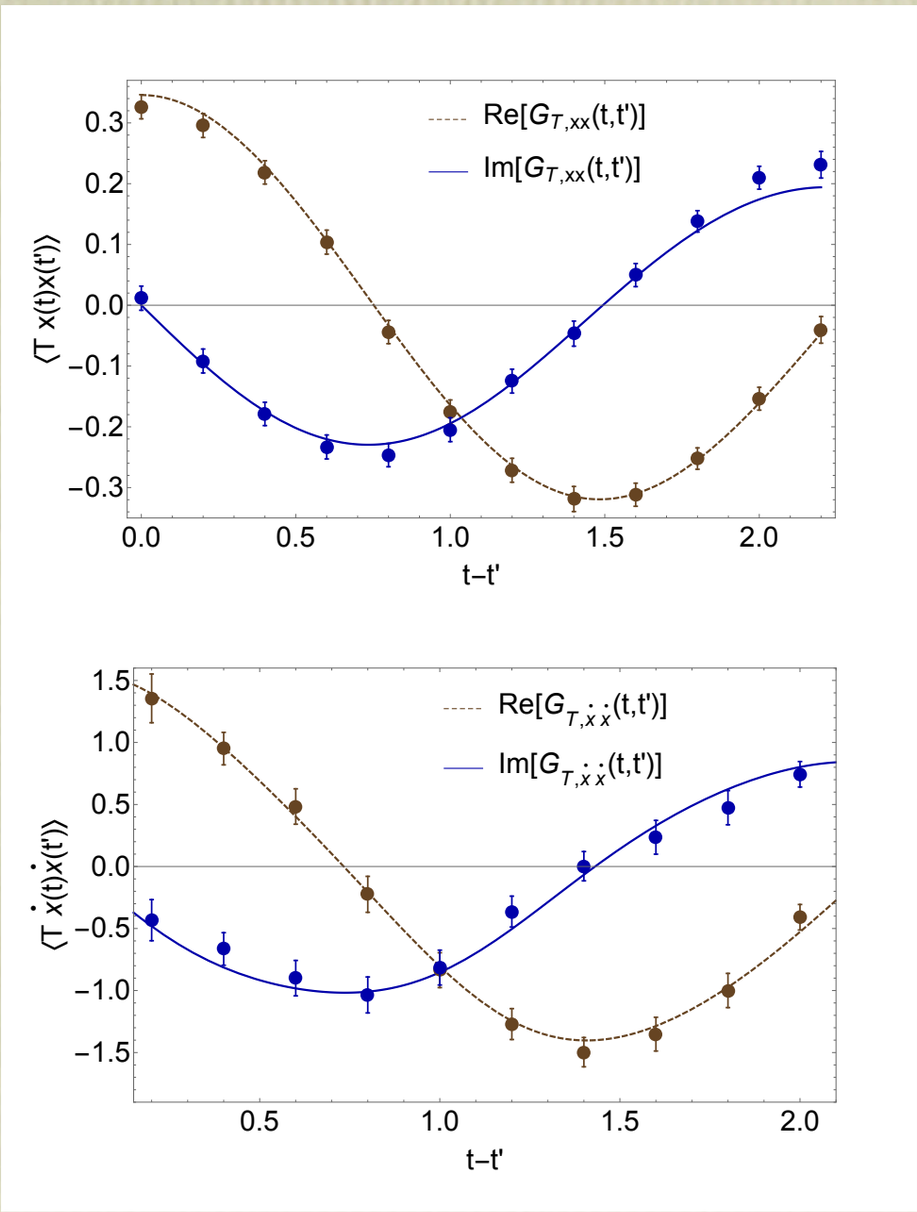
The worst sign problem



Histogram of $\mathbb{I}\mathrm{m}[S_{SK}]$ for $x \in \mathbb{R}^N$, $\mathcal{M}(T_{flow} = 0.2)$

Real time physics (0+1D)

- Complex Langevin only works for T<β
- Flow is required (from R^N)
- Jacobian is expensive and none of the estimators work efficiently
- Anisotropic proposals
- Tangent space in wrong homology class

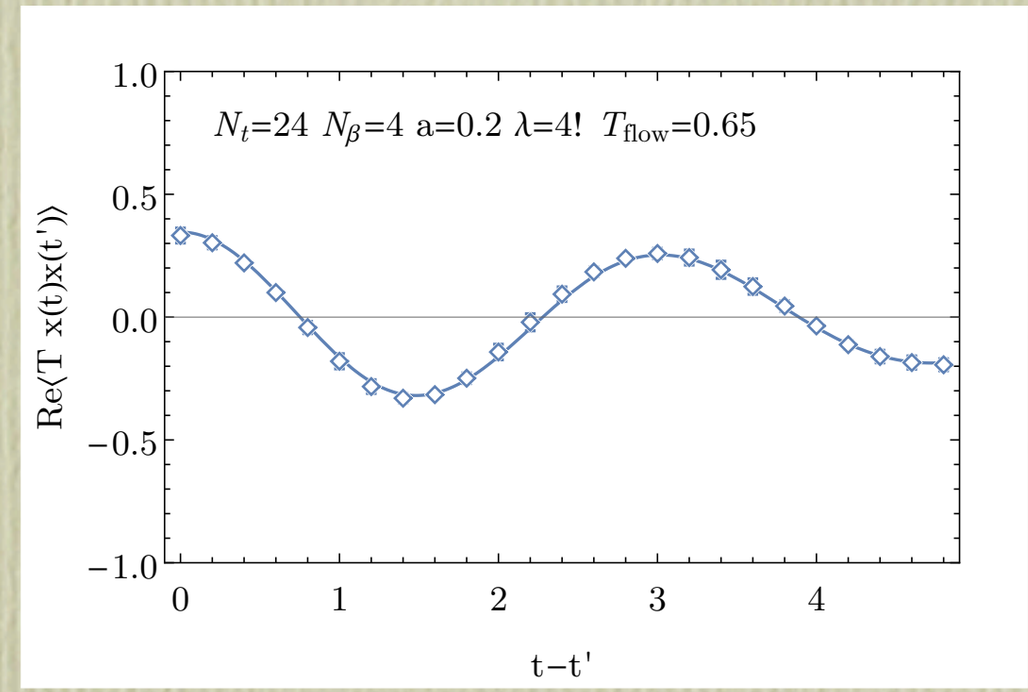


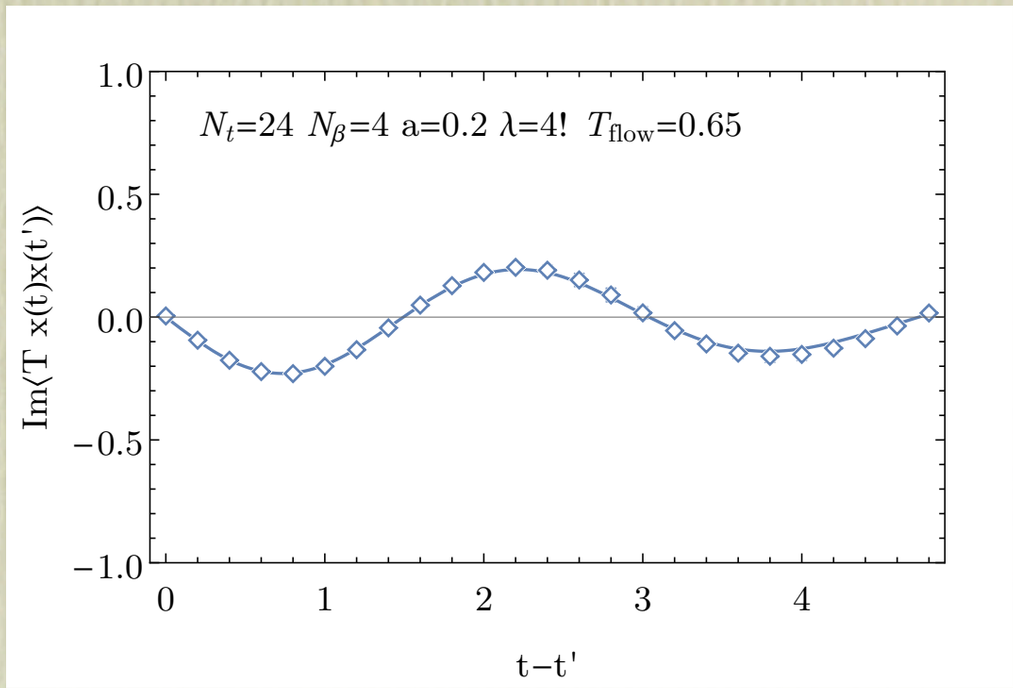
N_t=12 N_β=4 a=0.2 λ=4! dof=28

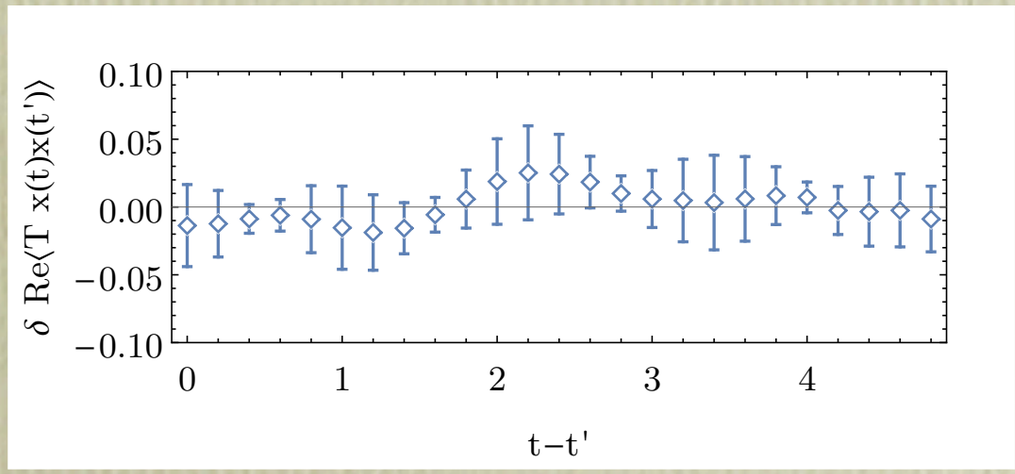
$$L = \frac{1}{2}\dot{x}^2 + \frac{1}{2}x^2 + \frac{\lambda}{4!}x^4$$

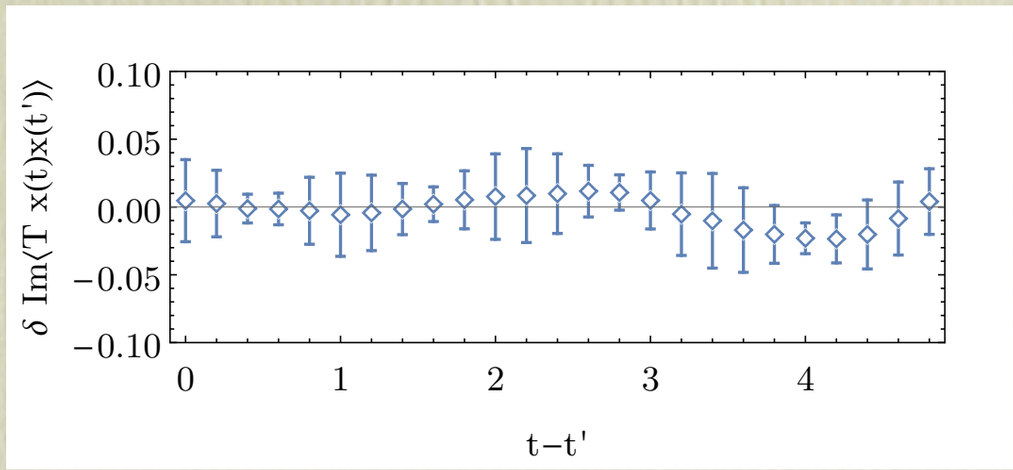
AA, G. Basar, P. F. Bedaque, S. Vartak, and N. C. Warrington, *Monte Carlo Study of Real Time Dynamics on the Lattice*, Phys. Rev. Lett. 117 (2016), no. 8 081602

Results

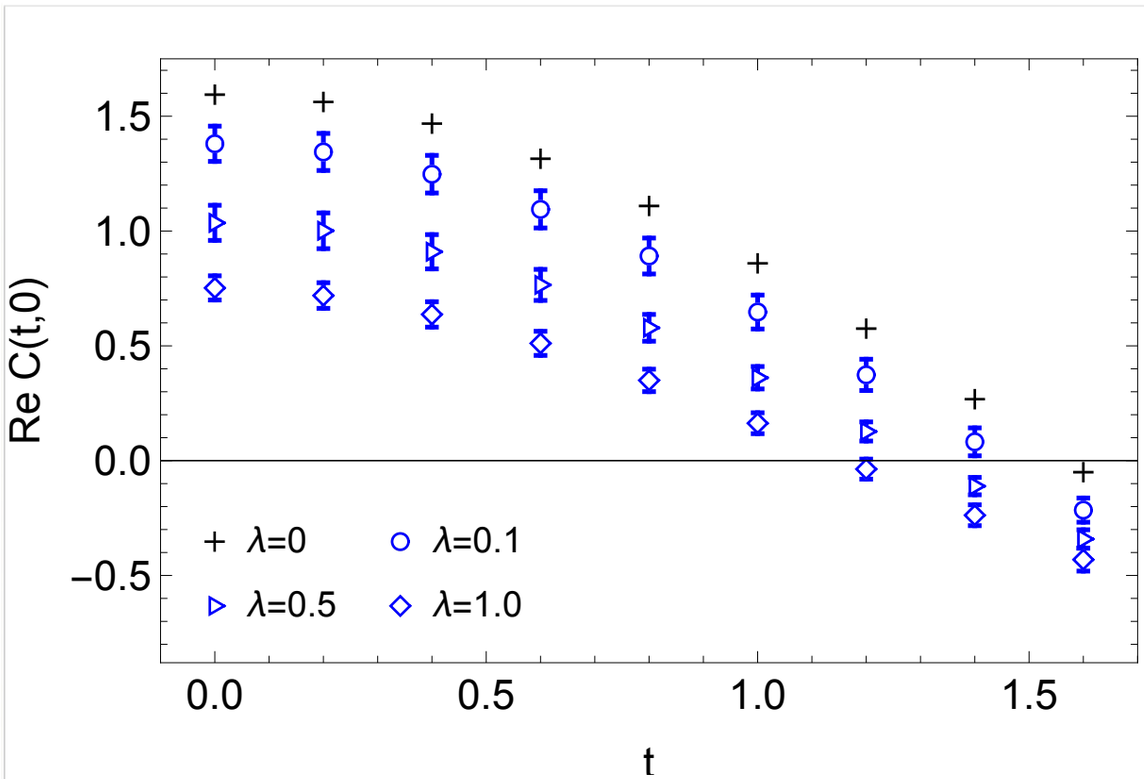

N_t=24 N_β=4 a=0.2 λ=4! $T_{\rm flow}$=0.65
Re⟨T x(t)x(t')⟩
t−t'

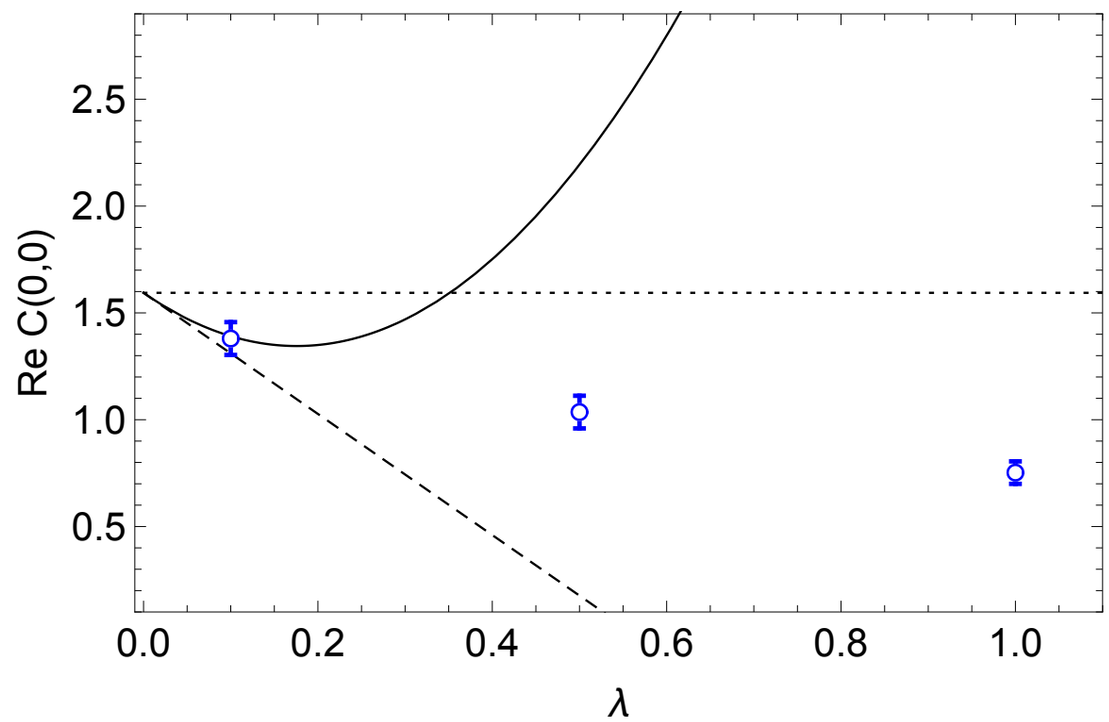

N_t=24 N_β=4 a=0.2 λ=4! $T_{\rm flow}$=0.65
Im⟨T x(t)x(t')⟩
t−t'


δ Re⟨T x(t)x(t')⟩
t−t'


δ Im⟨T x(t)x(t')⟩
t−t'

Results (1+1D)

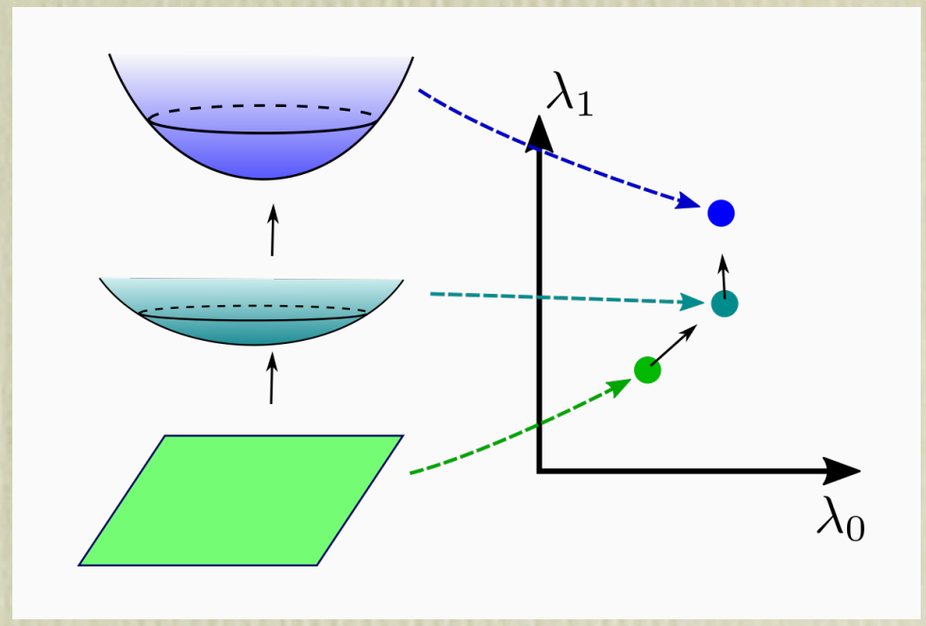




1+1D φ^4: n_t=8, n_x=8, n_β=2, λ=0.1,0.5,1.0

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

Massive Thirring model

Continuum action

$$S = \int d^3x \left[\bar{\psi}^a \left(\gamma_\mu \partial_\mu + \mu \gamma_0 + m \right) \psi^a + \frac{g^2}{2N_F} \bar{\psi}^a \gamma_\mu \psi^a \bar{\psi}^a \gamma_\mu \psi^a \right]$$

At zero density the model still attracts interest

- For small number of flavors, $N_F < (N_F)_c$, the massless model is expected to be chirally broken.
- For large number of flavors, $N_F > (N_F)_c$, chiral symmetry is restored.
- Numerical determinations for $(N_F)_c$ depend on the discretization used.

We are interested in the finite density results: we will take the model to be defined by the staggered discretization with N_F=2.

Massive Thirring model

Lattice action after Hubbard-Stratonovich rewriting

- A's are compact fields defined on links
- D is the staggered fermion discretization
- a runs from 1 to $N_F/2$

$$S_{\text{latt}} = \sum_{x,\mu} \frac{N_F}{g^2} \left(1 - \cos A_\nu(x)\right) + \sum_{x,y} \bar{\psi}^a D_{xy}(m, \mu; A) \psi^a(y)$$

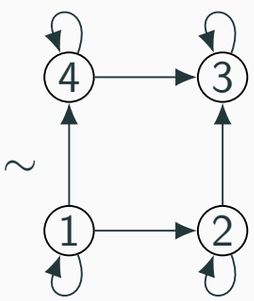
After integrating the fermionic fields the action is a function of A's

- A's are real periodic fields: integration manifold S_1^N
- after complexification $(S_1 \times R)^N$

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

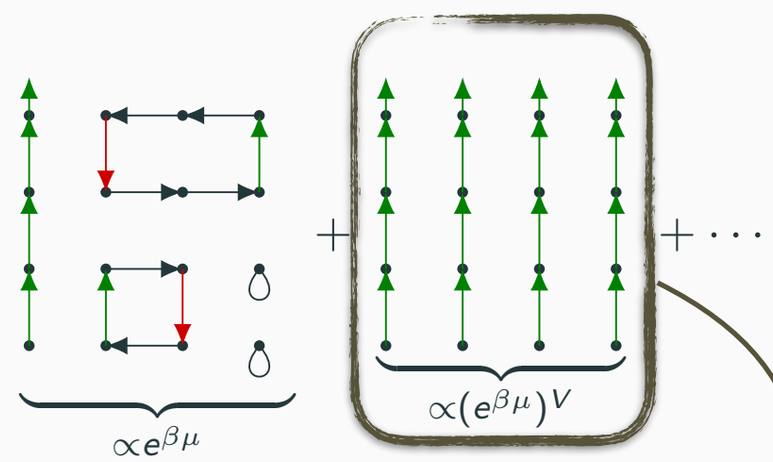
Ansatz

$$D = \begin{pmatrix} m & e^{iA_1(x_1)} & 0 & e^{\mu+iA_0(x_1)} \\ e^{-iA_1(x_1)} & m & e^{\mu+iA_0(x_2)} & 0 \\ 0 & e^{-\mu-iA_0(x_2)} & m & e^{-iA_1(x_3)} \\ e^{-\mu-iA_0(x_1)} & 0 & e^{iA_1(x_3)} & m \end{pmatrix} \sim$$



$\longrightarrow = e^{iA_1(x)}$ $\quad \uparrow = e^{iA_0(x)+\mu}$ $\quad \downarrow = e^{-iA_0(x)-\mu}$ $\quad$ $= m$

det $D =$

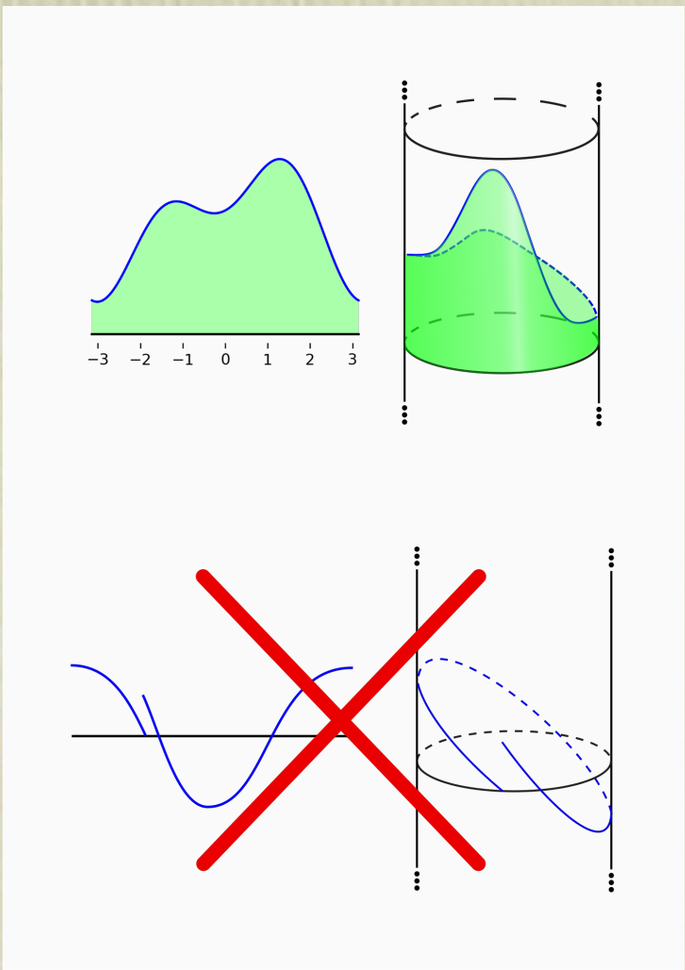


Ansatz is inspired by hopping expansion. For μ → ∞ we have

$$Z \approx \left[\int d^3A e^{\frac{1}{g^2}\left(\sum_\nu A_\nu\right)+\mu+\frac{1}{2}iA_0} \right]^{\beta V}$$

Ansatz

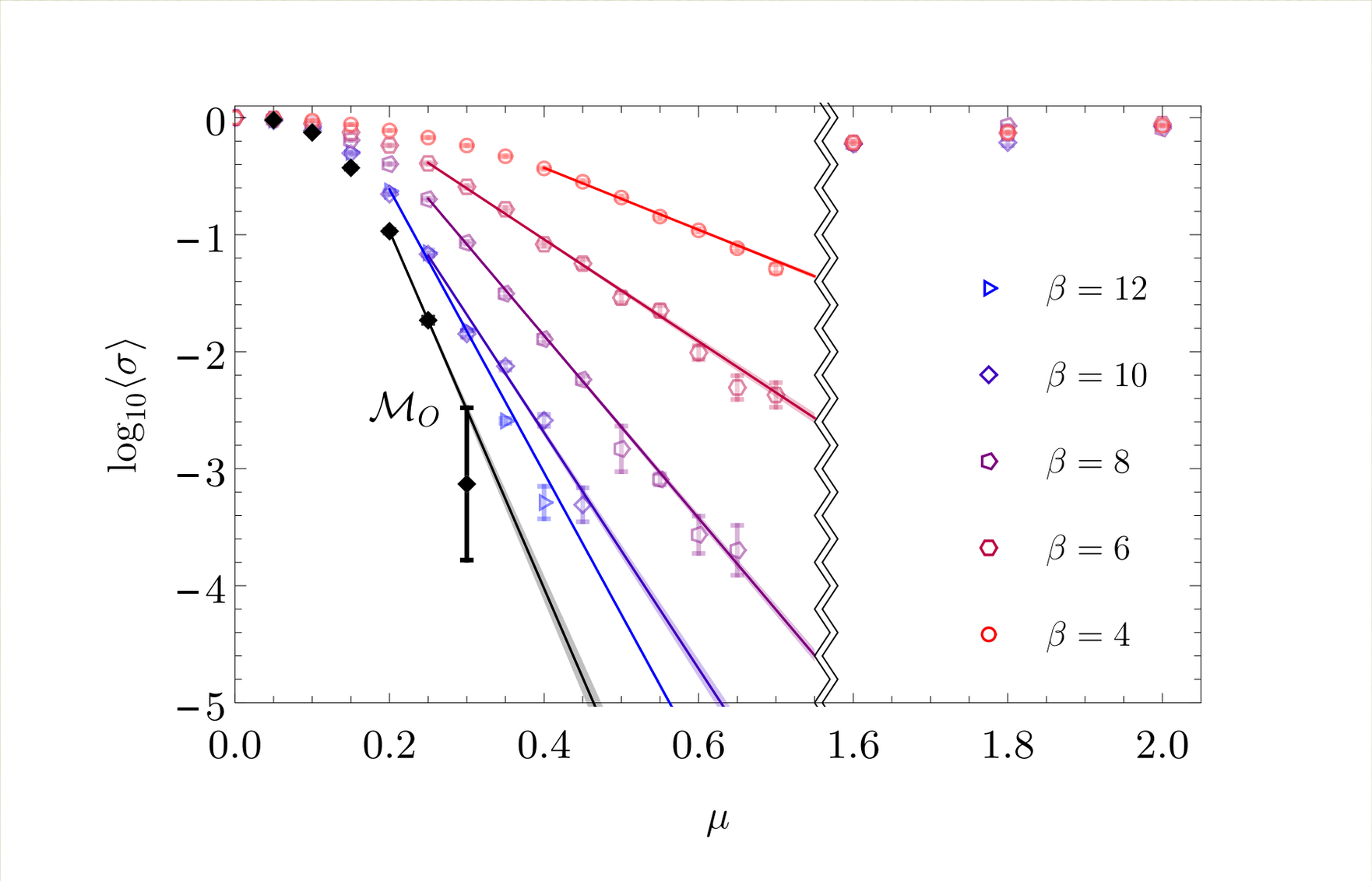
- For large μ the sign fluctuations can be removed by shifting the A_0 in the imaginary direction
- We propose then a map that only moves $A_0(x)$ in the complex plane (with correct periodicity)
- To keep the calculation of the Jacobian easy we propose that the shift in the imaginary direction for $A_0(x)$ depend only on the value of $A_0(x)$ and not on any other variables. The map $A \to \tilde{A}$ has only three parameters (λs):



$$\tilde{A}_0 = f(A_0)\,, \quad \tilde{A}_1 = A_1\,, \quad \tilde{A}_2 = A_2\,,$$
$$f(A_0) = A_0 + i[\lambda_0 + \lambda_1 \cos A_0 + \lambda_2 \cos(2A_0)]\,.$$

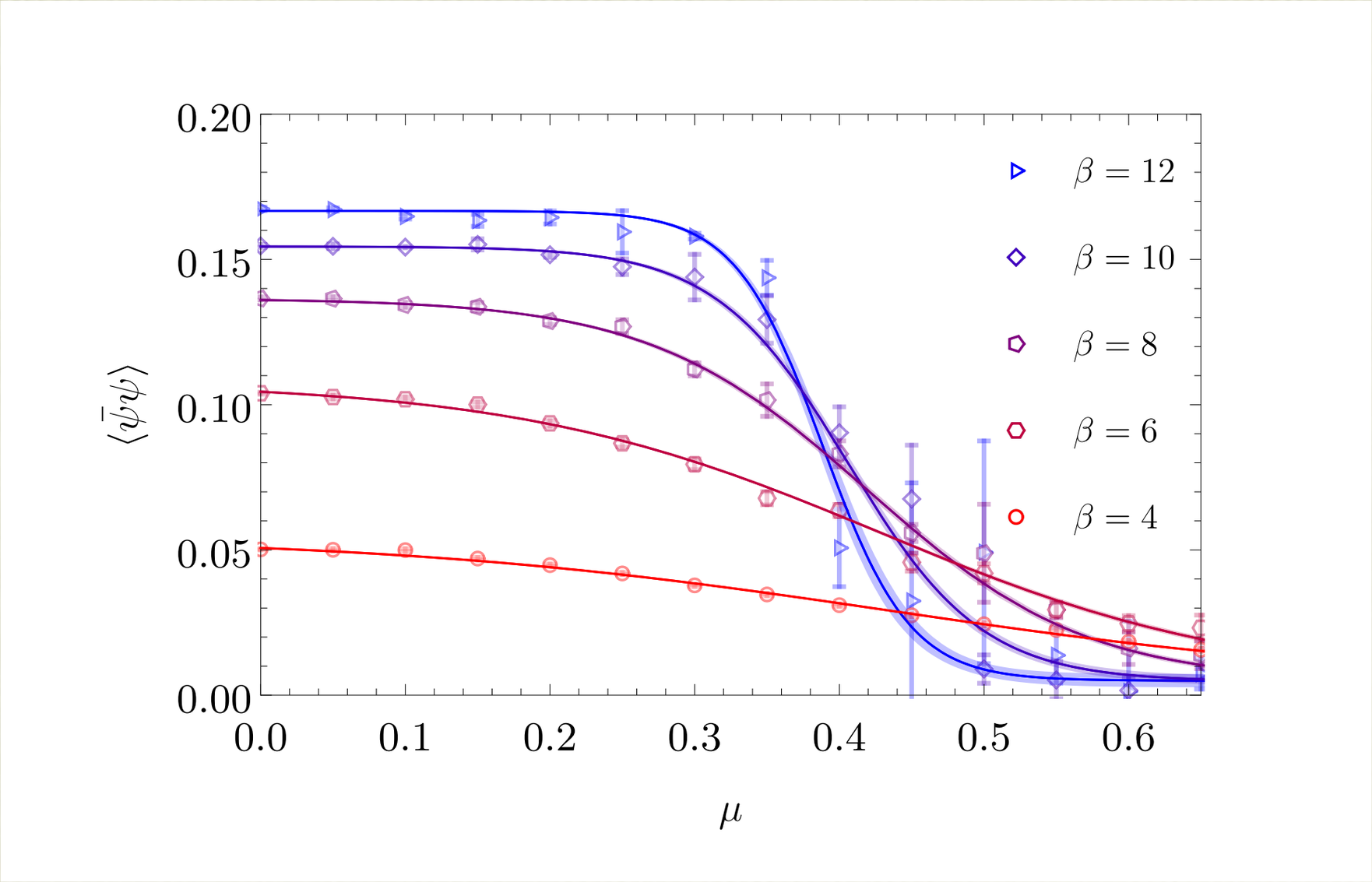
$$\det J = \prod_x [1 + i f'(A_0(x))]$$

Sign fluctuations



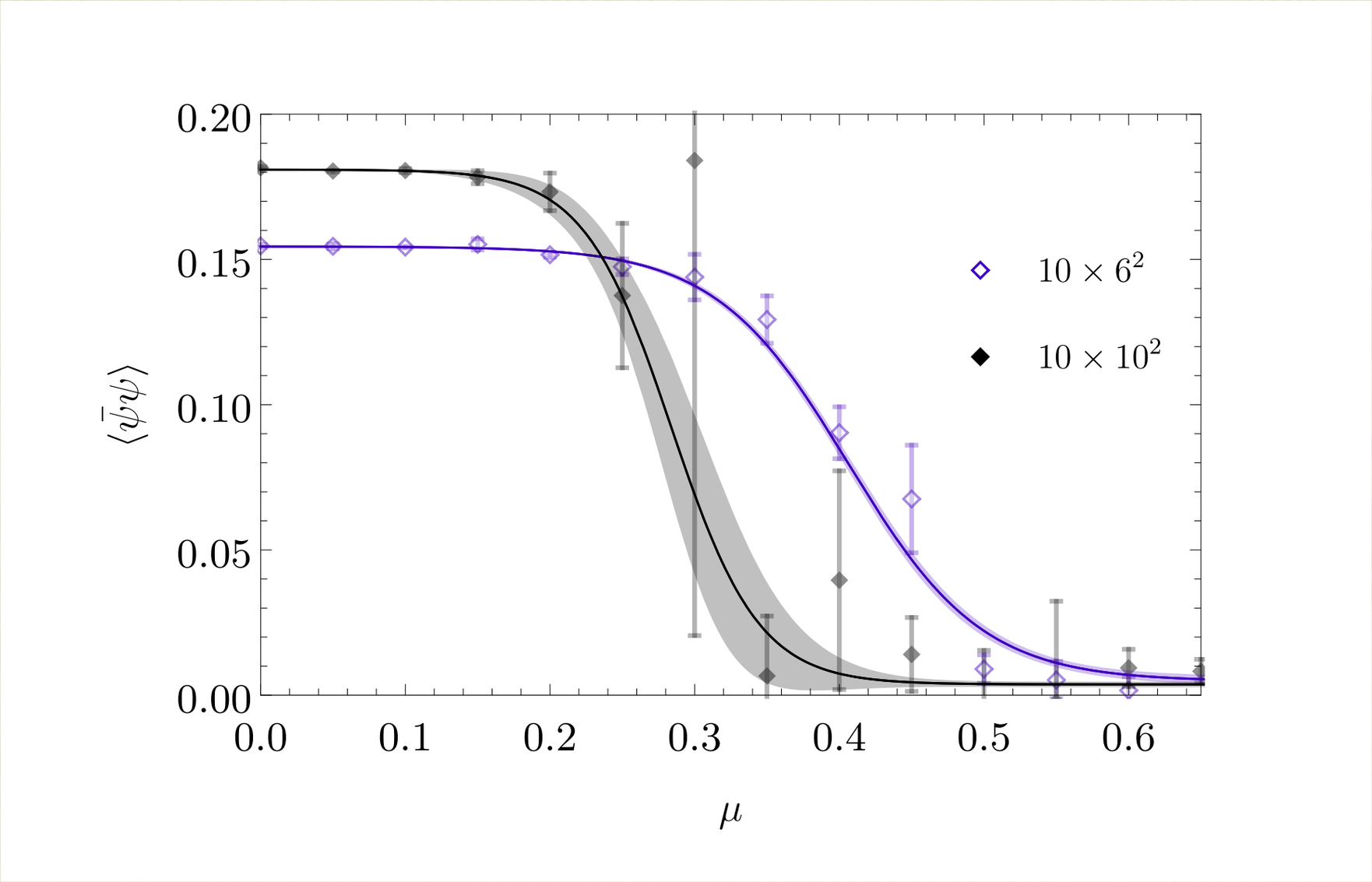
$m = 0.1$, $g = 1.08 \Rightarrow m_f = 0.46(1)$, $m_b = 0.21(1)$ $\quad m_b/m_f \ll 2$

Chiral condensate

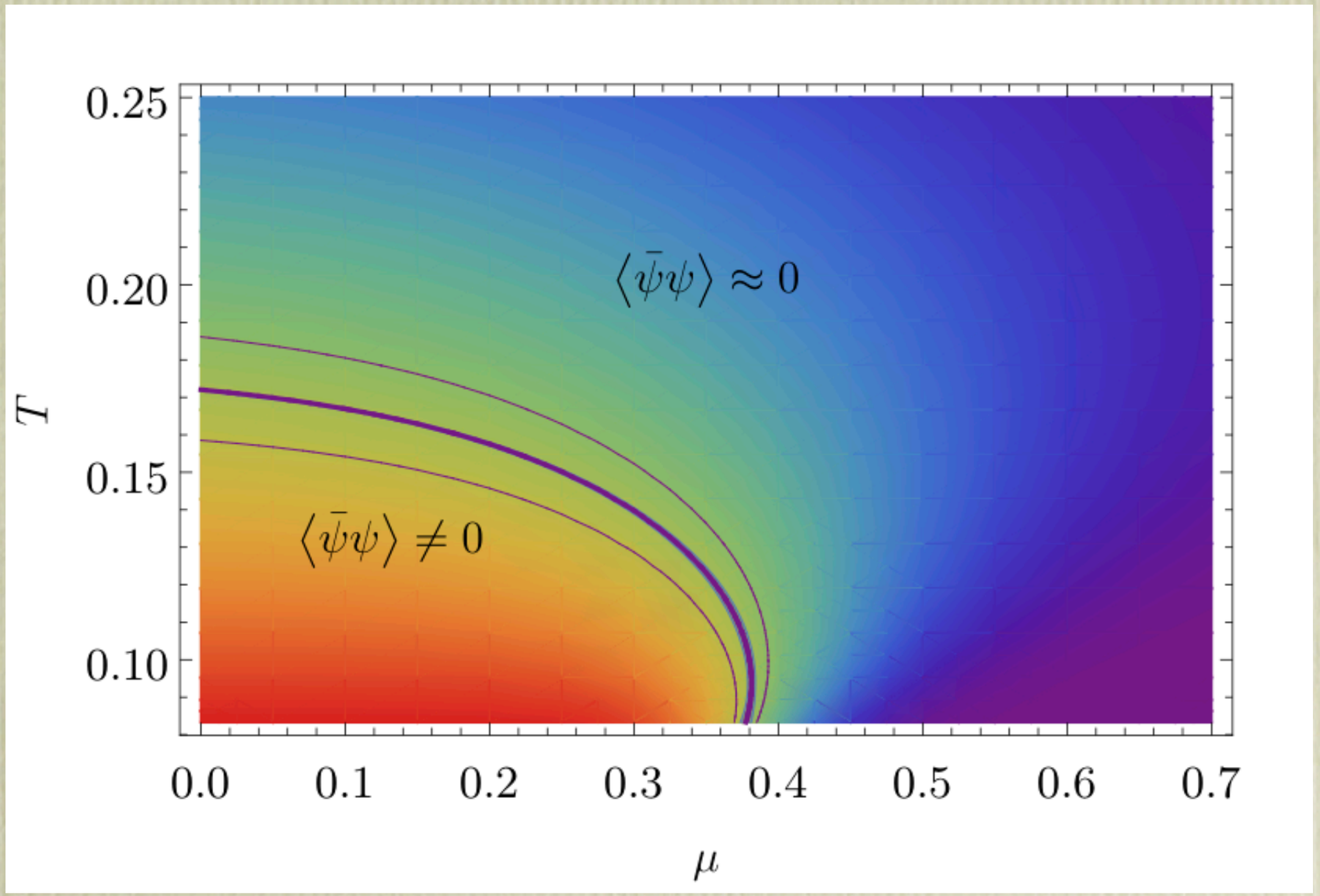


$$\langle\bar{\psi}\psi\rangle(\mu) = c_0 + c_1 \tanh[c_2(\mu - c_3)]$$

Chiral condensate volume scaling



Phase diagram



Conclusions and outlook

- The basic idea is to use complexification and contour deformation to eliminate or reduce the phase fluctuations of the action.
- 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).
- These methods can be used to attack bosonic and fermionic QFTs that have a sign problem.