Sign problem and the generalized thimble method

Andrei Alexandru

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

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ICTS, Bangalore

THE GEORGE WASHINGTON UNIVERSITY
WASHINGTON, DC

The plan

- Importance sampling and sign problem
- Complexification and contour deformation
- Single thimble and contraction algorithm
- Generalized thimble method
- Case study: Massive Thirring model
- Conclusions and 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.)
- 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

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

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

- 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): $e^{-iS_I(\phi_1)} + \ldots + e^{-iS_I(\phi_N)} \ll N$

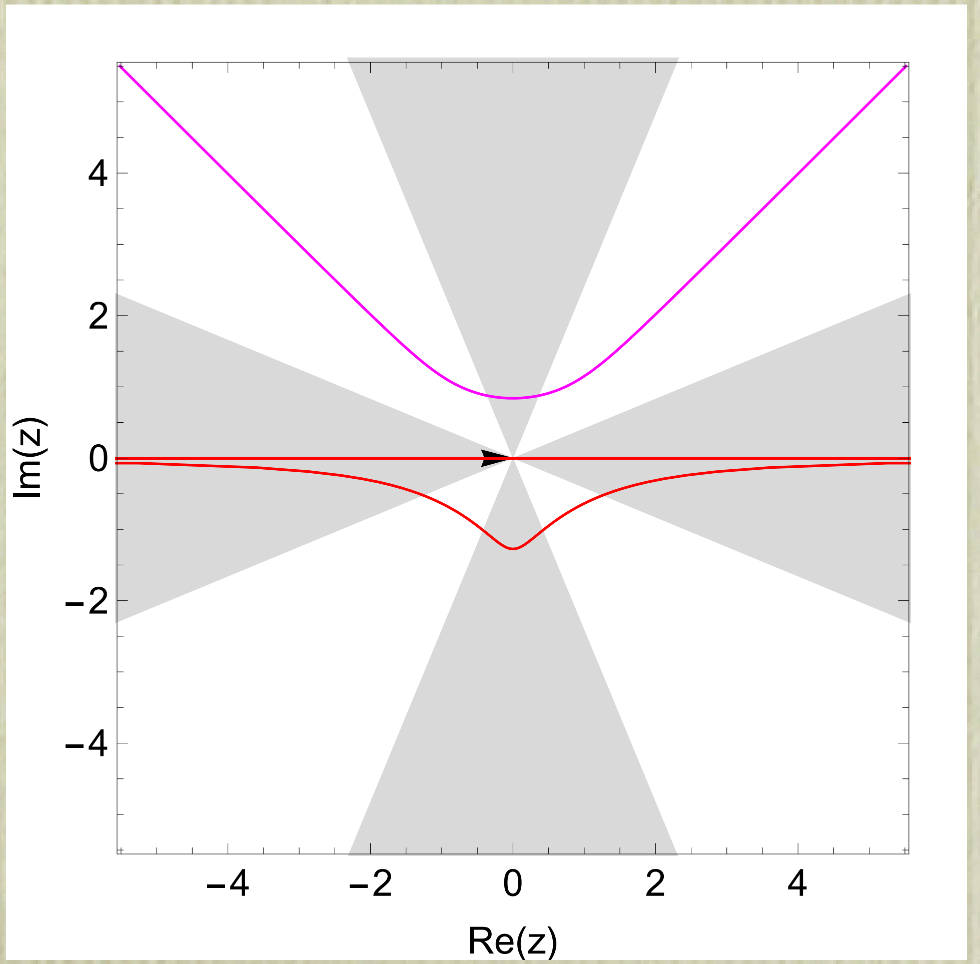
- The cost of the calculation is inversely proportional to the phase average: $N \propto \left\langle e^{-iS_I(\phi)} \right\rangle^{-2}$

- For example in QCD

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

- In QCD the calculation cost increases exponentially with the volume

Contour deformation

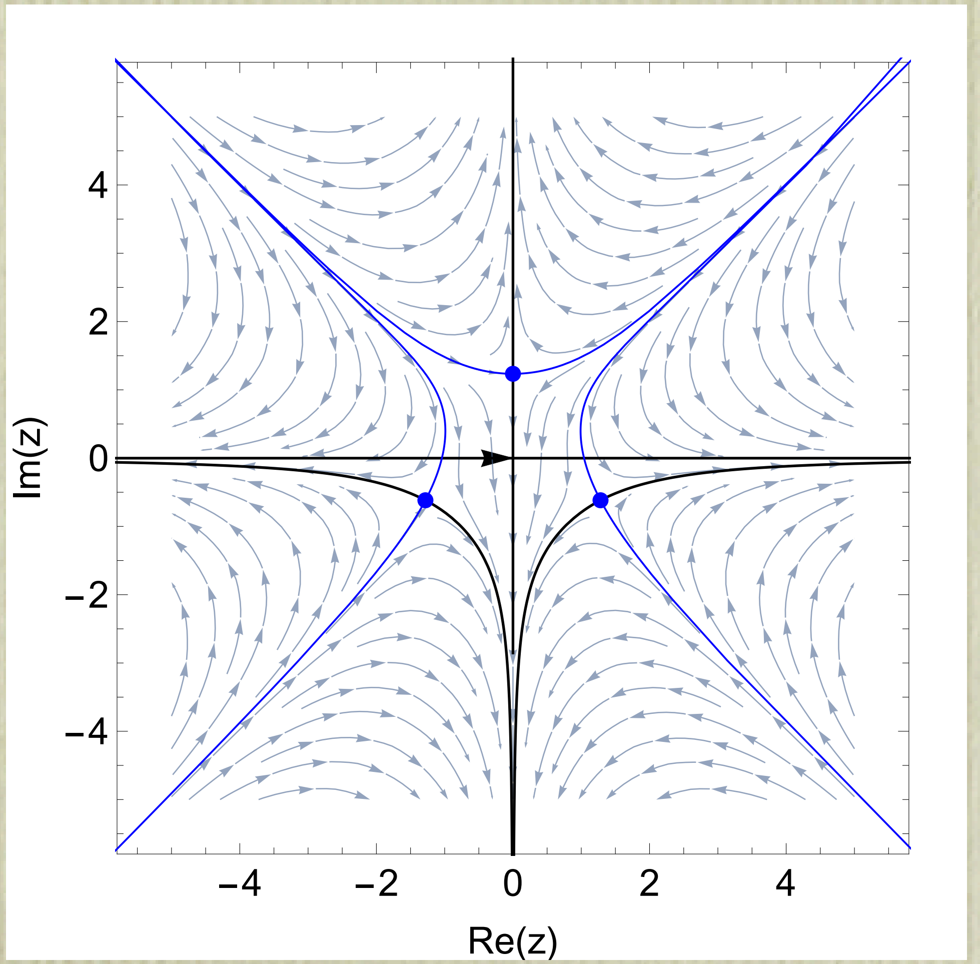


$$Z = \int_{-\infty}^{\infty} \mathrm{d}x\, e^{-S(x)}$$

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

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

Holomorphic gradient flow and Lefschetz thimbles



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

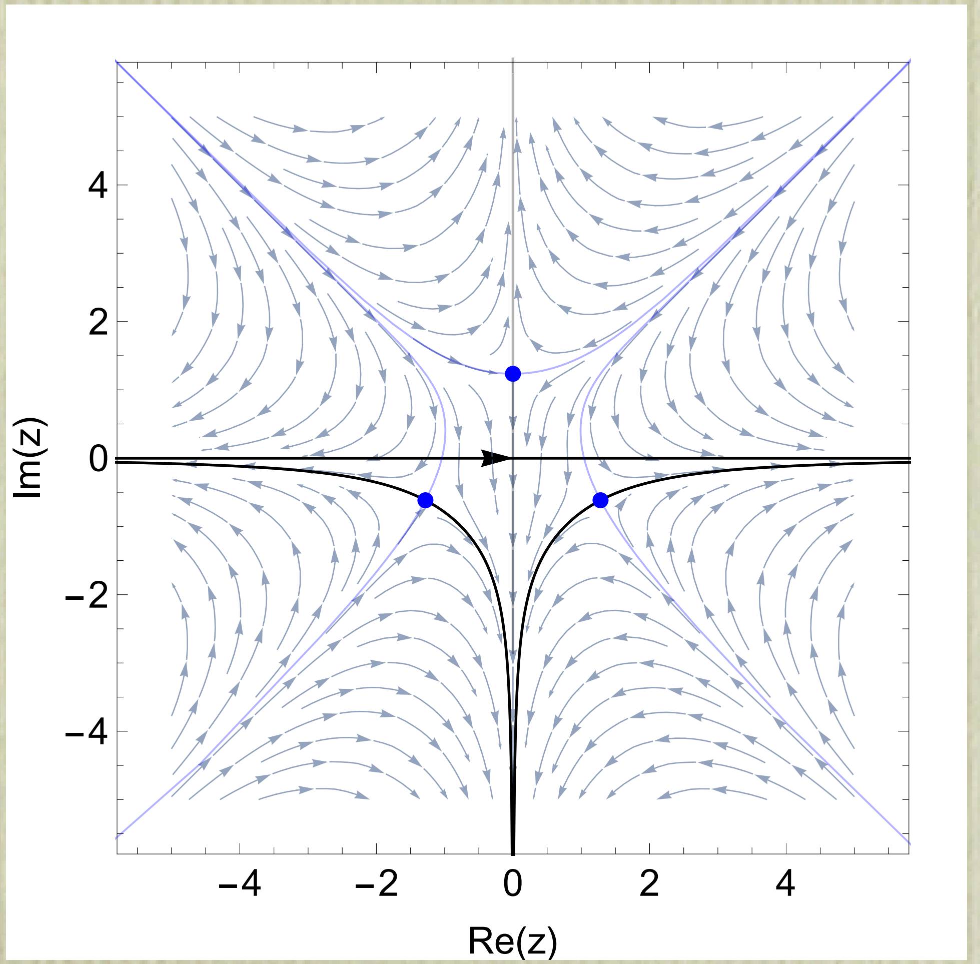
$$\frac{dS}{dz} = 0 \quad \text{(critical points)}$$

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

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

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



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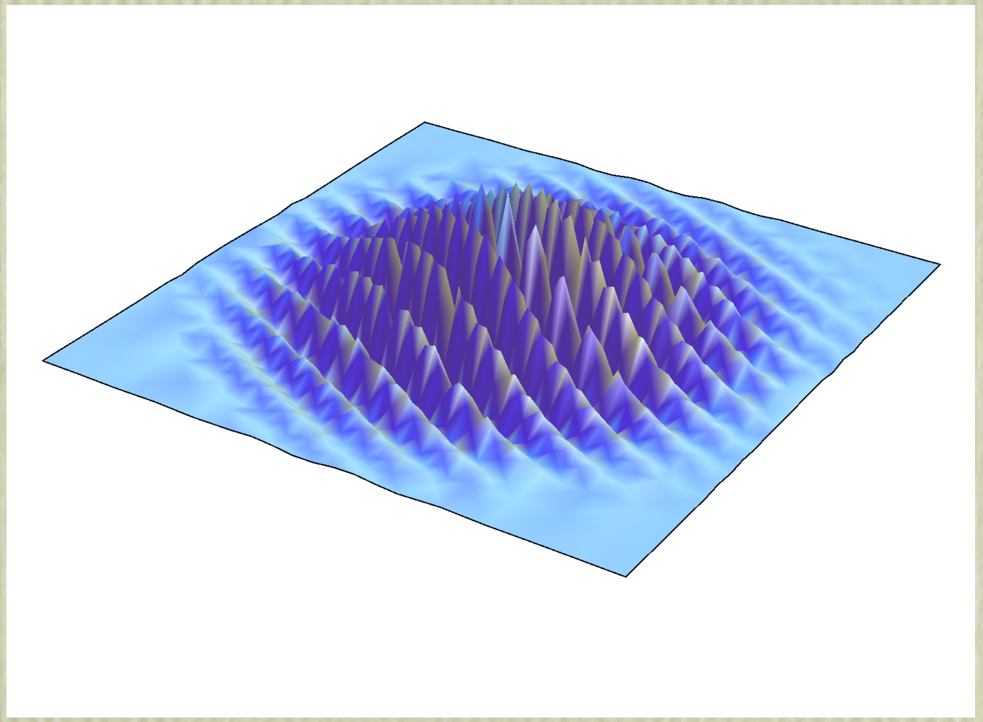
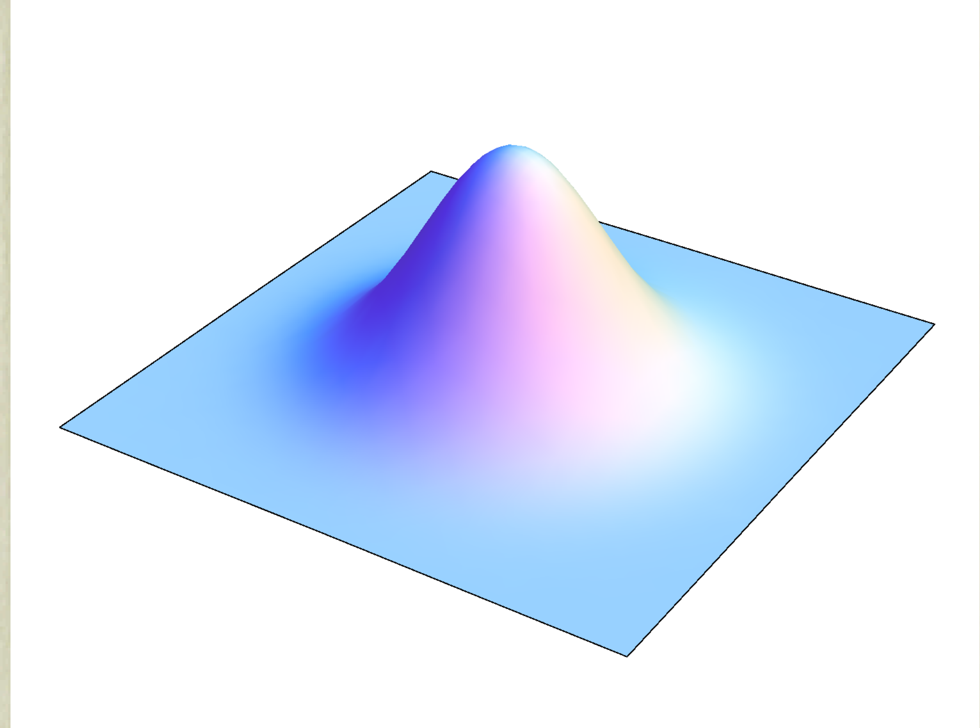
$$Z = \sum_\sigma n_\sigma \int_{J_\sigma} dz \, e^{-S(z)}$$

Lefschetz thimble



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



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

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

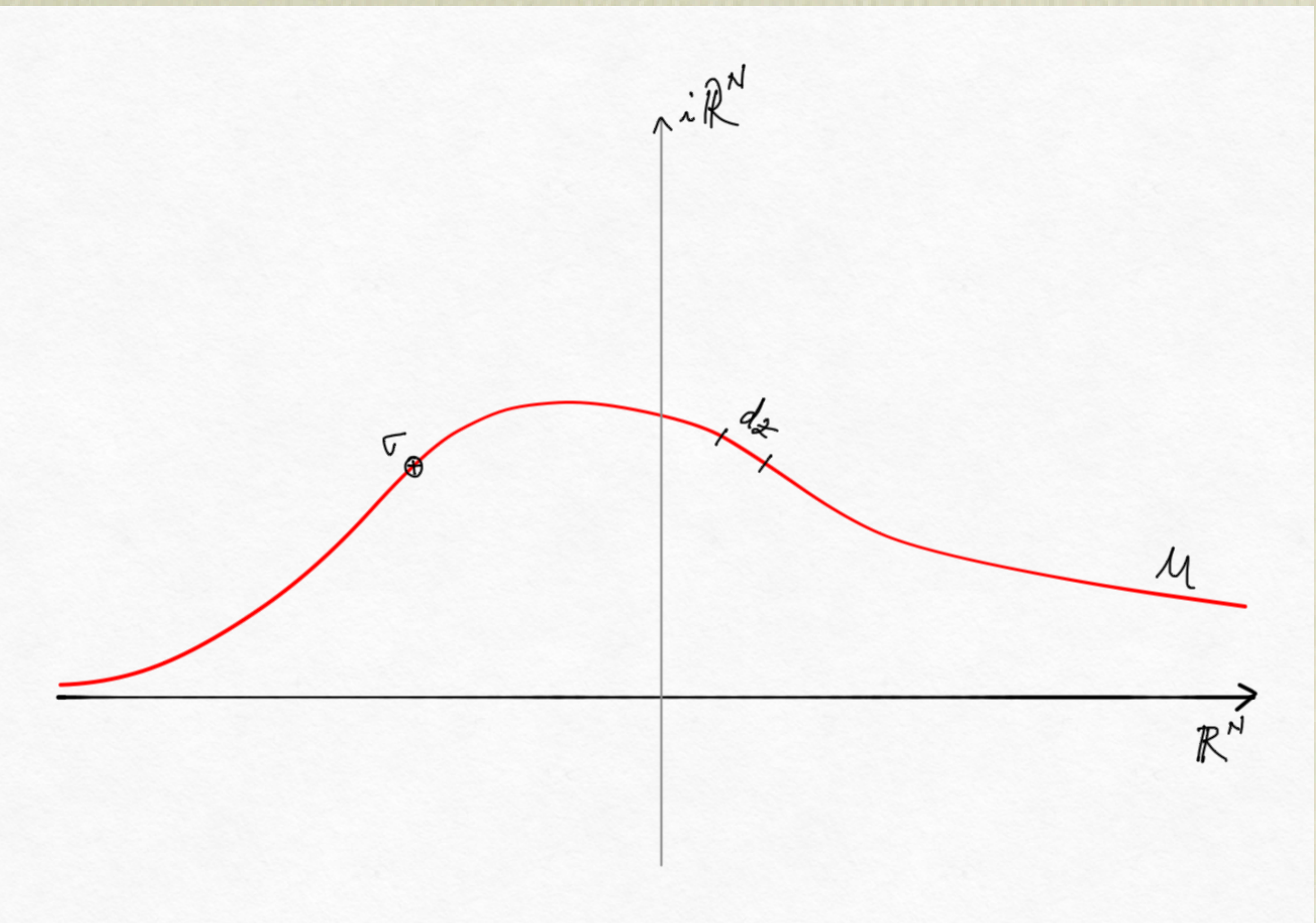
Single thimble

$$\langle O\rangle = \int_{\mathcal{M}} \mathrm{d}z\, e^{-S_R(z)} O(z) \Big/ \int_{\mathcal{M}} \mathrm{d}z\, e^{-S_R(z)}$$ ($e^{-iS_I(\sigma)}$ factors out)

$$P(z) \propto |\mathrm{d}z|\, e^{-S_R(z)}$$

$$\langle O\rangle = \frac{\langle O\phi\rangle_{|\mathrm{d}z|}}{\langle \phi\rangle_{|\mathrm{d}z|}}$$

$$\phi = \frac{\mathrm{d}z}{|\mathrm{d}z|}$$ (residual phase)



The algorithm

$$\langle O \rangle = \frac{1}{Z_R}\int_{\mathcal{M}} \mathrm{d}z_f \, e^{-S_R(z_f)} O(z_f) = \frac{1}{Z_R}\int_{\mathcal{M}} \mathrm{d}z_n \left\| \frac{dz_f}{dz_n} \right\| e^{-S_R(z_f)} O(z_f)$$

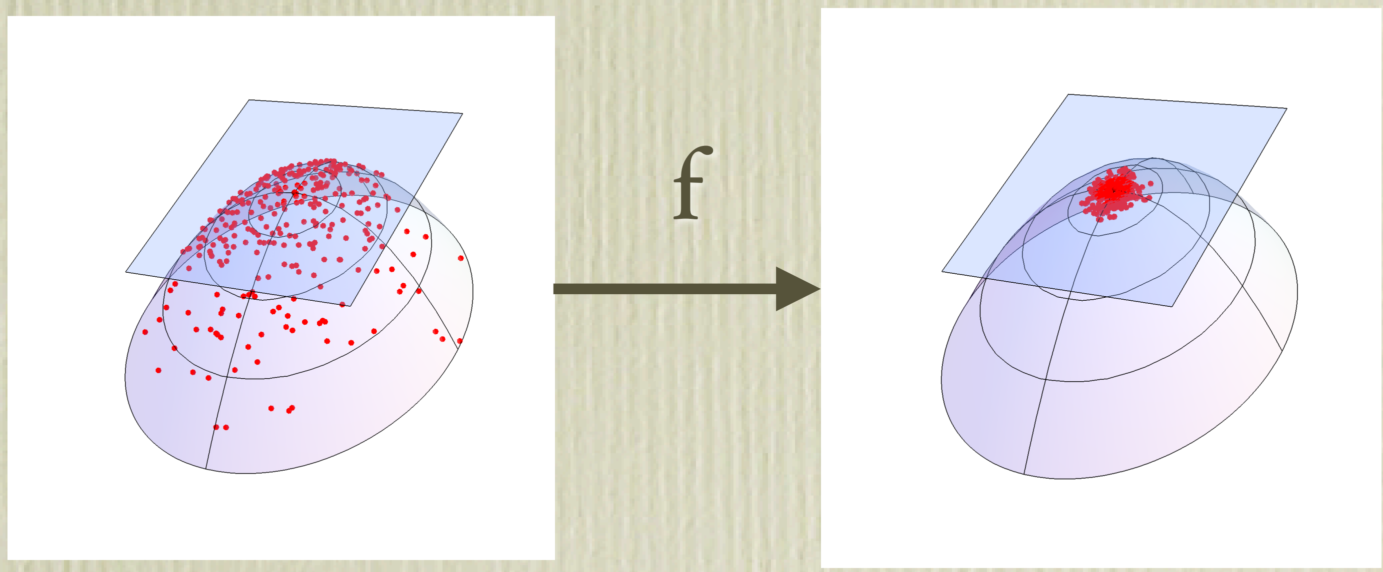
f is the downward flow

$f(z_f; T) = z(T)$

$$\frac{dz}{d\tau} = -\overline{\frac{dS}{dz}} \text{ and } z(0) = z_f$$

f^{-1} is the upward flow

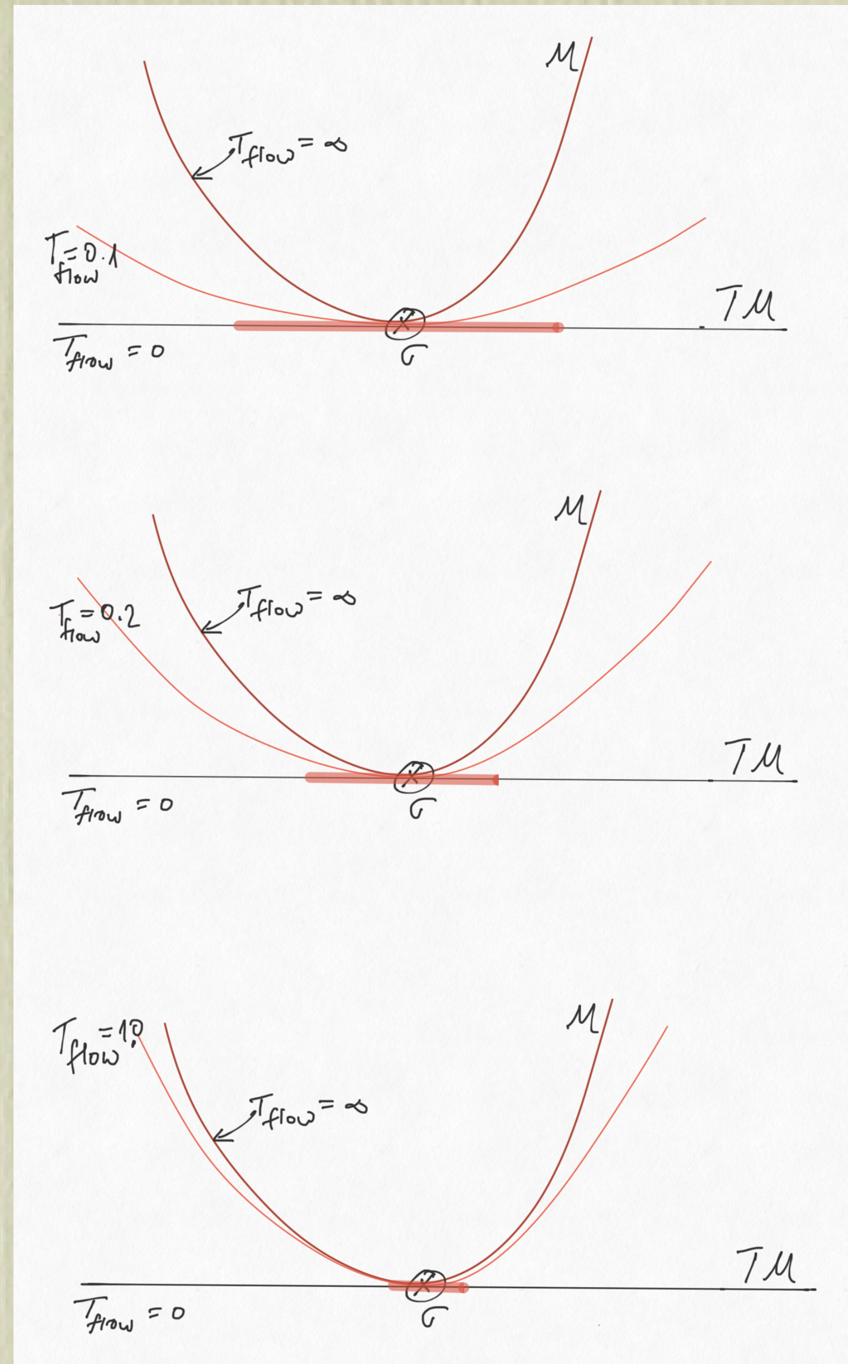
$f^{-1}(z; T) = f(z; -T)$



Flow manifold

$$\langle O \rangle = \frac{1}{Z_R} \int_{\mathcal{M}} \mathrm{d}z_n \left\| \frac{dz_f}{dz_n} \right\| e^{-S_R(z_f)} O(z_f)$$

$$\approx \frac{1}{\tilde{Z}_R} \int_{T\mathcal{M}} \mathrm{d}z_n \left\| \frac{dz_f}{dz_n} \right\| e^{-S_R(z_f)} O(z_f)$$



$$z(0) = z_0 \xrightarrow{\overline{\partial S/\partial \tau}} z = z(T_{\mathrm{flow}})$$

$$S_{\mathrm{eff}}(z_0) = \left[S(z) - \det \left\| \frac{dz}{dz_0} \right\| \right]_R$$

Case study: Thirring model 0+1

- $0 + 1$ model with staggered fermions and auxiliary bosonic fields.
- The action is $S = S_f + S_g = \bar{\chi} K \chi + \beta \sum_t (1 - \cos\phi_t)$
- The fermionic kernel is

$$K_{t,t'} = \frac{1}{2}\left(e^{\mu + i\phi_t}\delta_{t+1,t'} - e^{-\mu - i\phi'_t}\delta_{t-1,t'}\right) + m\delta_{t,t'}$$

- After fermionic integration, the partition function is

$$Z(m, \mu, \beta) = \int \prod_t \frac{d\phi_t}{2\pi} e^{-S_g(\phi)} \det K(m, \mu)$$

J. M. Pawlowski, I.-O. Stamatescu, and C. Zielinski, *Simple QED- and QCD-like Models at Finite Density*, Phys. Rev. D92 (2015)

H. Fujii, S. Kamata, and Y. Kikukawa, *Lefschetz thimble structure in one-dimensional lattice Thirring model at finite density,* arXiv:1509.0817

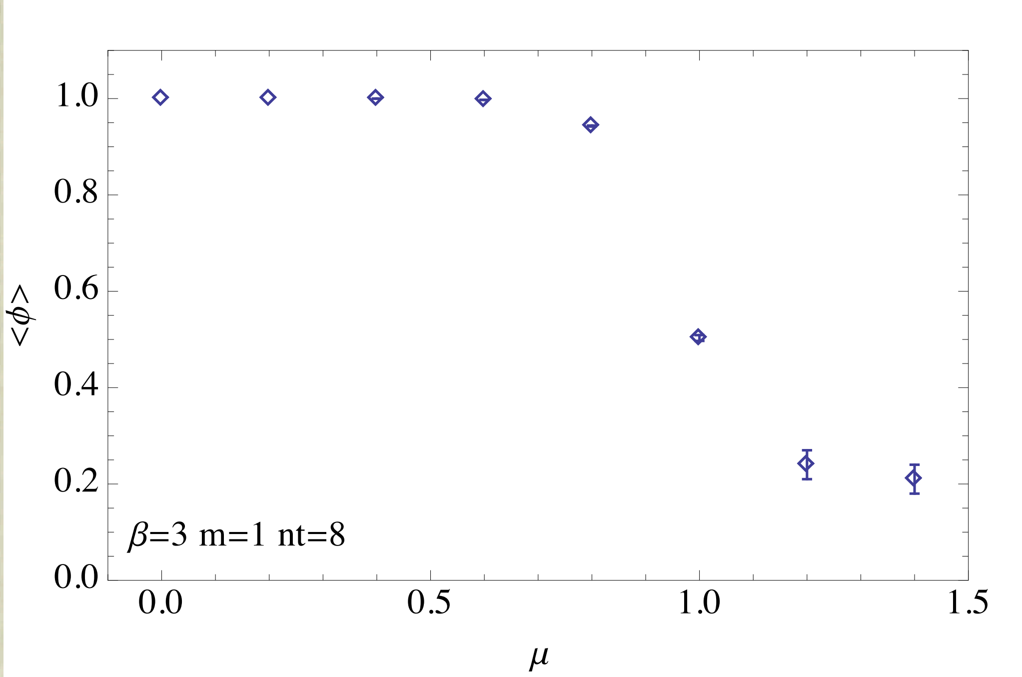
Thirring model 0+1

- This model has a complex measure and direct MC simulations are not possible

- Phase quenched simulations run into a sign problem at high μ

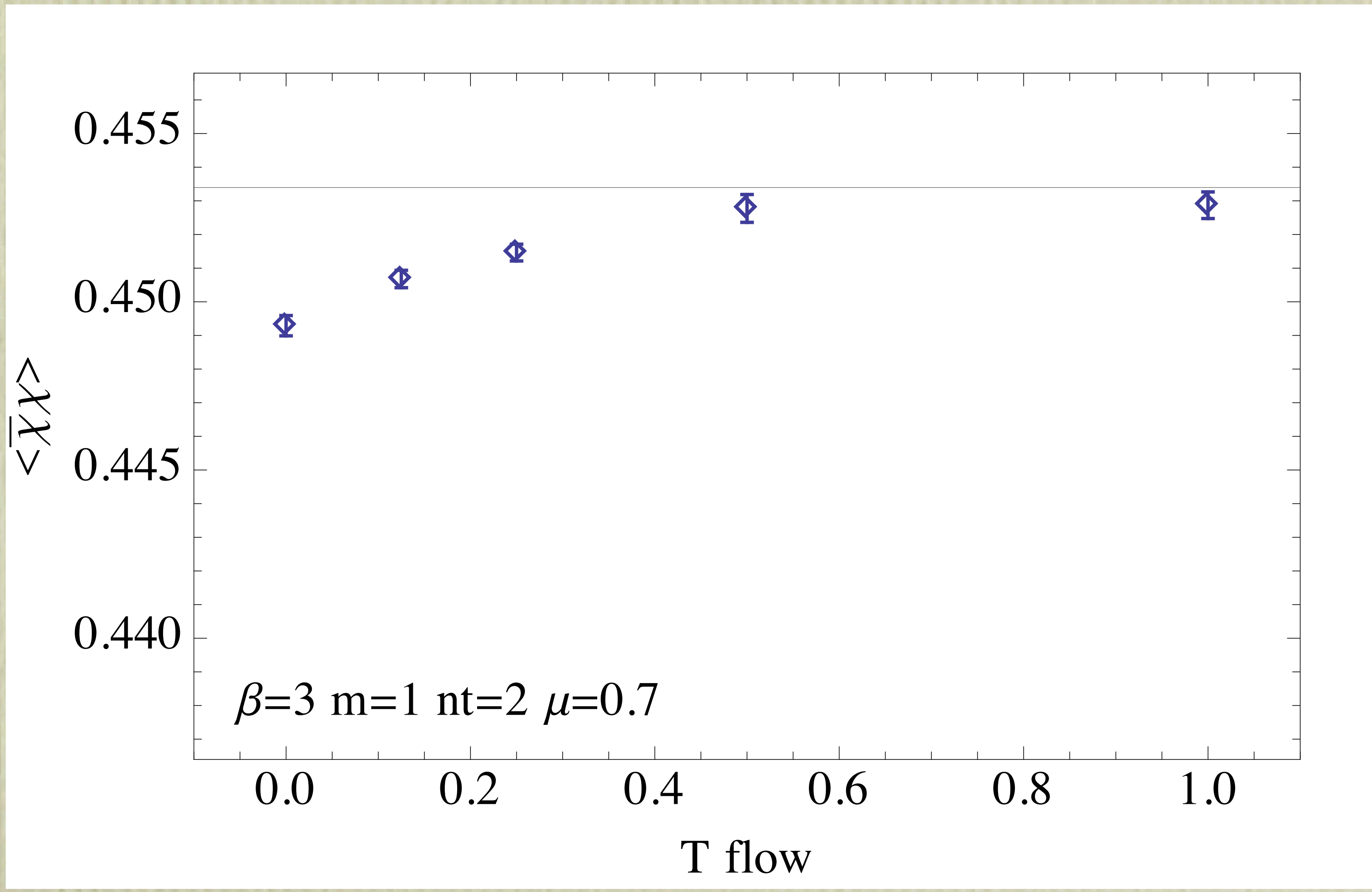
$$\langle O \rangle = \frac{\langle O\phi \rangle_0}{\langle \phi \rangle_0}$$

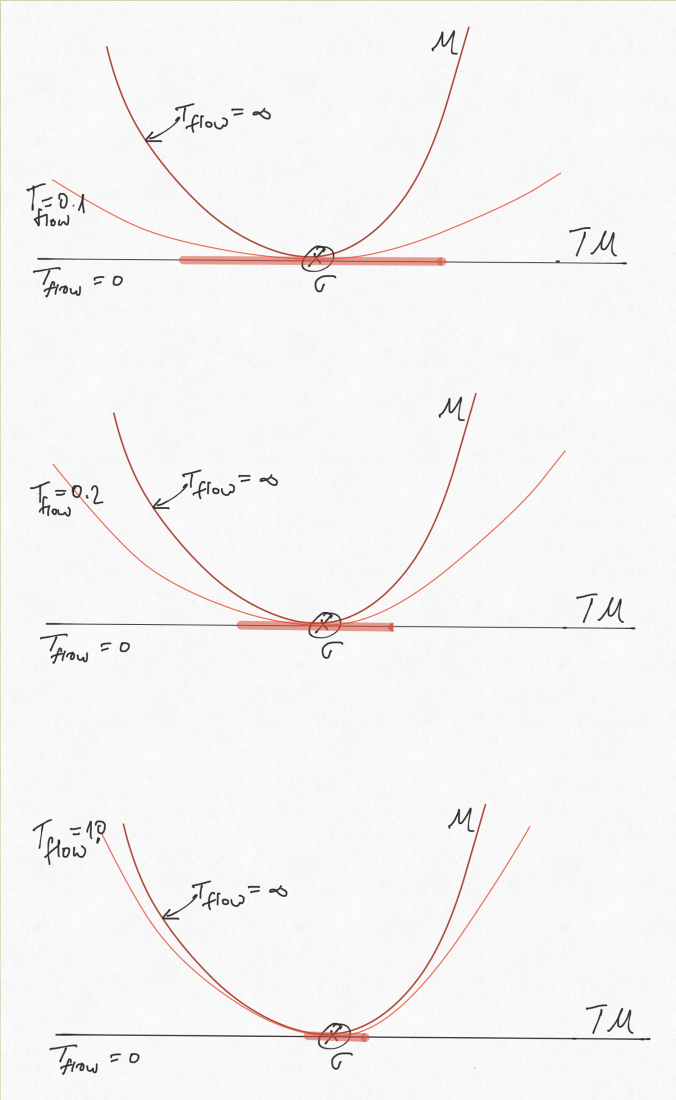
$$\langle \cdot \rangle_0 \propto e^{-S_g} |\det K| \quad \phi = \frac{\det K}{|\det K|}$$



Numerical results

Algorithm check



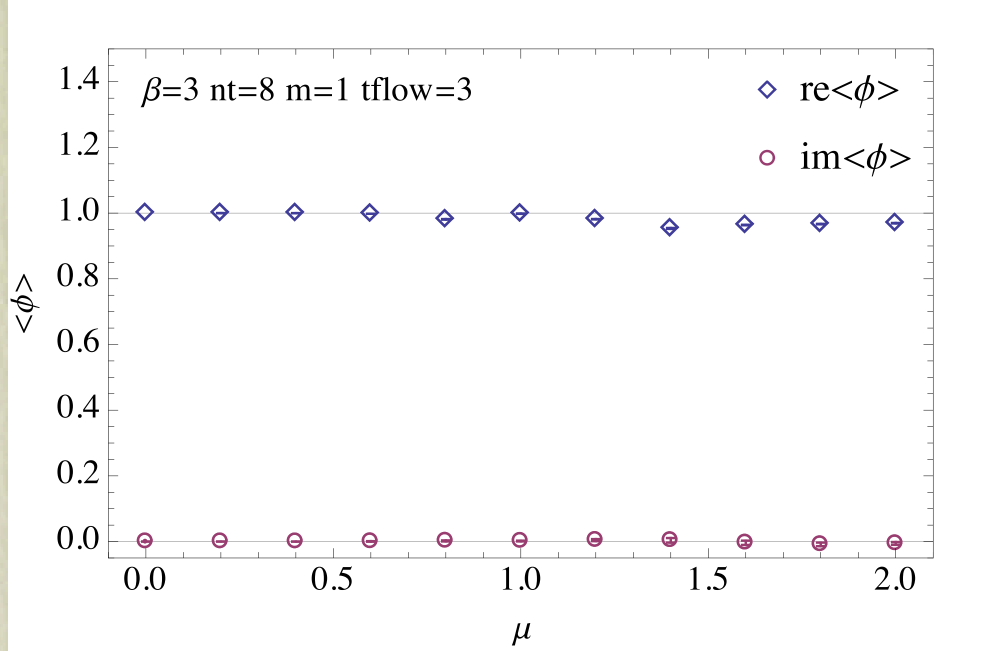


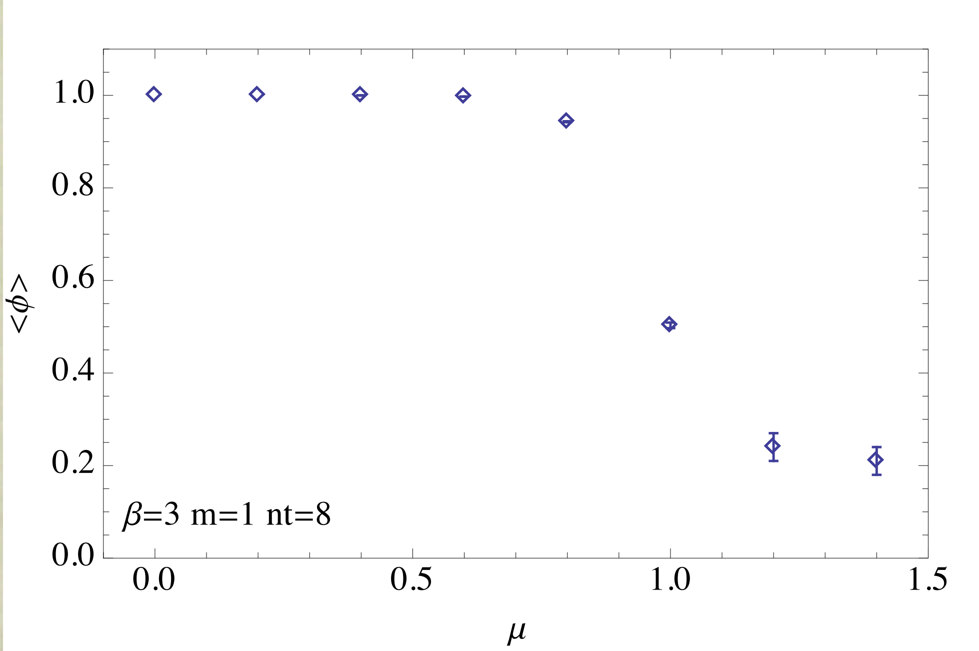
Residual phase

- The Jacobian of the map function is not real, $\boxed{\det J \notin \mathbb{R}}$
- We use only its magnitude in the updating process

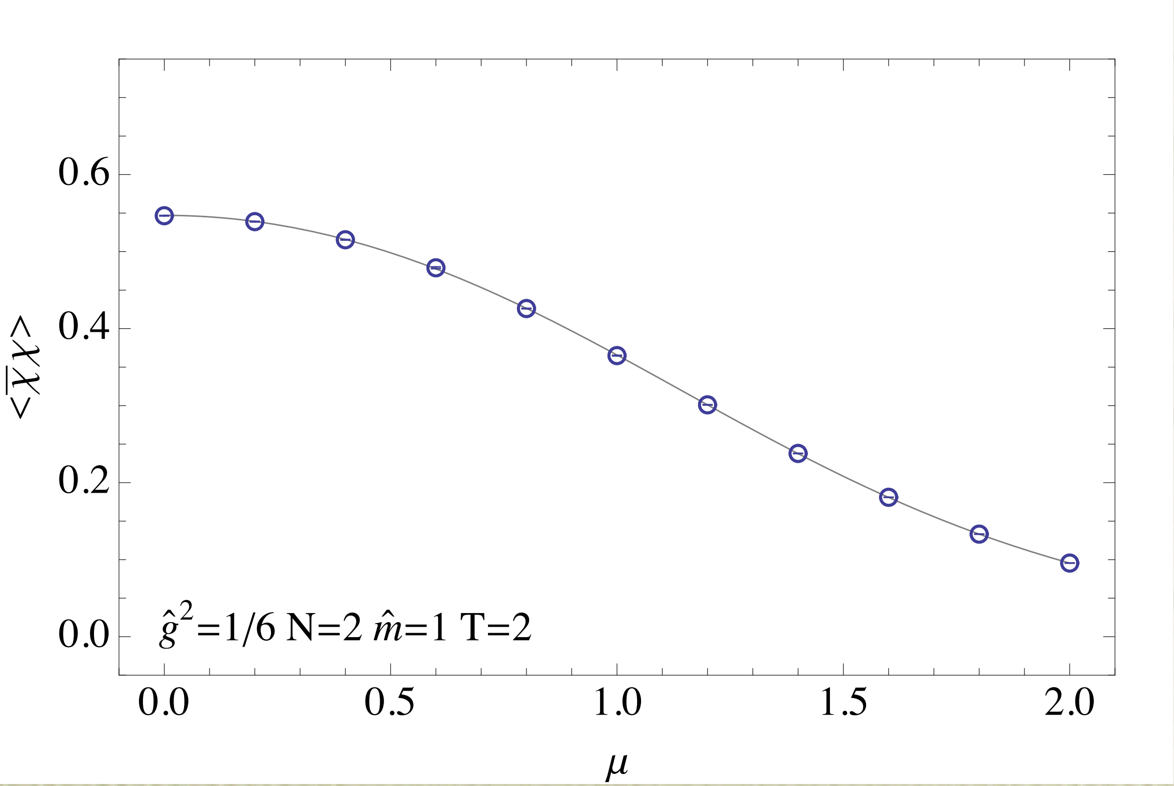
$$S_{\text{eff}} = S_R - \log|\det J|\,.$$

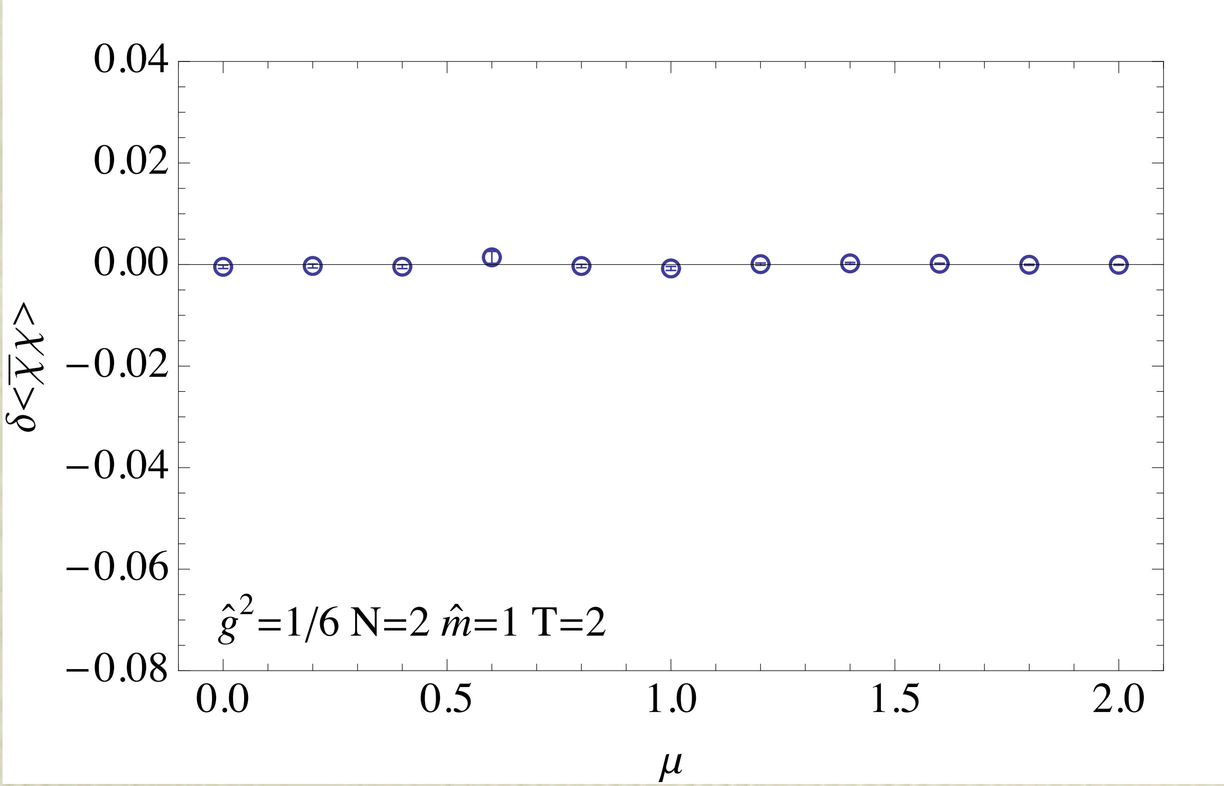
- The residual phase $\phi = \det J/|\det J|$ is folded in the observable.
- This is *not* the same phase as in the phase quenched theory.
- The sign fluctuations of the residual phase are observable but mild in our model.



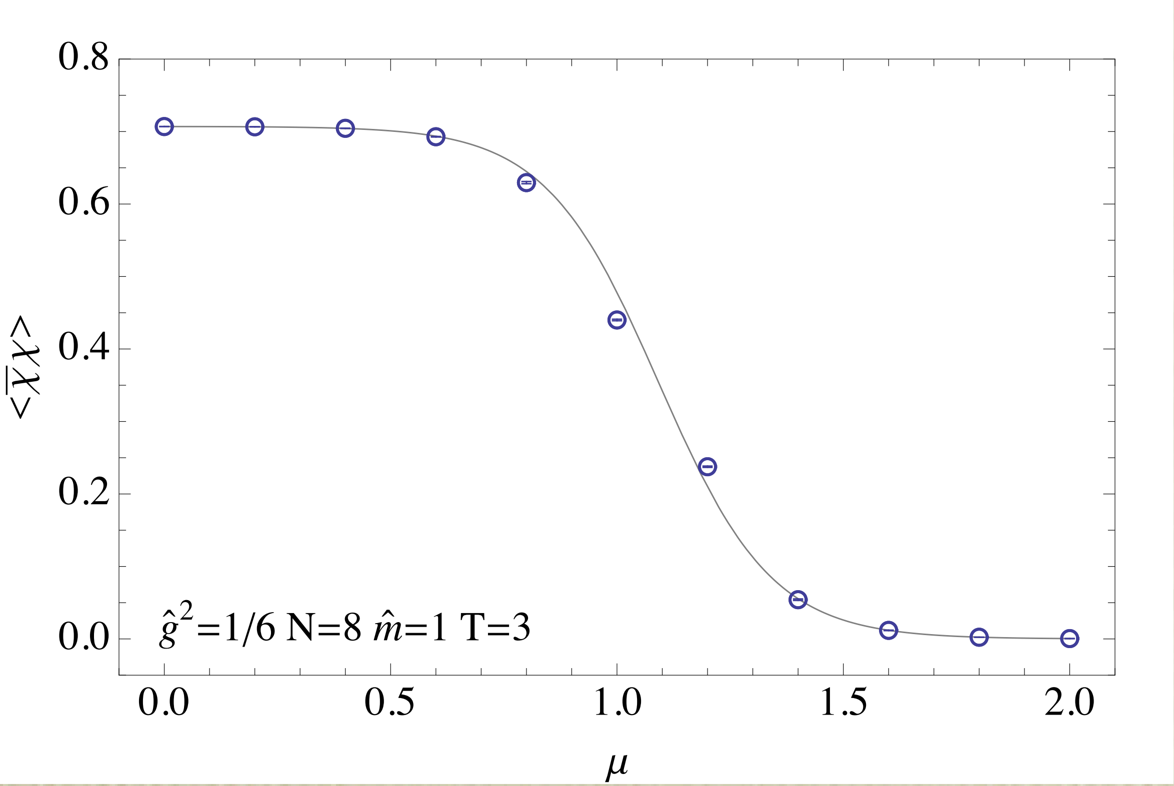


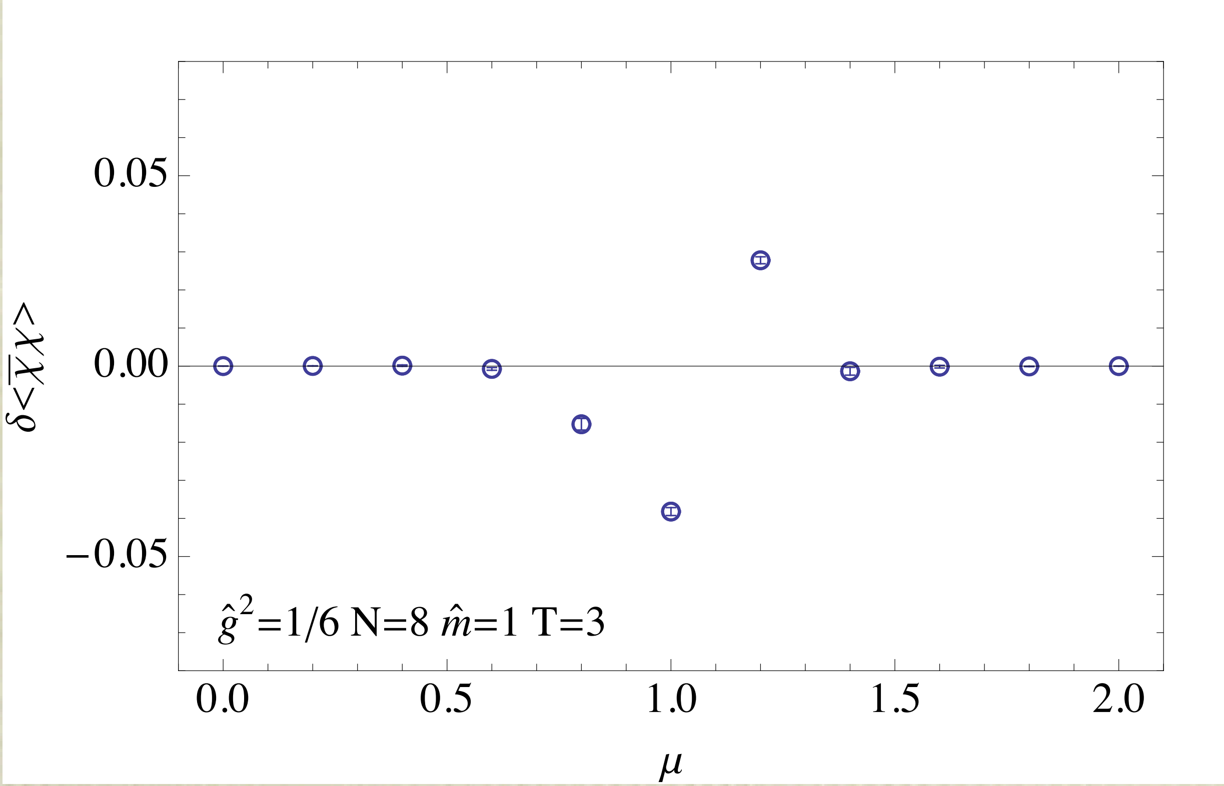
High temperature



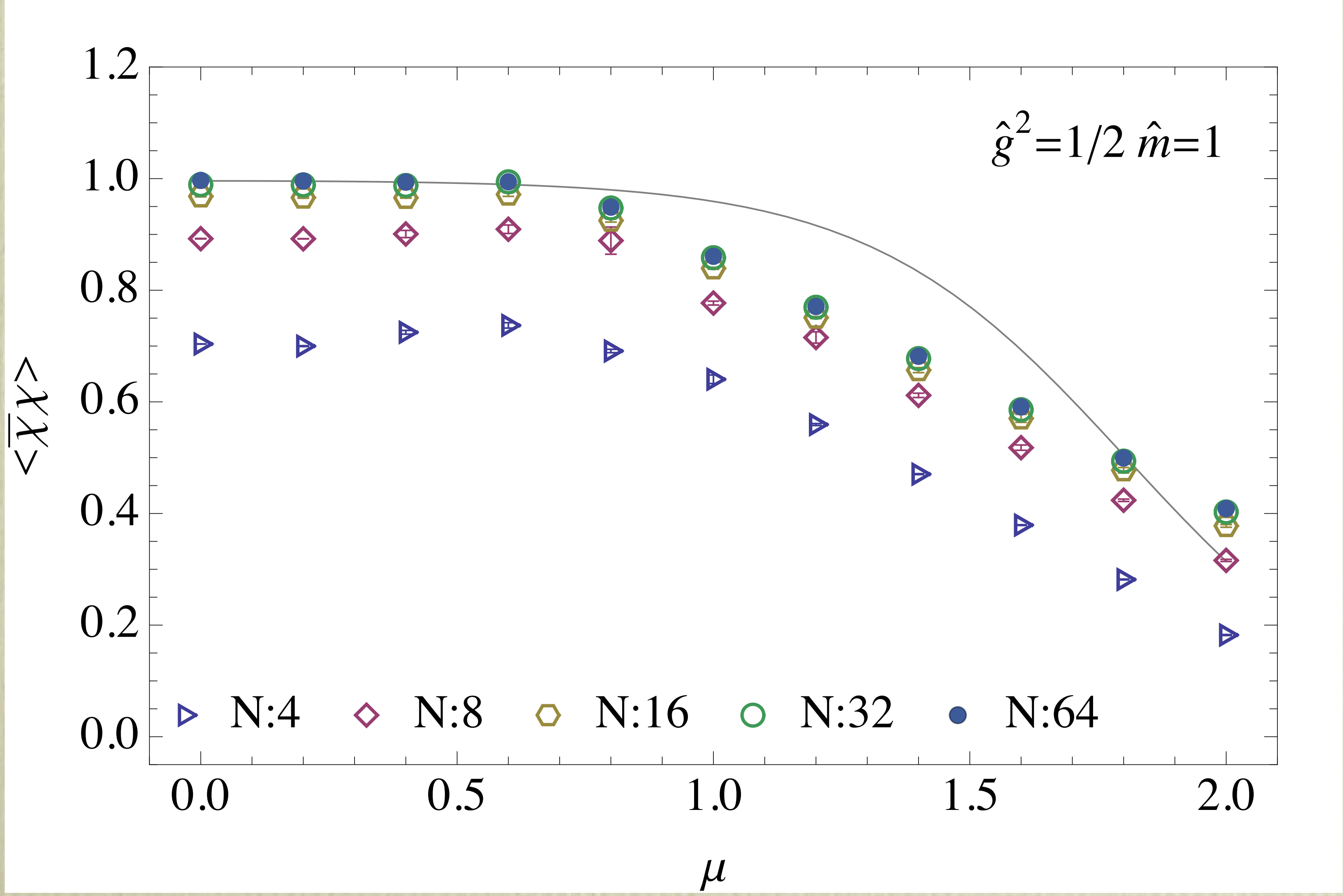


Low temperature



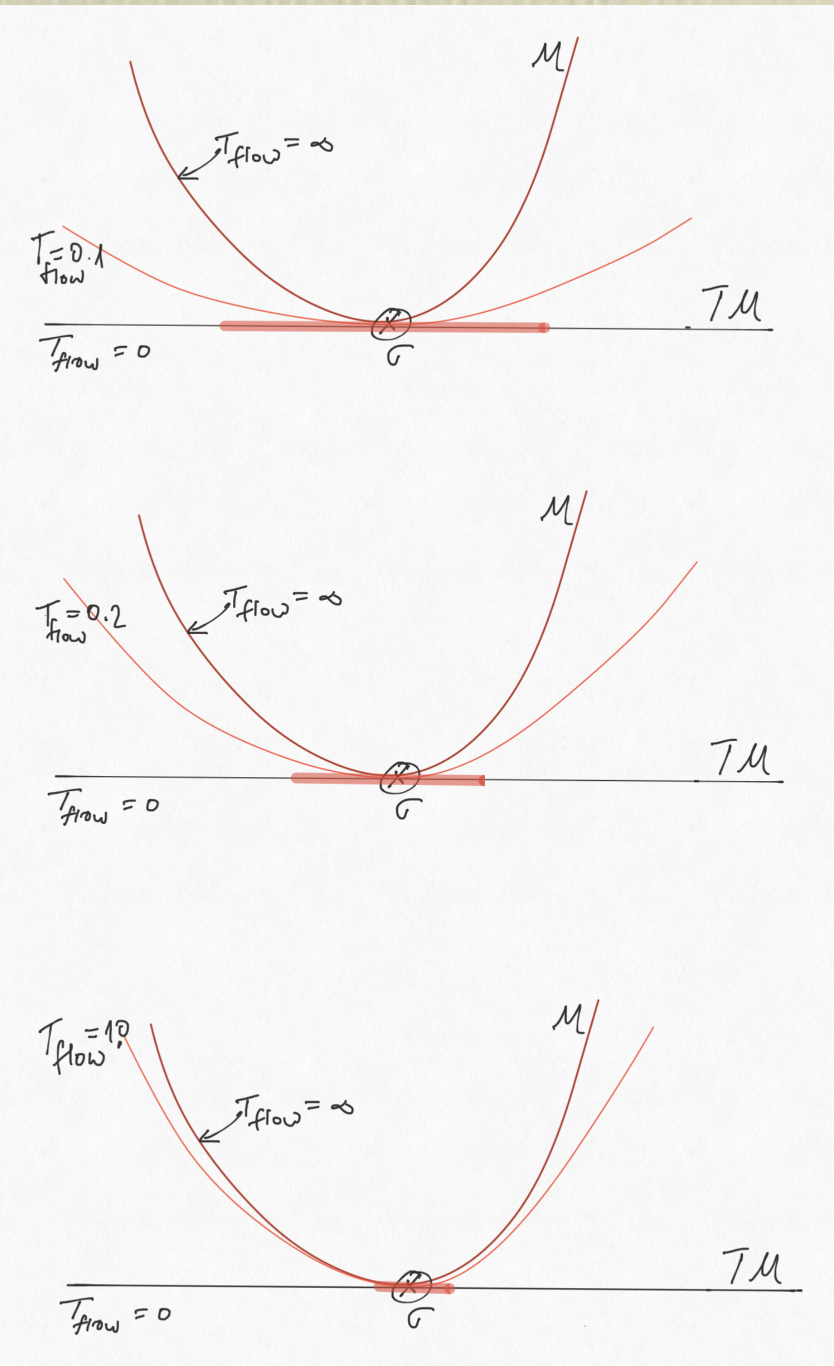


Continuum limit

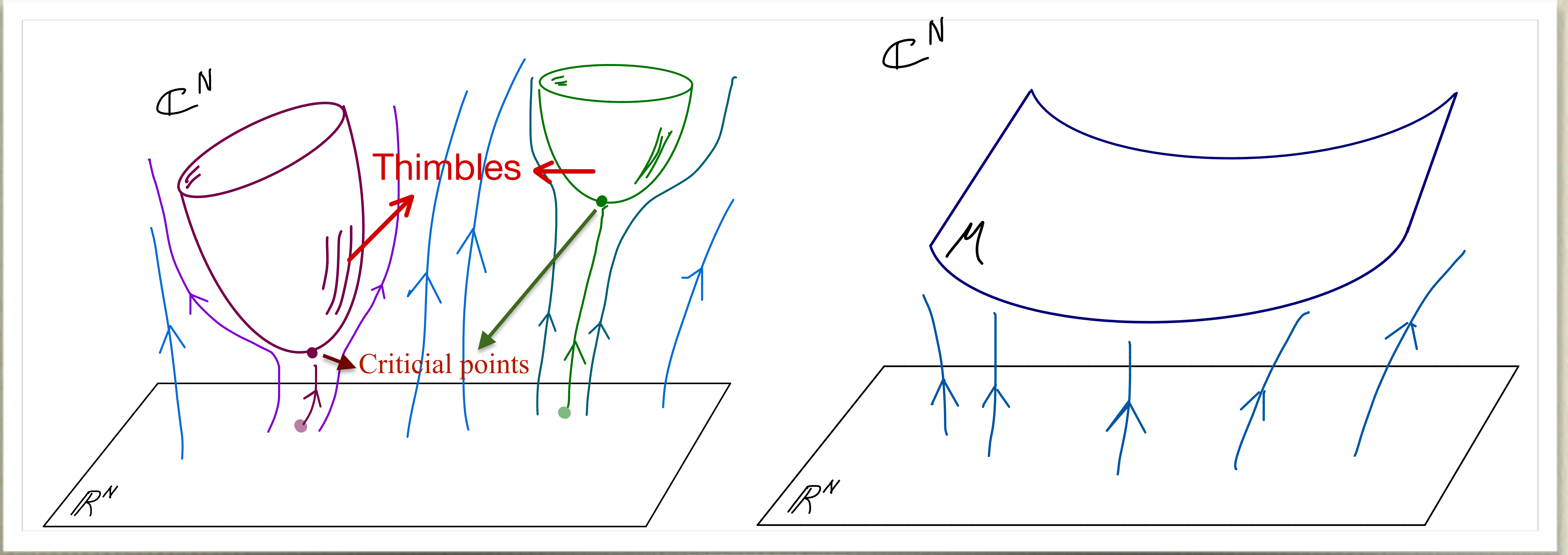


Generalized thimble method

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

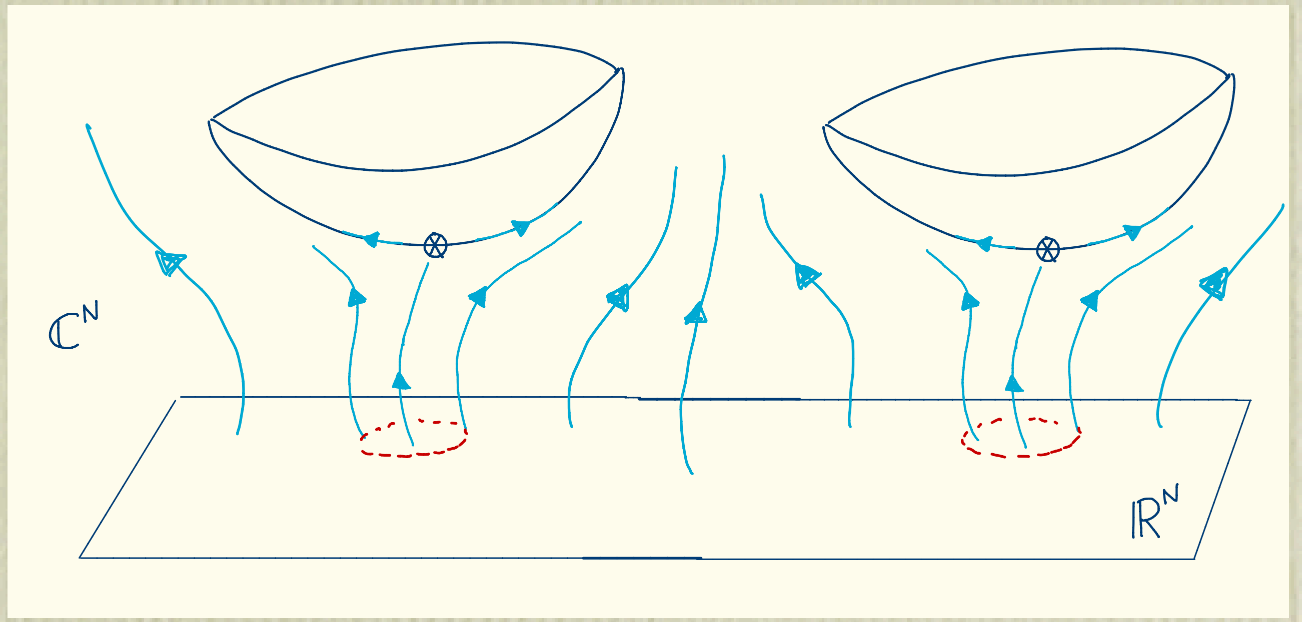


Manifolds generated by holomorphic gradient flow



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

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

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

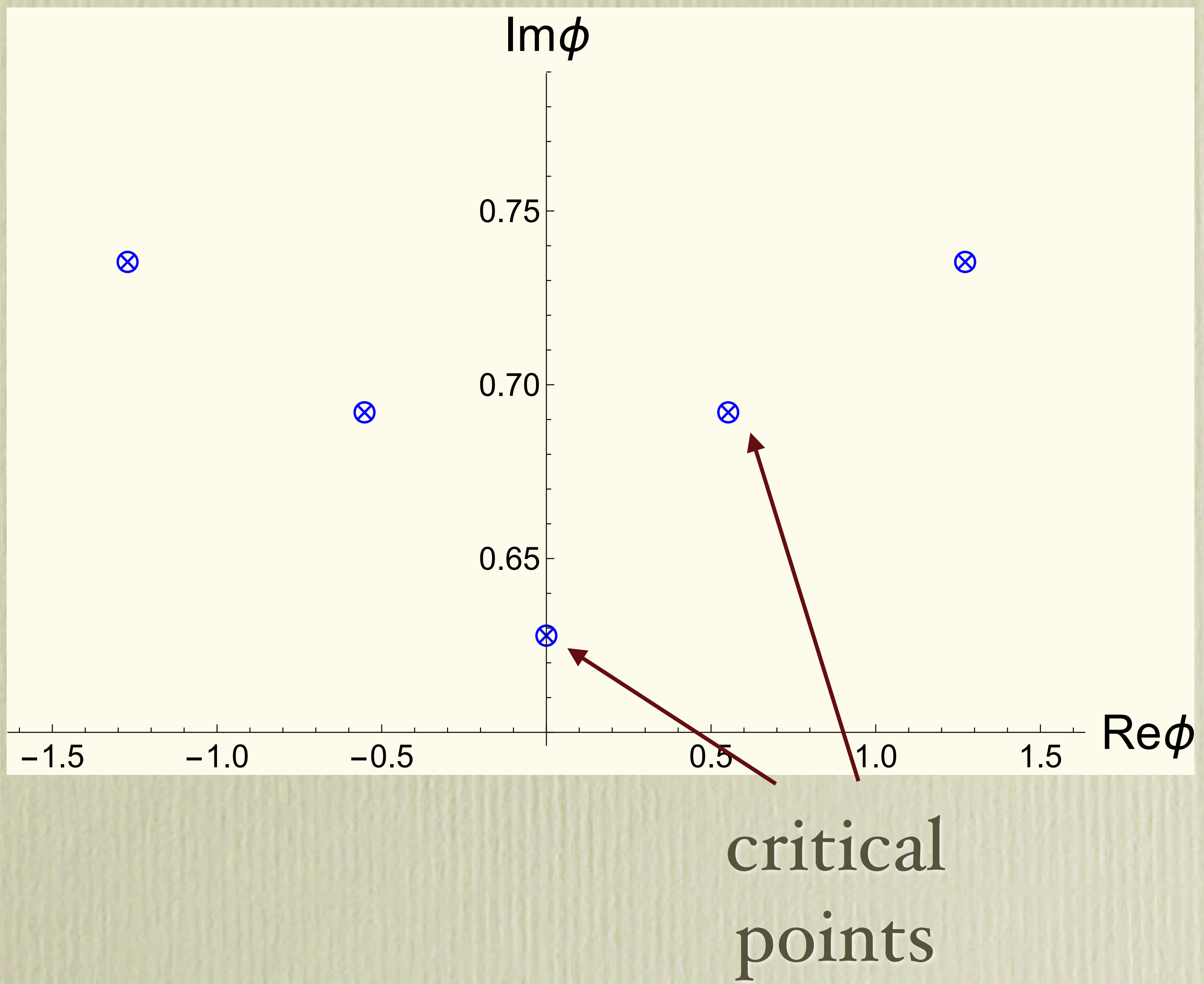
Auxiliary field A's

$$S = \int d^2x \, \left[\frac{N_F}{2g^2} A_\mu A_\mu + \bar{\psi}^\alpha (\partial\!\!\!/ + \mu\gamma_0 + iA\!\!\!/ + m)\psi^\alpha\right]$$

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: $\phi = \frac{1}{L^2} \sum_x A_0(x)$



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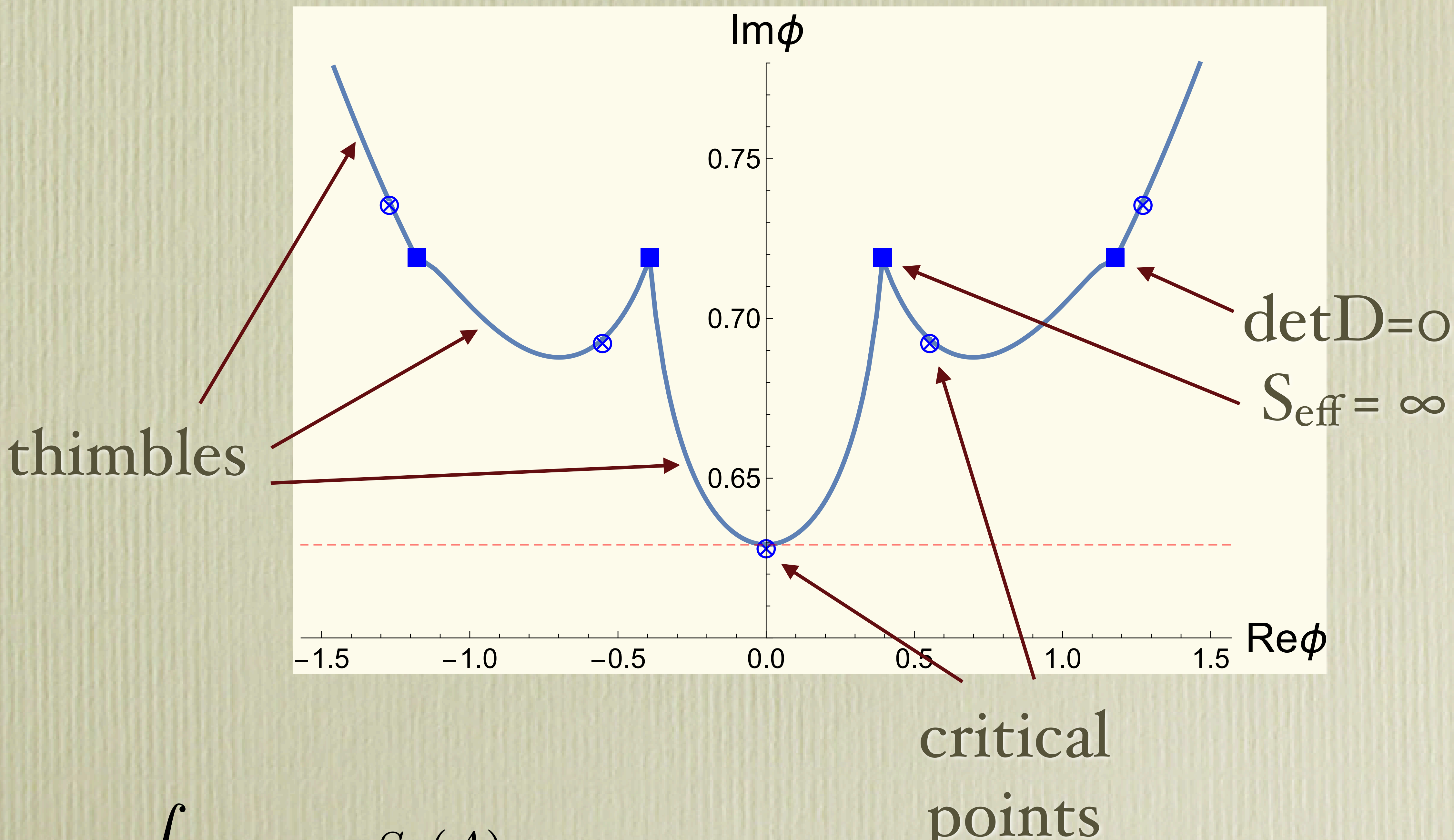
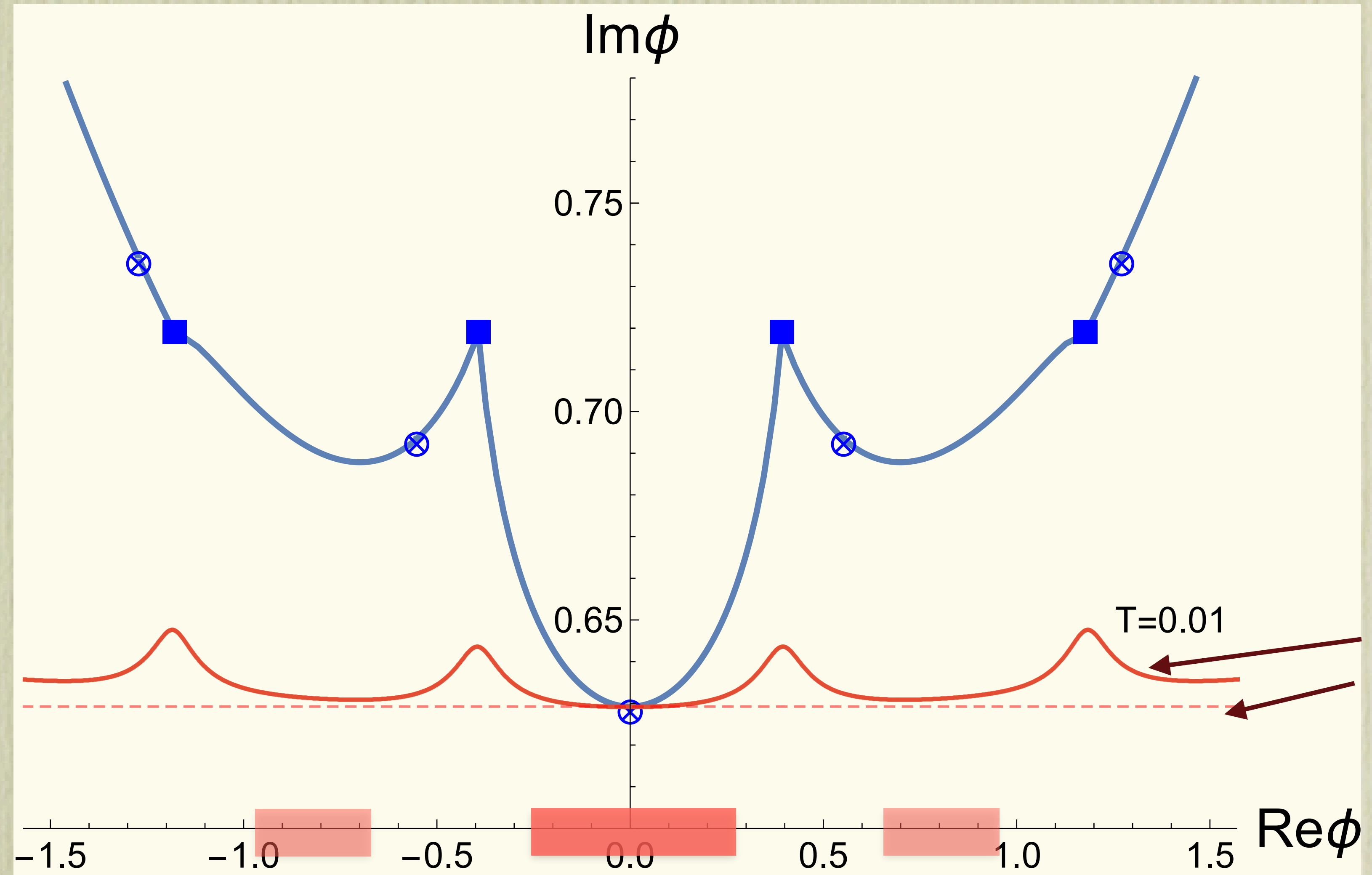


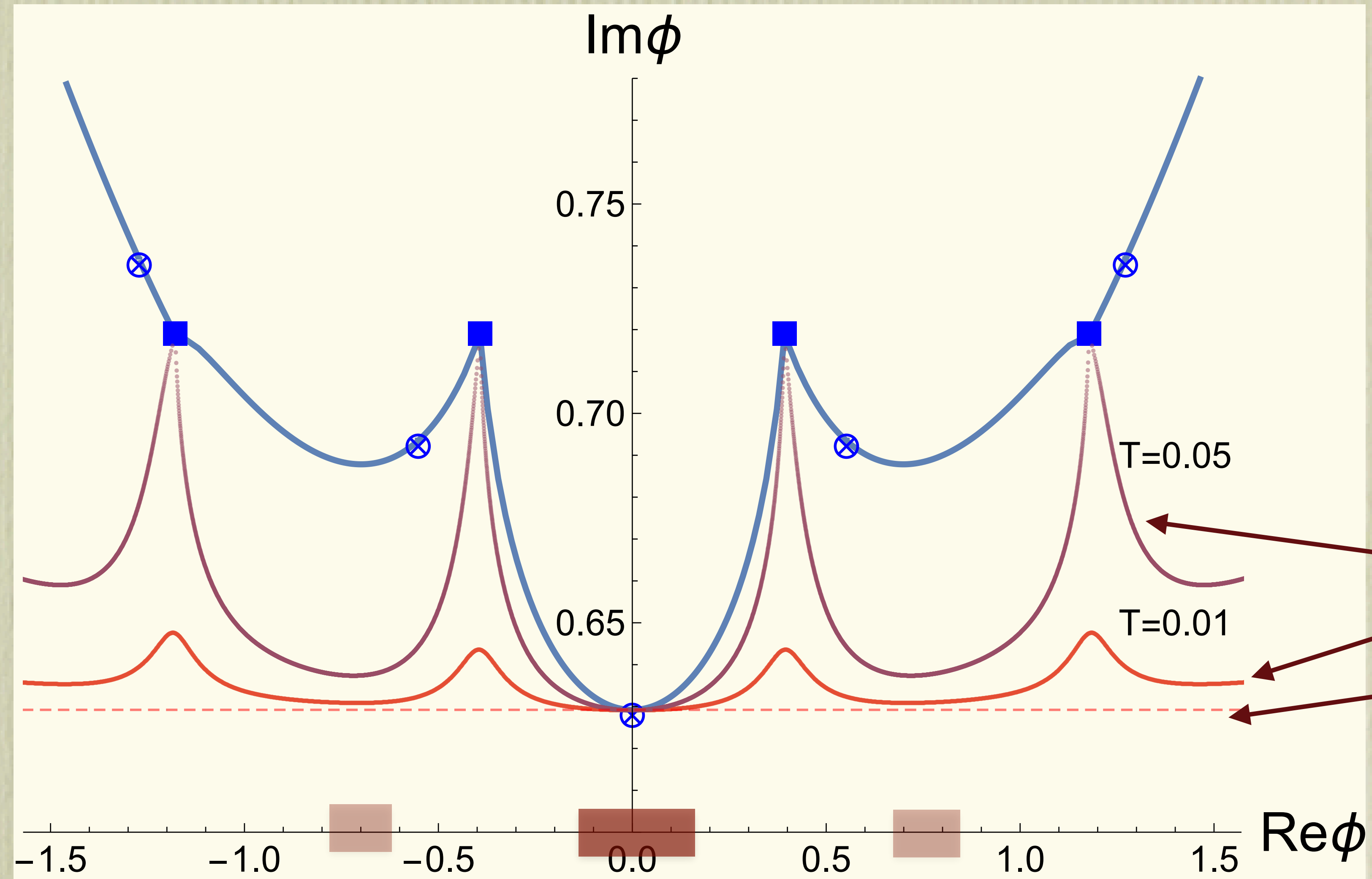
$$Z = \int \mathcal{D}A \, e^{-S_g(A)} \det D(A, \mu)$$

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



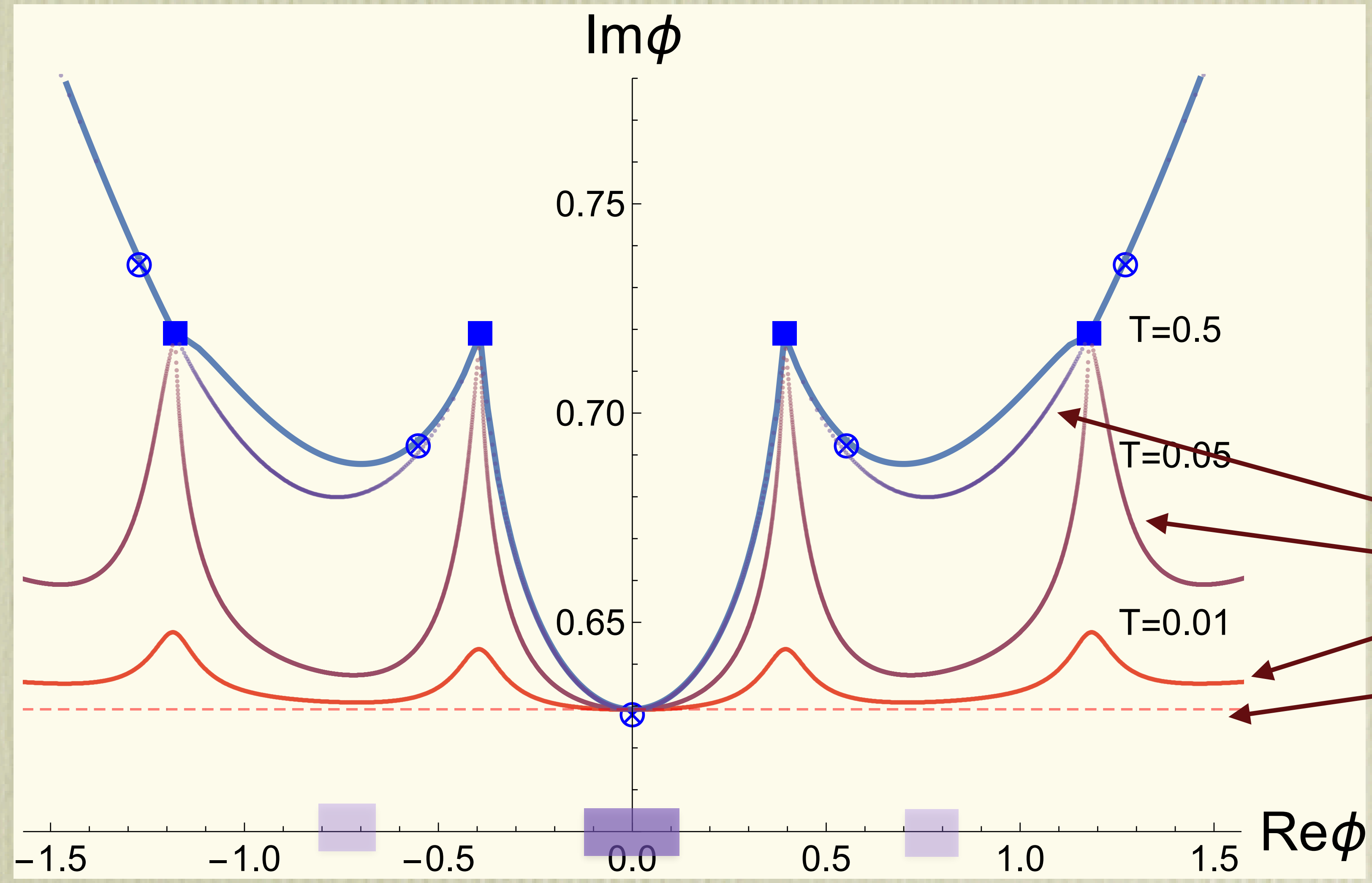
same homological class

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



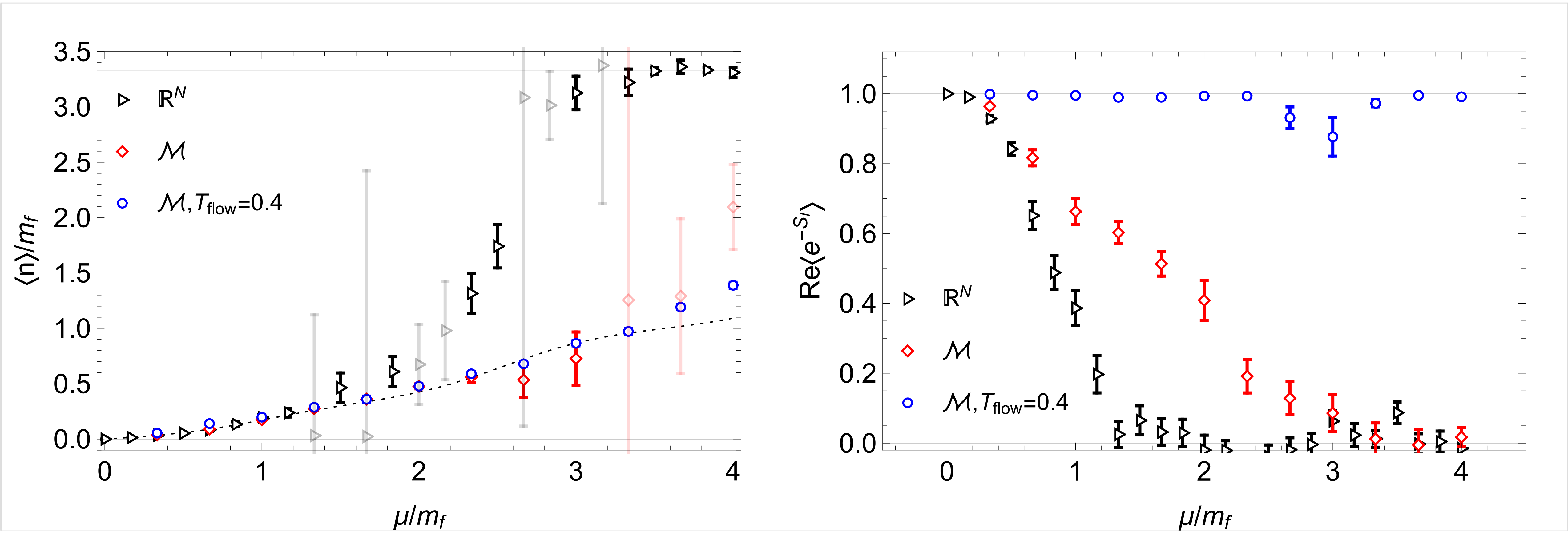
flowed tangent space

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

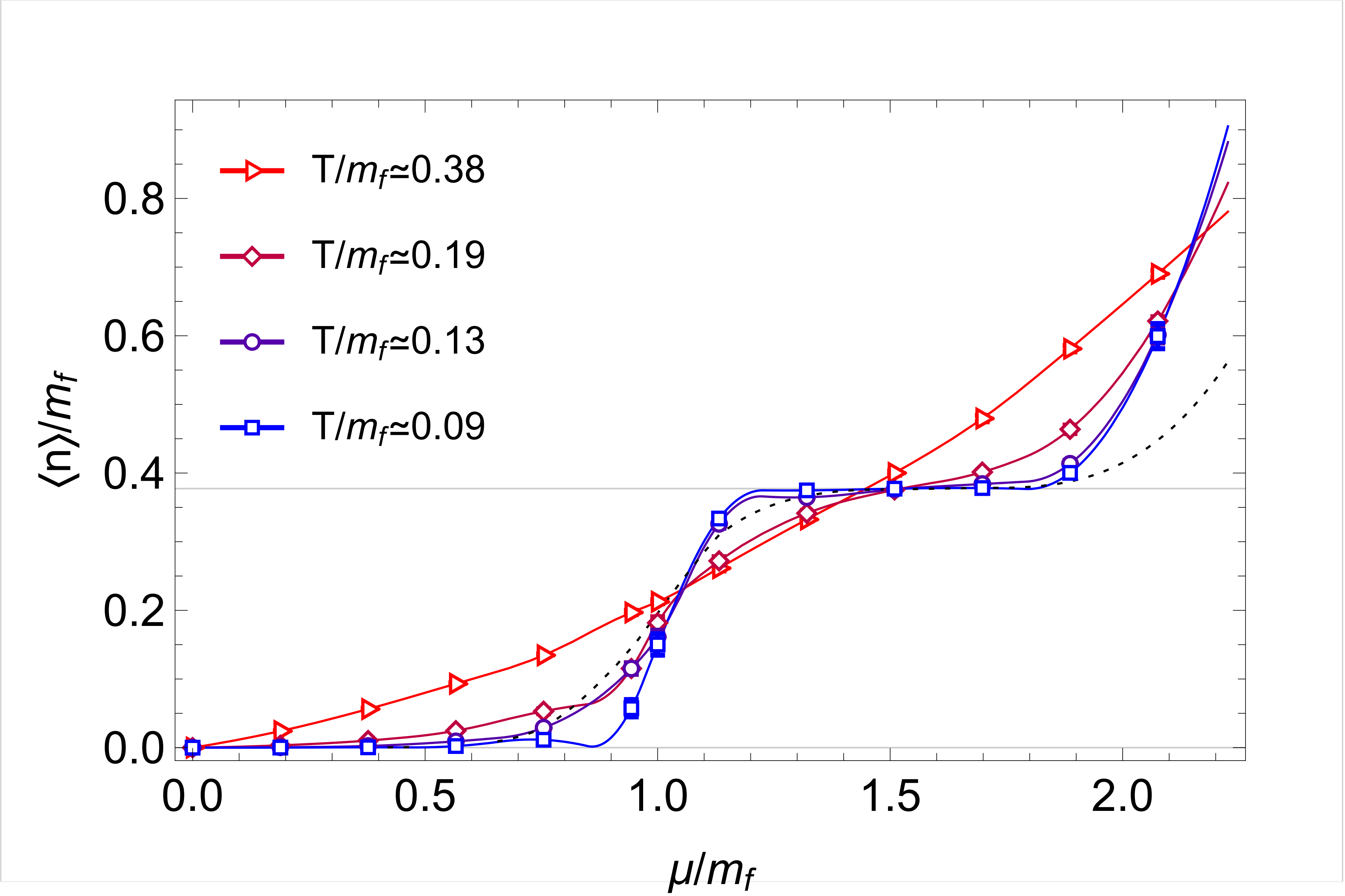


flowed tangent space

Sign problem

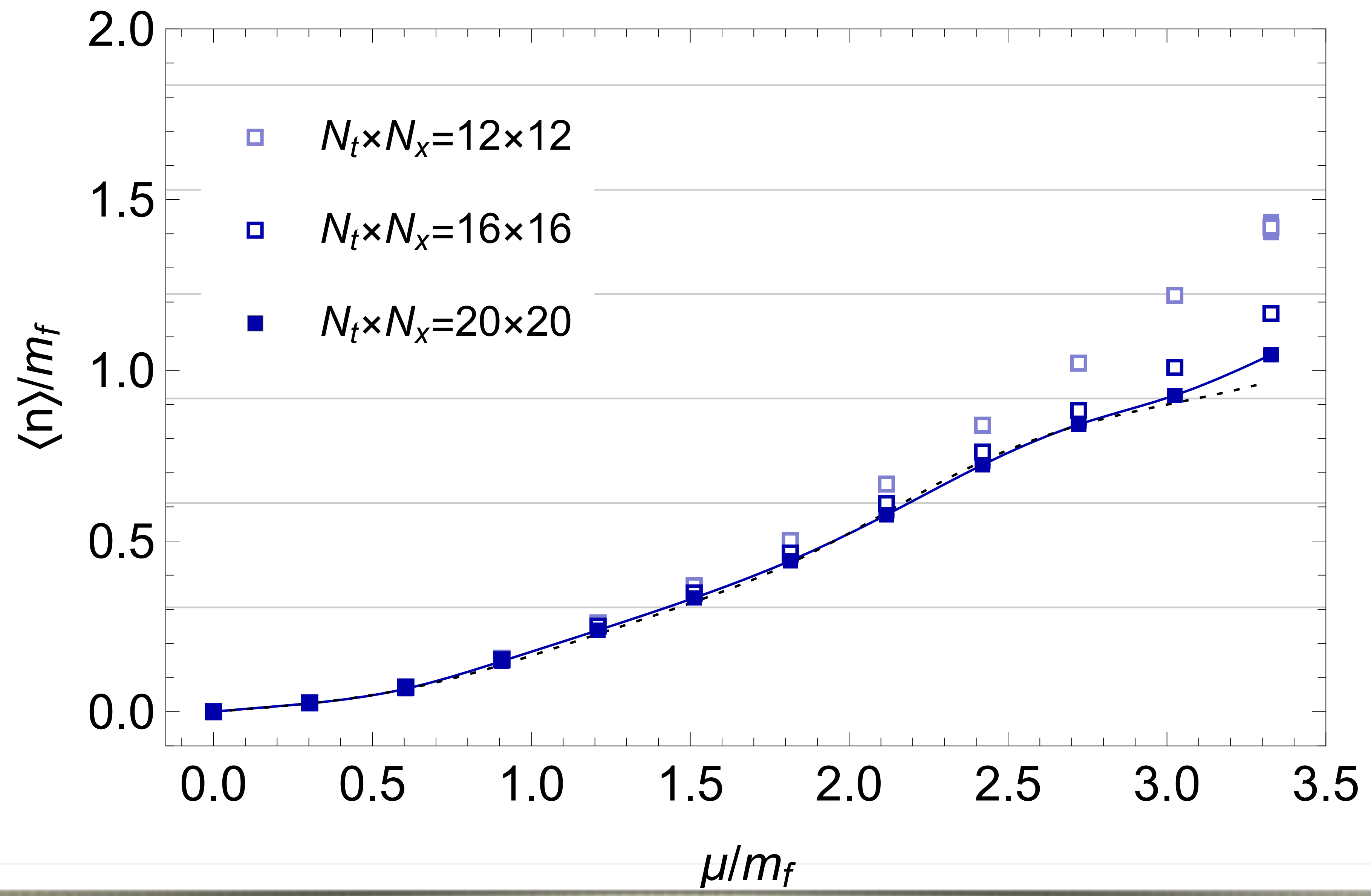


Silver blaze (cold limit)

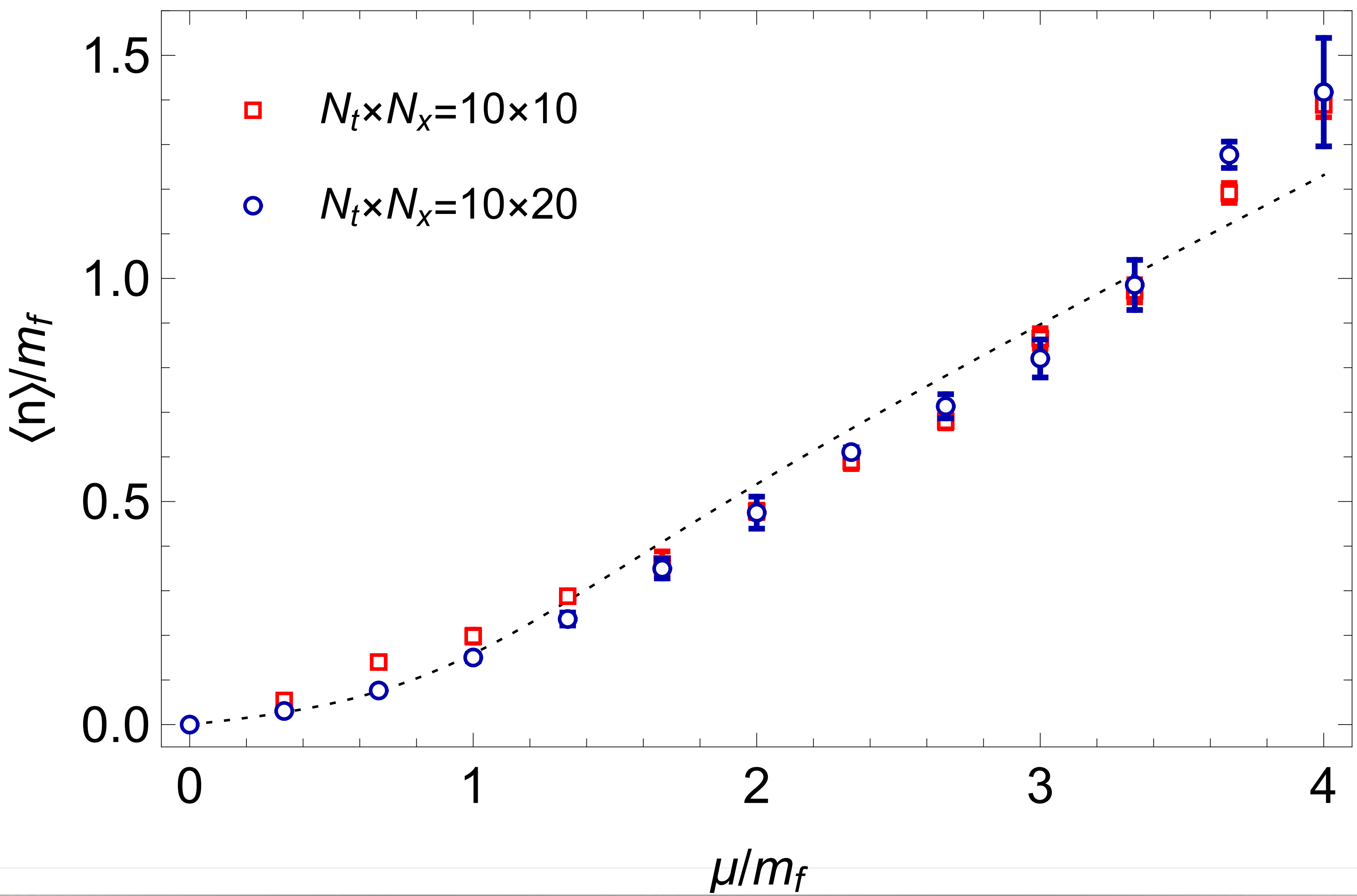


Y. Tanizaki, Y. Hidaka, and T. Hayata, *Lefschetz-thimble approach to the Silver Blaze problem of one-site fermion model*, [arXiv:1610.00393].

Continuum limit



Thermodynamic limit



Conclusions

- Complex manifold integration is feasible for both bosonic and fermionic systems; the residual phase fluctuations are mild.
- Field complexification serves as a knob to control the sign problem.
- Lefschetz thimble decomposition is a limiting case of the holomorphic gradient flow, difficult to sample if multiple thimbles contribute.
- Holomorphic gradient flow generates a continuous family of manifolds : sign problem $\Leftrightarrow$ multimodal distributions
- Useful to attack problems with fermions, QFT, real time dynamics, etc.