Monte Carlo calculations using the holomorphic gradient flow

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arXiv:1510.0325 arXiv:1512.0876 arXiv:1604.00956
arXiv:1605.08040 arXiv:1606.02742 arXiv:1609.01730
arXiv:1703.02414 arXiv:1703.06404

Excited QCD, Sintra
May 2017

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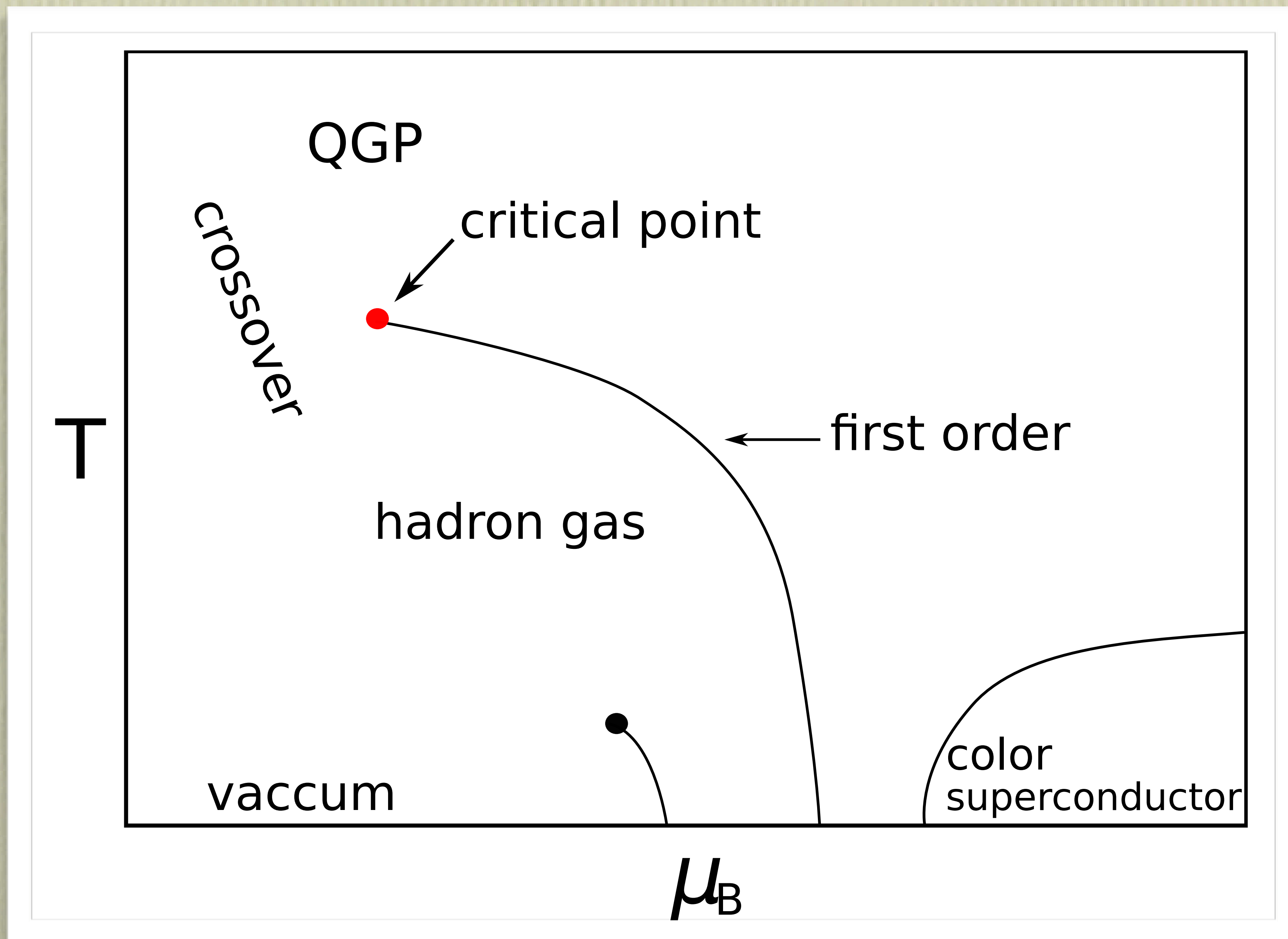
Motivation



complex

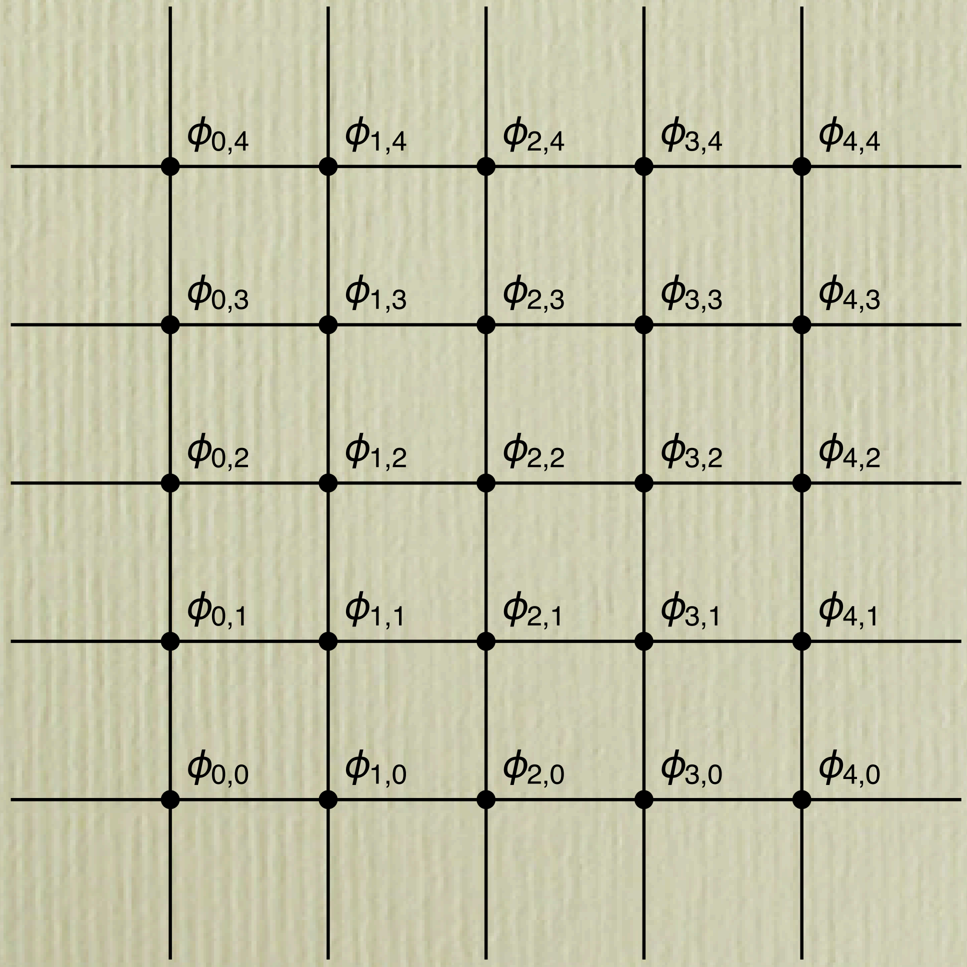
$$Z_{GC}(T,V,\mu) = \int \mathcal{D}U e^{-S_g(U)} \det M(U,\mu)$$

The plan

- Lefschetz thimbles
- Holomorphic gradient flow
- Case study: Massive Thirring model
- Case study: Real time dynamics
- Conclusions and outlook

Lattice discretization

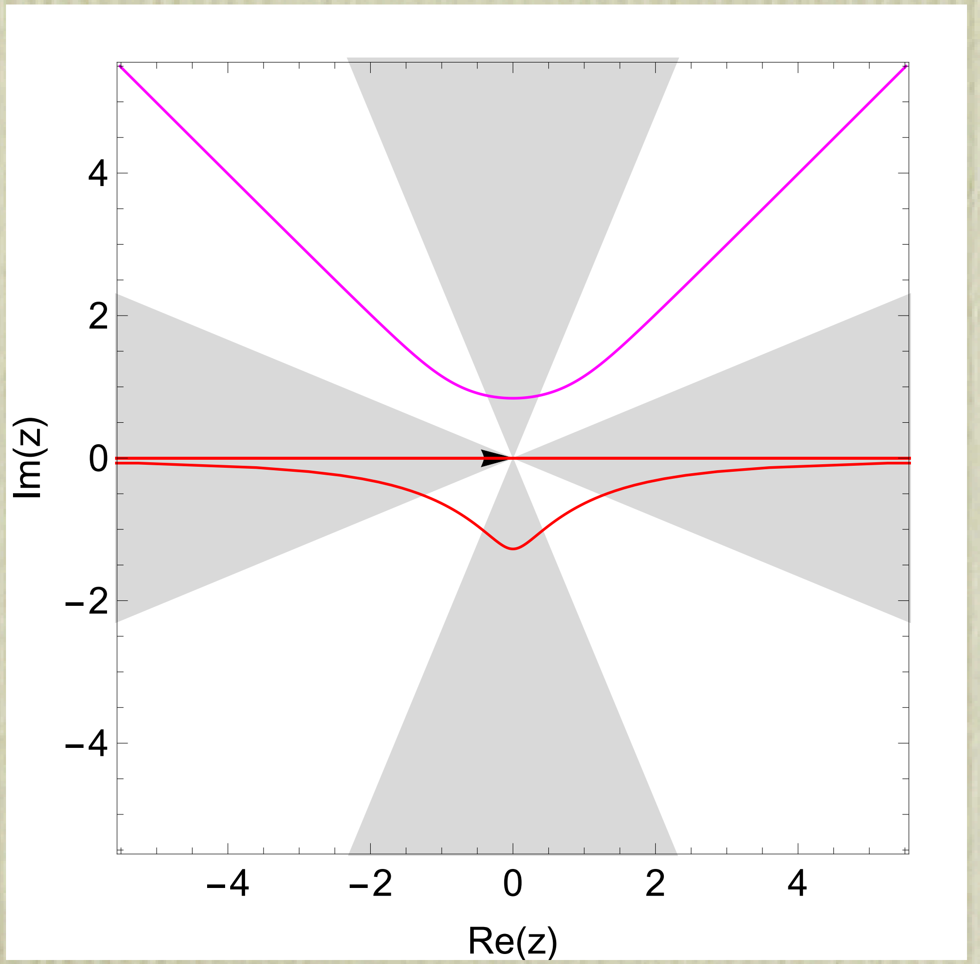
$$S = \int d^4x \left[\partial_0\phi^*\partial_0\phi + \nabla\phi^*\cdot\nabla\phi + (m^2-\mu^2)|\phi|^2 + \mu\underbrace{(\phi^*\partial_0\phi - \phi\partial_0\phi^*)}_{j_0(x)} + \lambda|\phi|^4\right]$$



$$S = a^4\sum_x \left[\frac{e^{\mu a}\phi^*_{x+\hat{0}} - \phi^*_x}{a}\,\frac{e^{-\mu a}\phi_{x+\hat{0}} - \phi_x}{a} + \sum_{\nu=1}^{3}\left|\frac{\phi_{x+\hat{\nu}} - \phi_x}{a}\right|^2 + m^2|\phi_x|^2 + \lambda|\phi_x|^4 \; - h(\phi_{x,1} + \phi_{x,2})\right].$$

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

Contour deformation

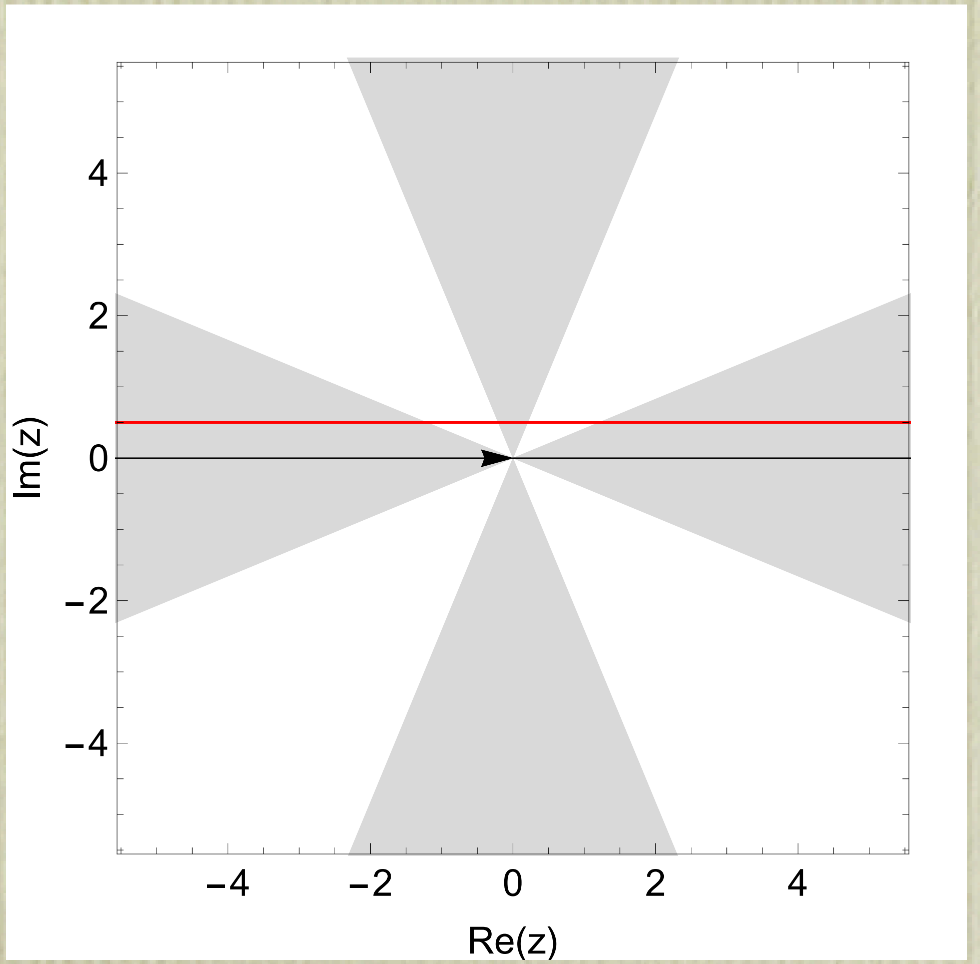


$$Z = \int_{-\infty}^{\infty} \mathrm{d}x \, e^{-S(x)}$$

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

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

Contour deformation



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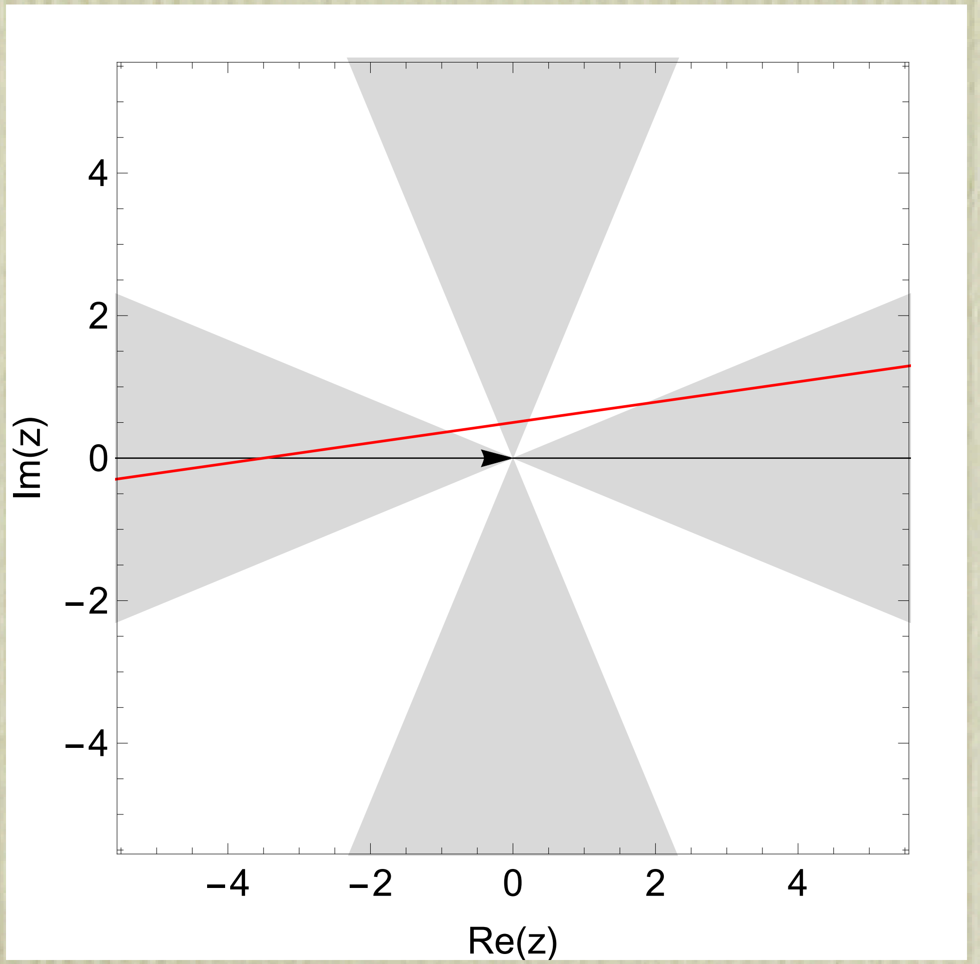

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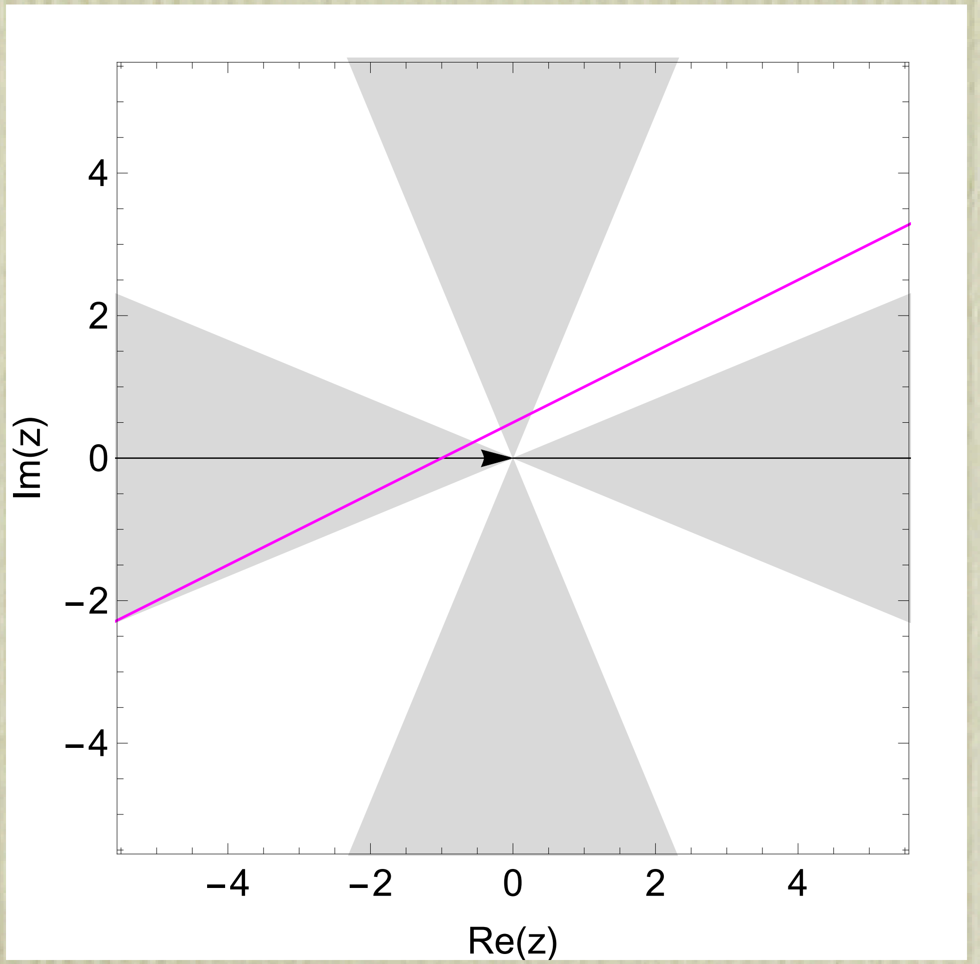

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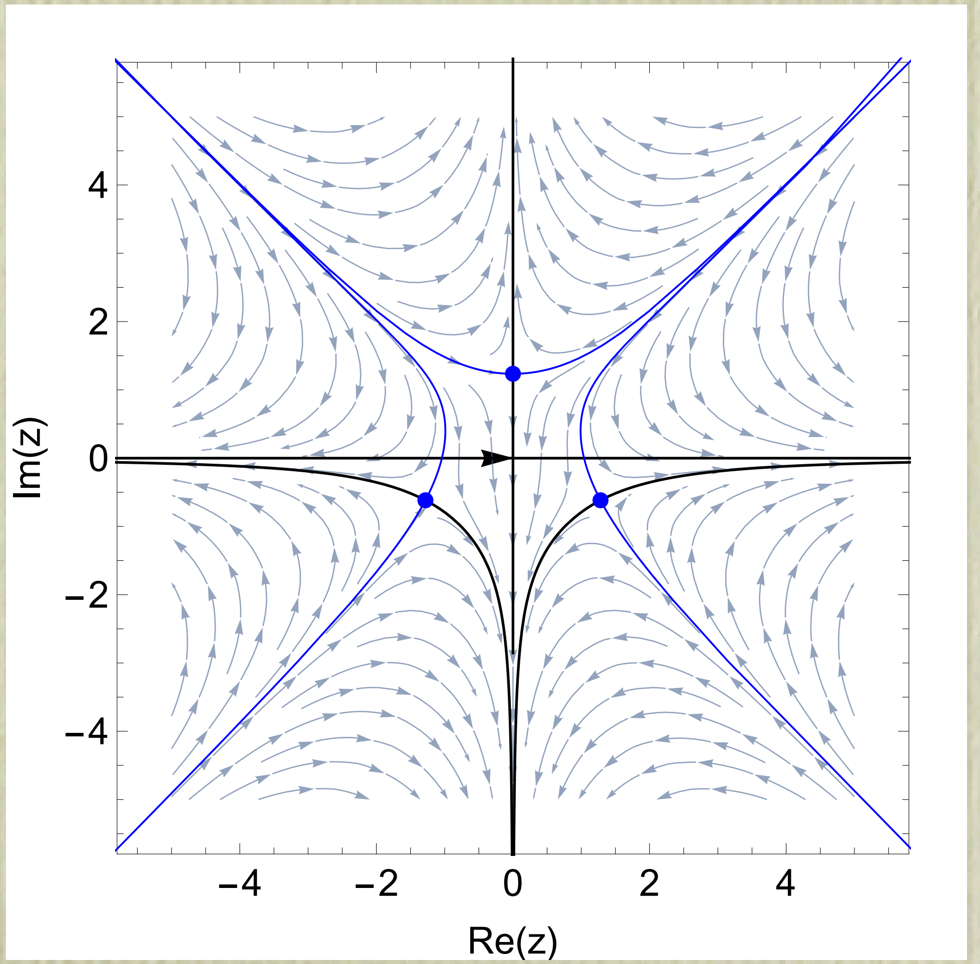
Lefschetz thimble



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

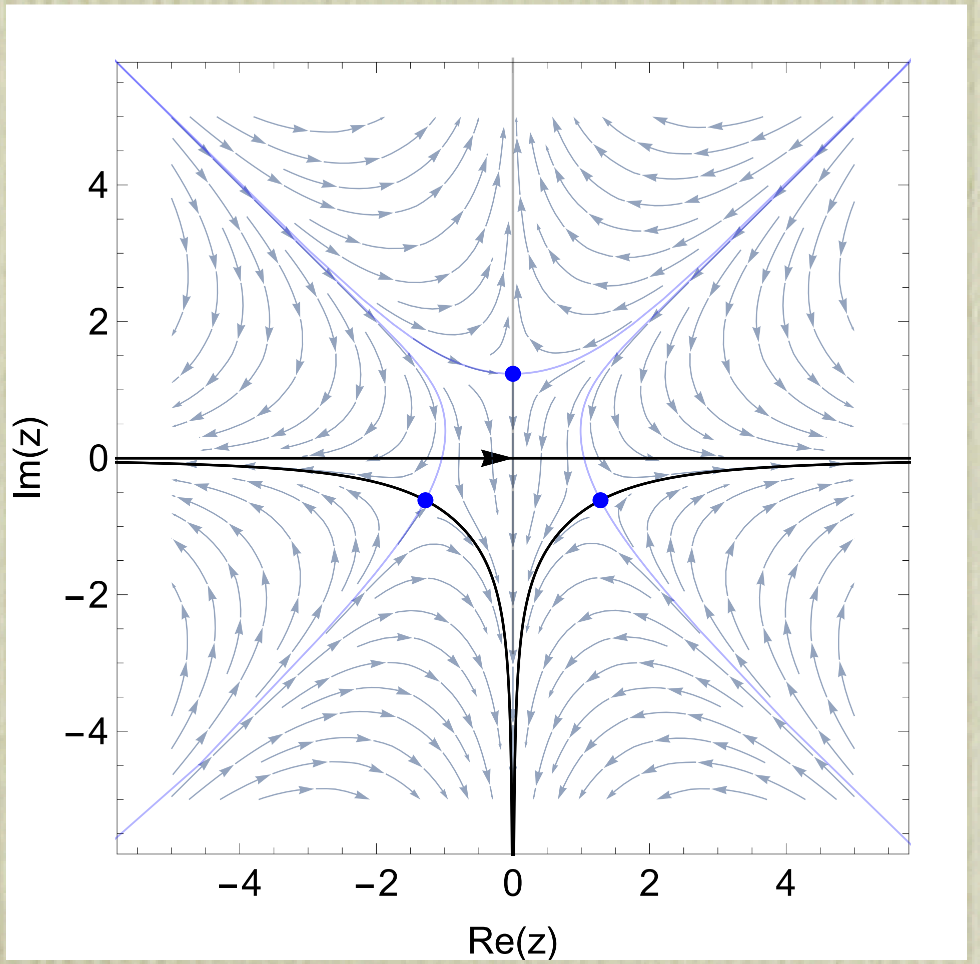
$$\frac{dS}{dz} = 0 \quad \text{(critical points)}$$

$$\frac{dz}{d\tau} = \overline{\frac{dS}{dz}} \quad \text{(upward flow)}$$

$$\frac{dz}{d\tau} = -\overline{\frac{dS}{dz}} \quad \text{(downward flow)}$$

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

Lefschetz thimble



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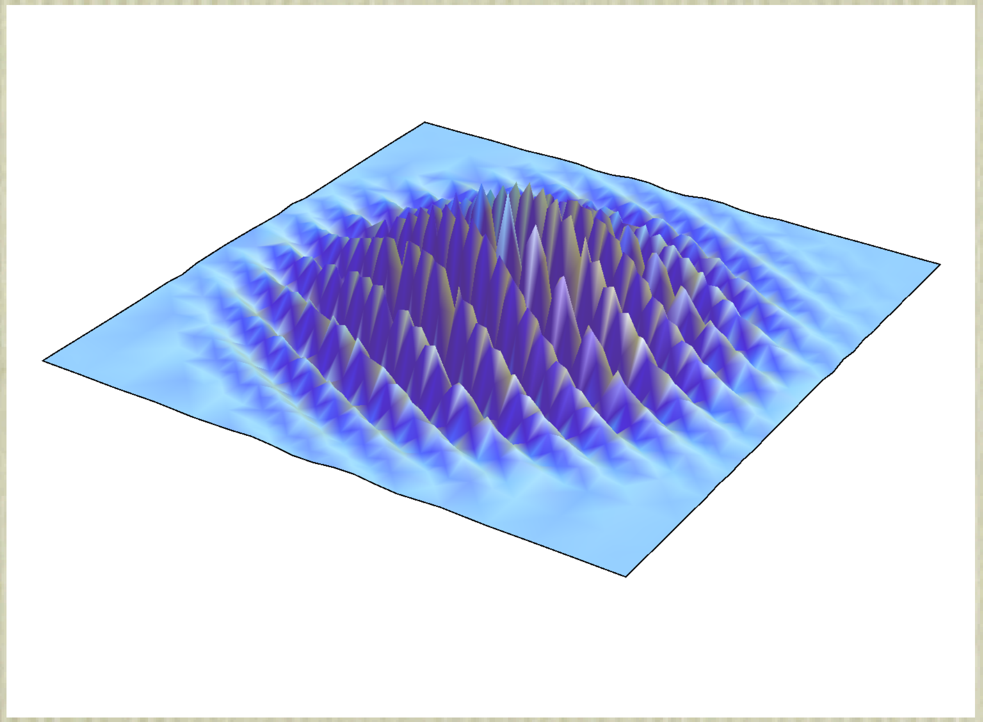
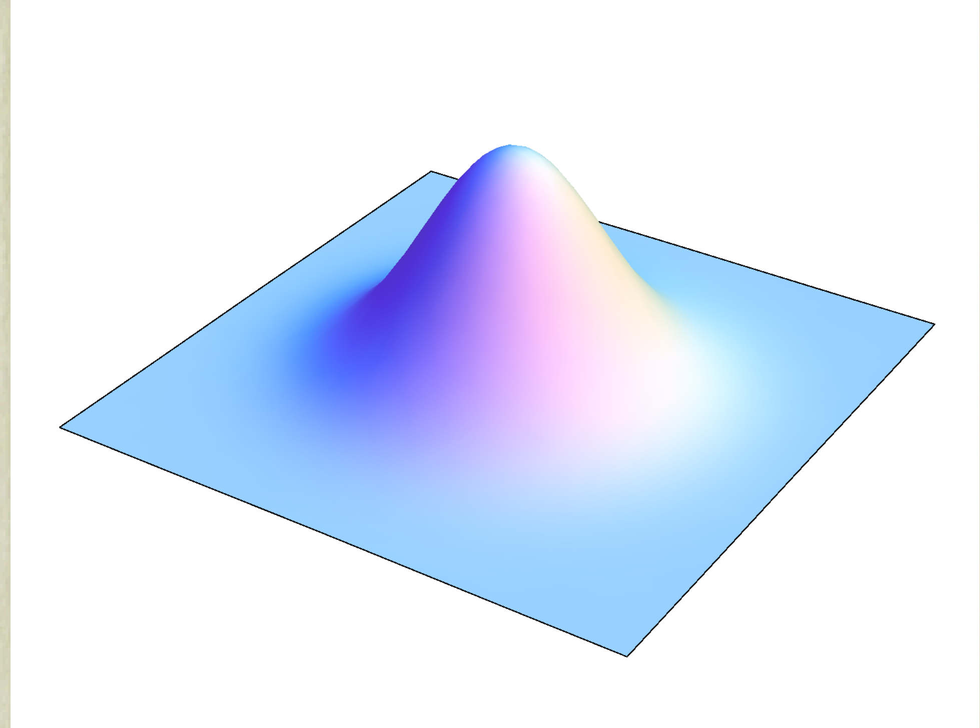
$$Z = \sum_\sigma n_\sigma \int_{J_\sigma} dz \, e^{-S(z)}$$

Lefschetz thimble



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



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

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

Beyond thimbles

- Most prior Monte-Carlo investigations focused on sampling a single thimble
- In general there are many thimbles (at least one for each solution of the equation of motion)
- The hope is that only one thimble dominates either in the thermodynamic or continuum limit
- Otherwise we need to identify all critical points and determine which ones contribute, setup a proper sampling algorithm, etc (very difficult)

Beyond thimbles

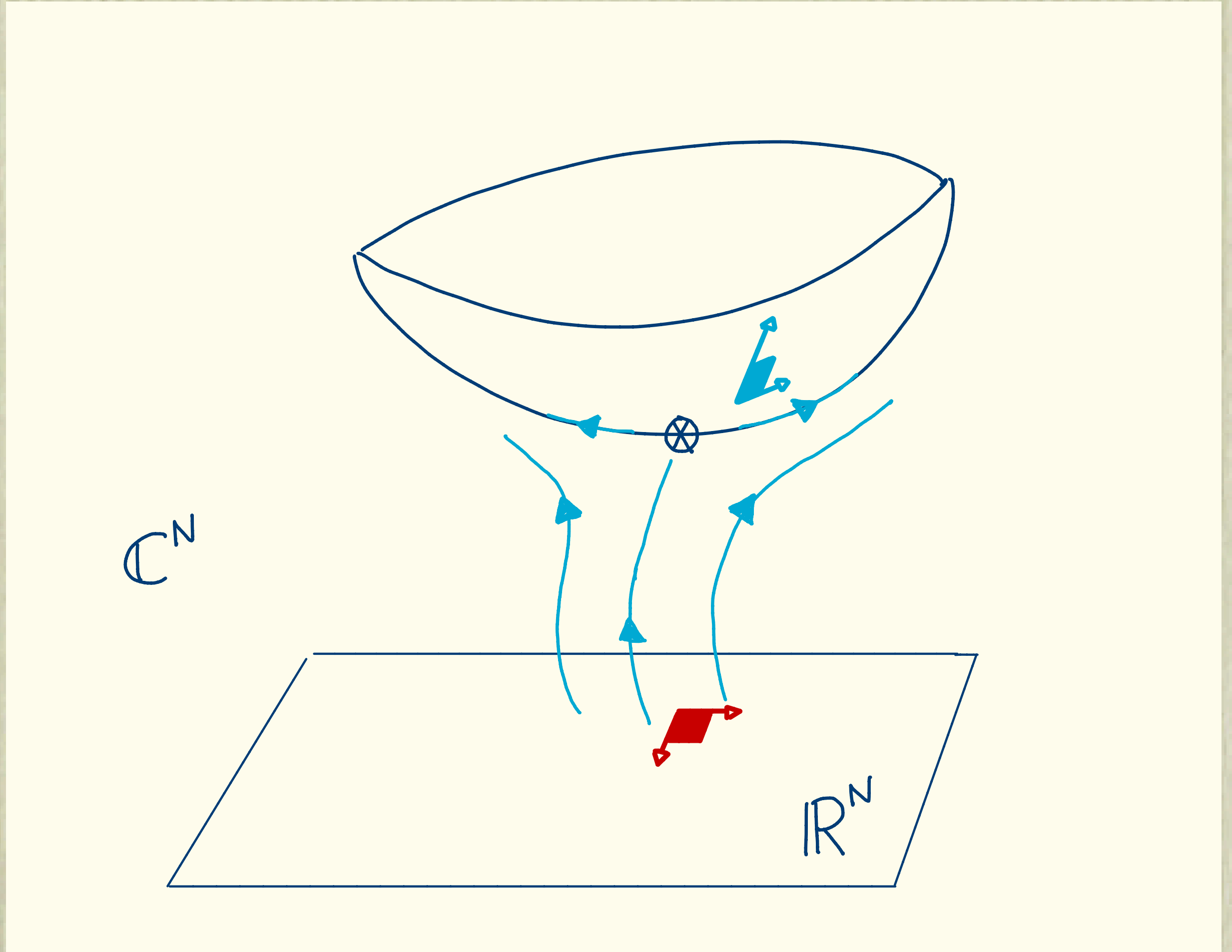
- We take a different route: use manifolds generated from the original integration domain using the holomorphic gradient flow

- As we increase the flow time from 0 to infinity we interpolate between the original integration domain and the thimble decomposition

- If we flow too little we have a sign problem

- If we flow too much we have ergodicity problems

Manifolds generated by holomorphic gradient flow

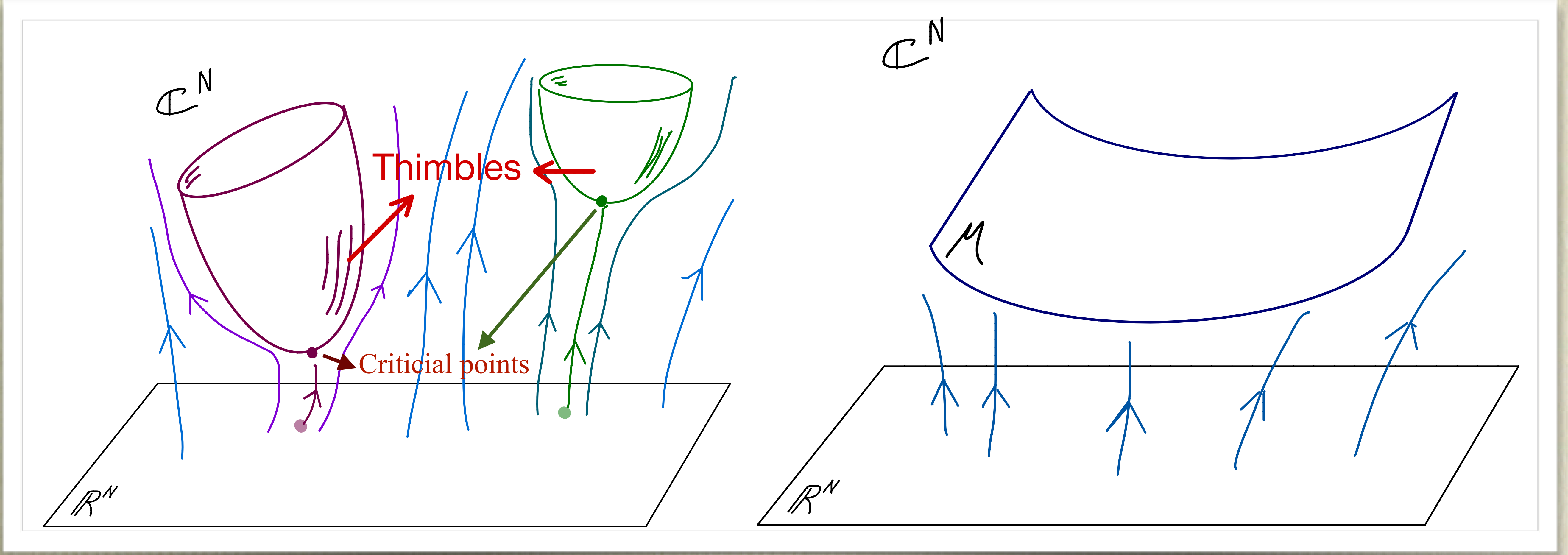


$$\frac{d\phi_a}{d\tau} = \overline{\frac{\partial S}{\partial \phi_a}}, \qquad \phi_a \equiv x_a + i y_a$$

$$\begin{cases} \dfrac{dx_a}{d\tau} = \dfrac{\partial S_R}{\partial x_a} = \dfrac{\partial S_I}{\partial y_a} \\ \dfrac{dy_a}{d\tau} = \dfrac{\partial S_R}{\partial y_a} = -\dfrac{\partial S_I}{\partial x_a} \end{cases}$$

- Real part of the action increases (gradient flow)
- Imaginary part of the action remains constant (Hamiltonian flow)

Manifolds generated by holomorphic gradient flow

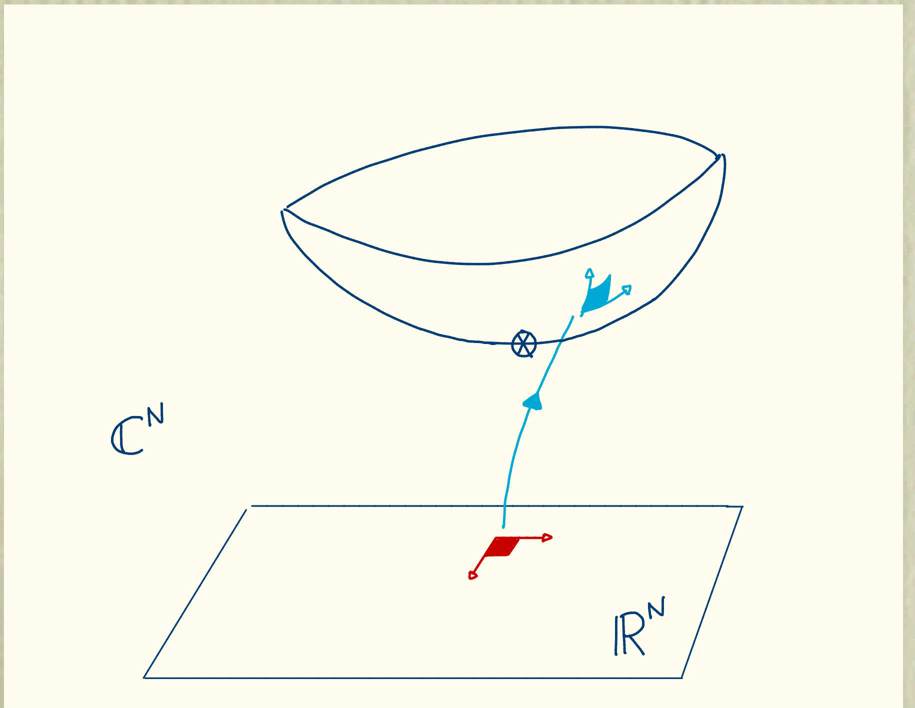


$$T_{\text{flow}} \to \infty \quad \Rightarrow \quad \mathcal{M} \to \text{sum over thimbles}$$

Basic idea

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

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



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

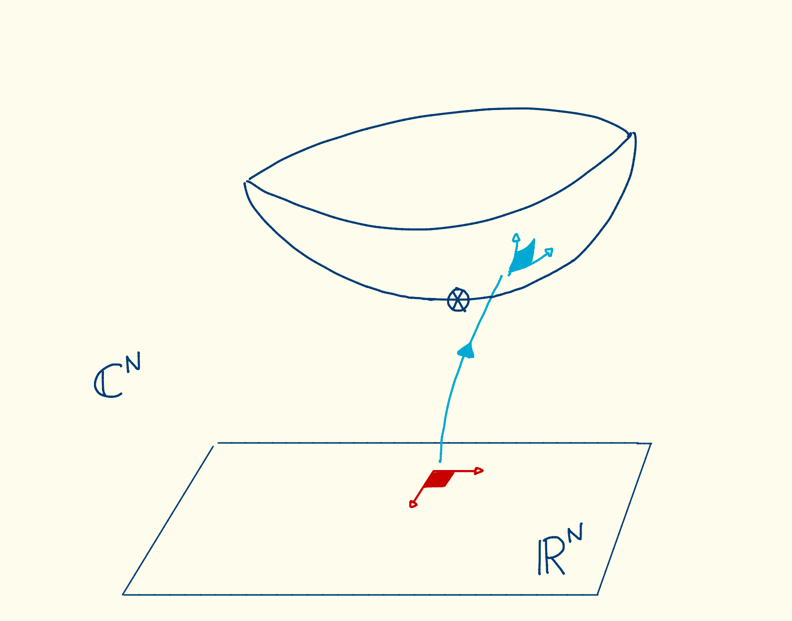
$$\Phi(x) = e^{i[S_I(z(x)) - \mathrm{Im}\,\det J(x)]}$$

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

Basic idea

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

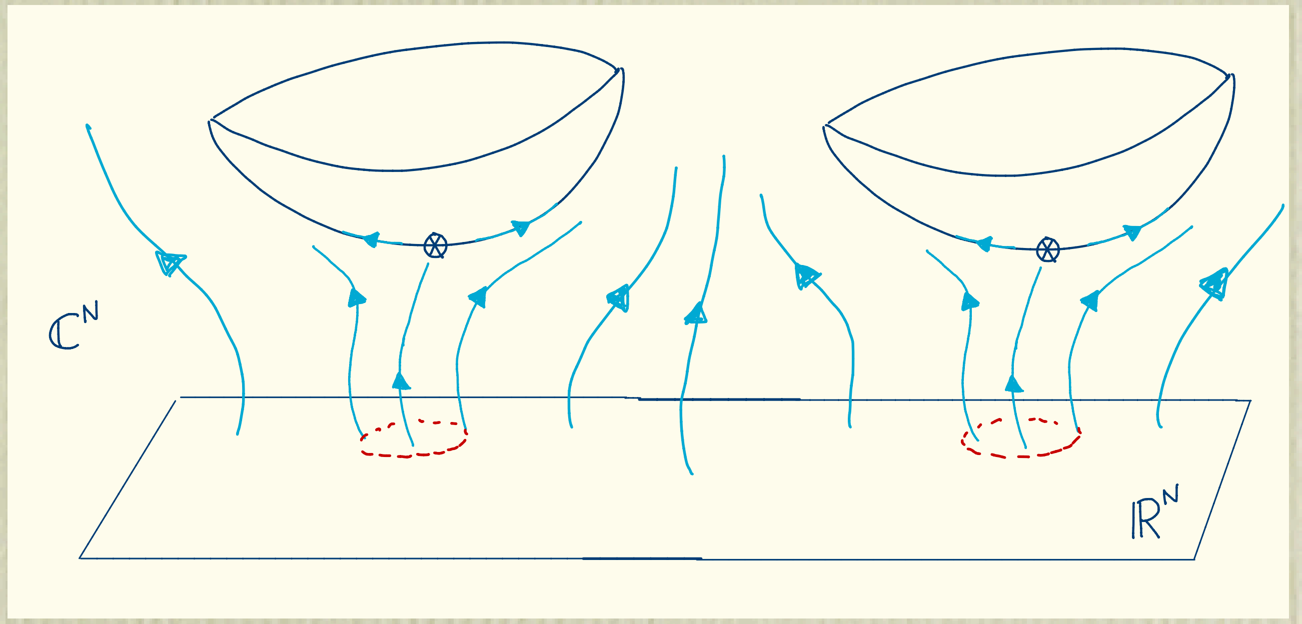
$$\frac{dJ}{d\tau} = \overline{H(z)J}\,, \quad J(0) = I \quad H(z)_{ij} = \frac{\partial^2 S}{\partial z_i \partial z_j}$$



- The differential equations are integrated for a fixed amount of “time”: T_{flow}
- This is expensive, especially the calculation of J
- Sampling is done based on the effective action and the phase is reweighted at the end

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

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

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

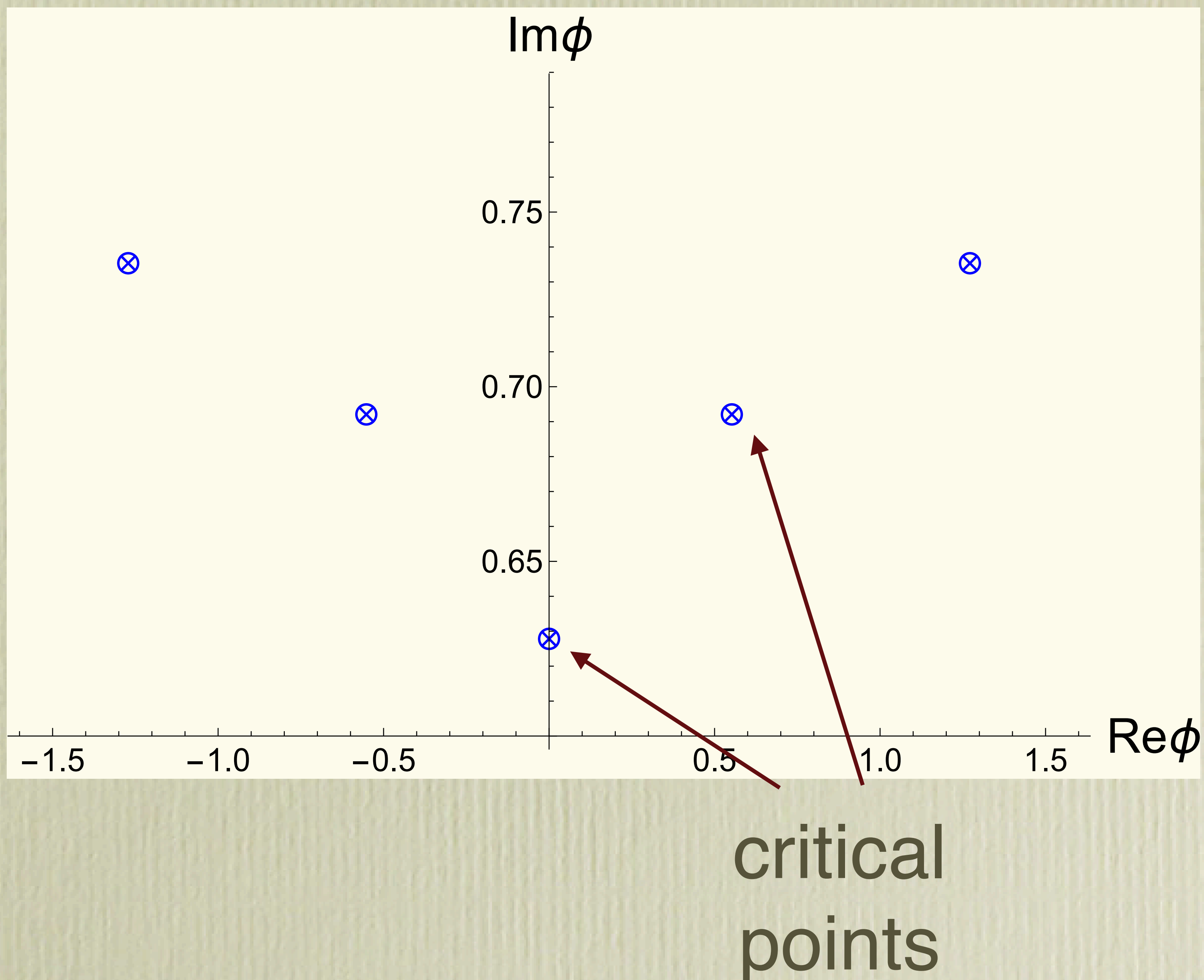
Auxiliary field A's

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

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



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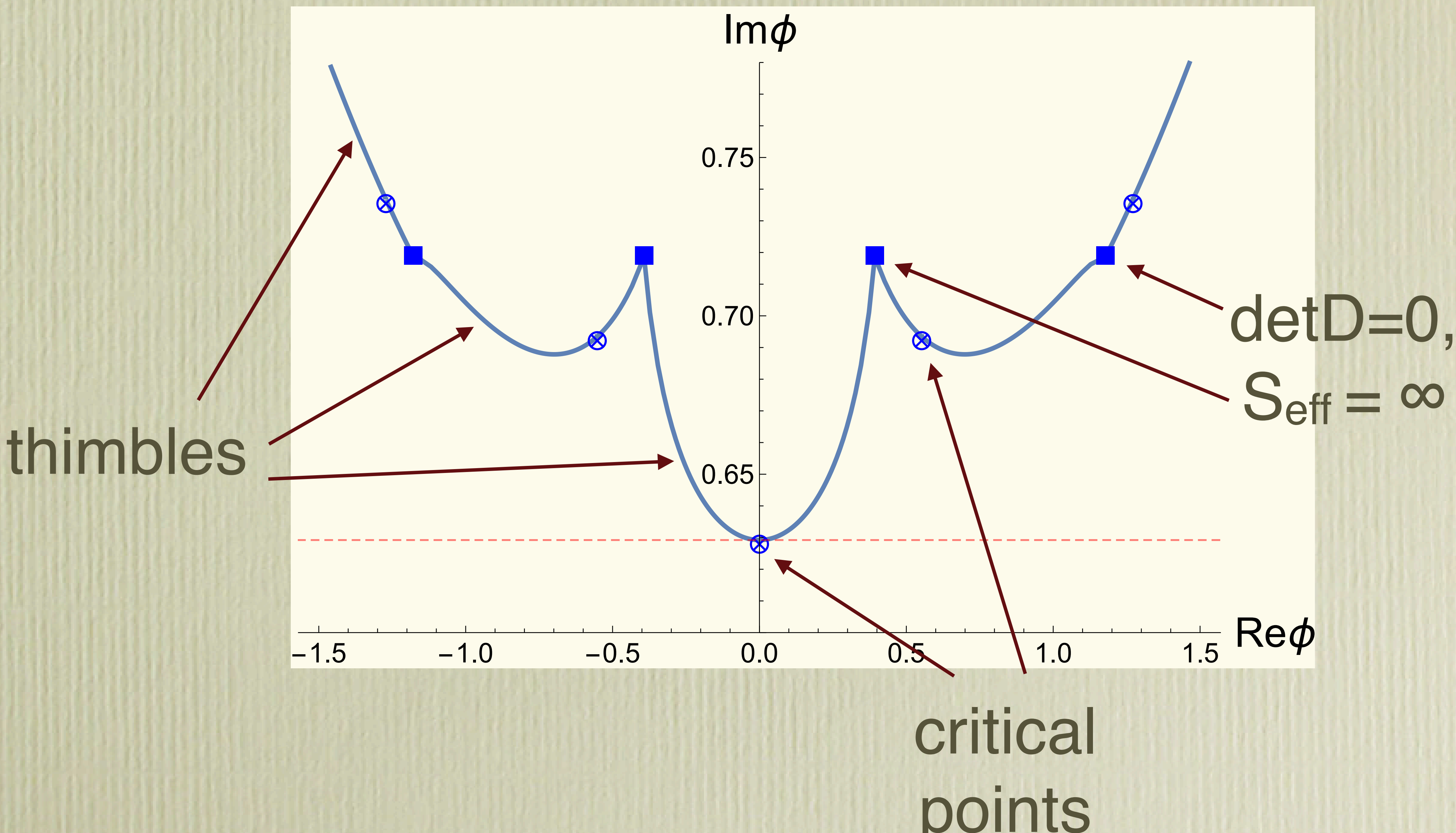

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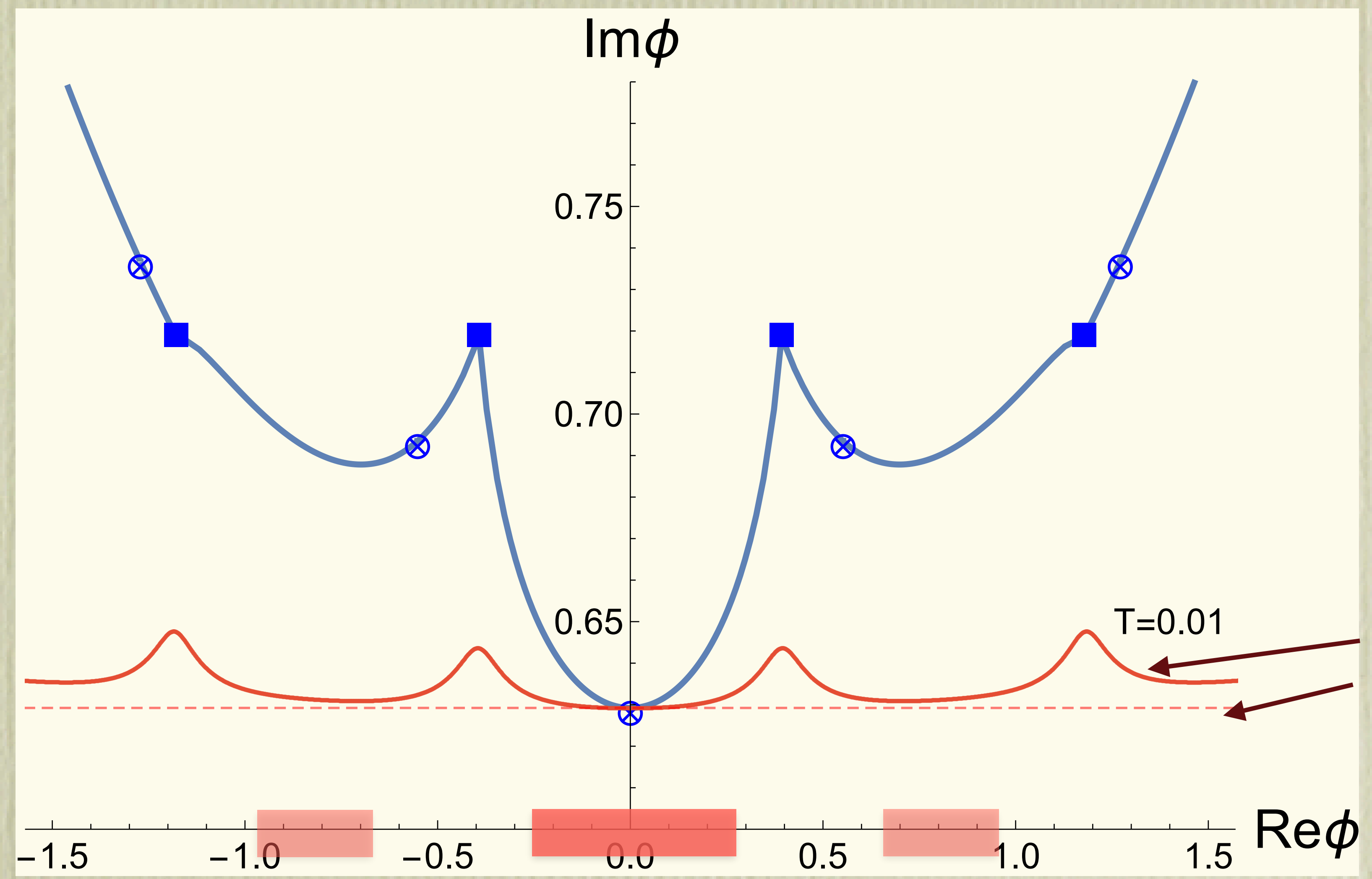
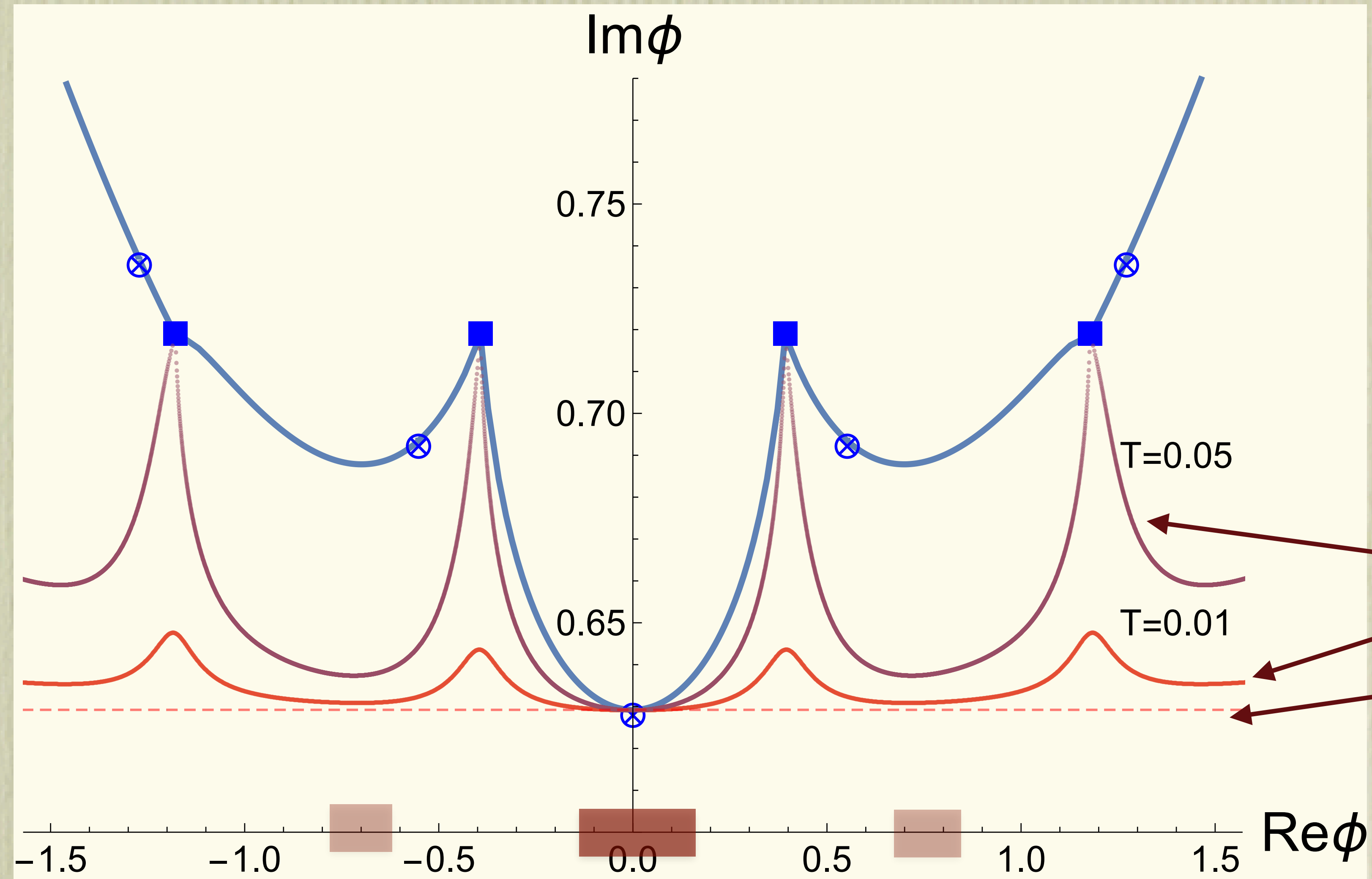


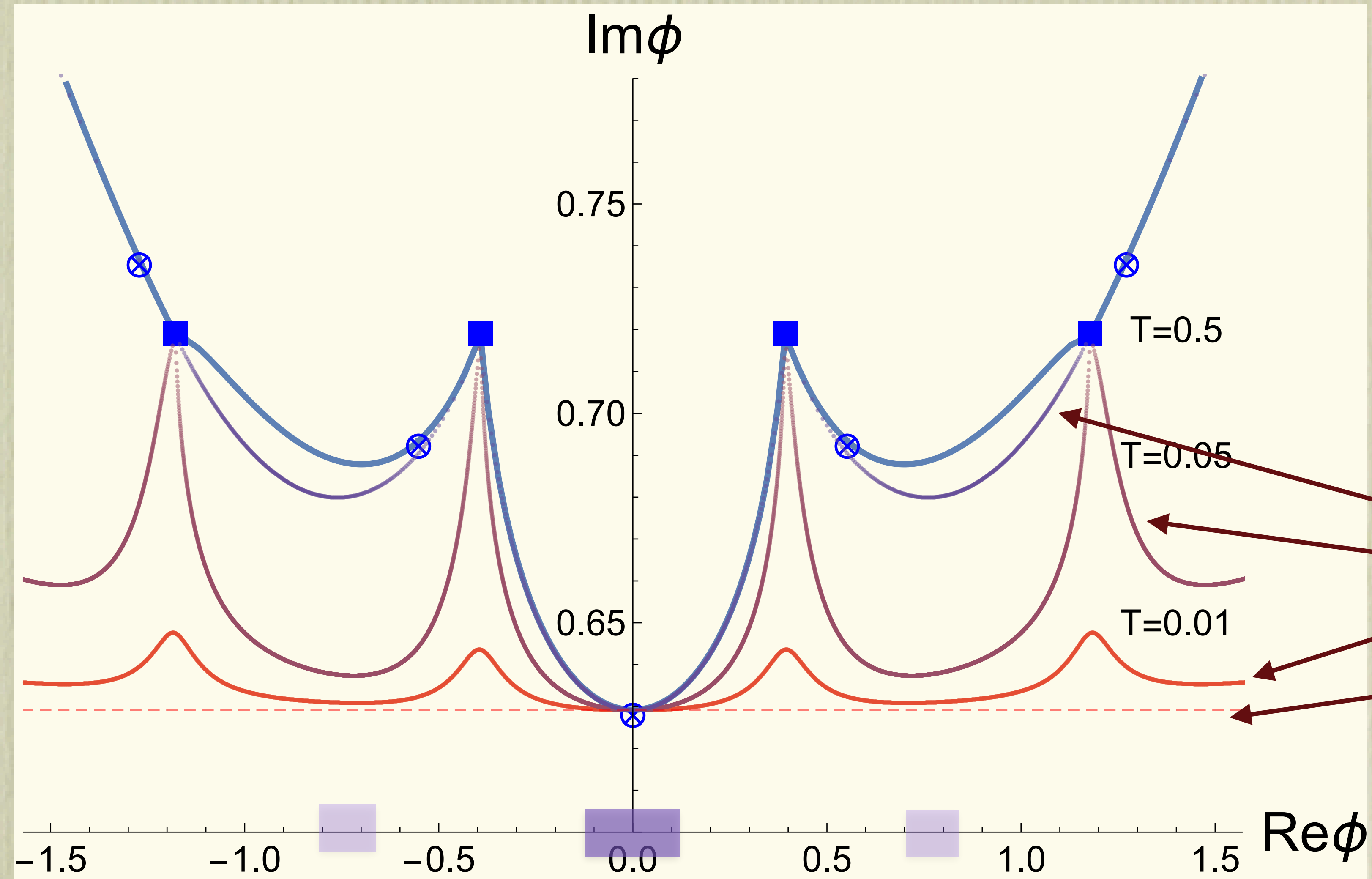
same homological class

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



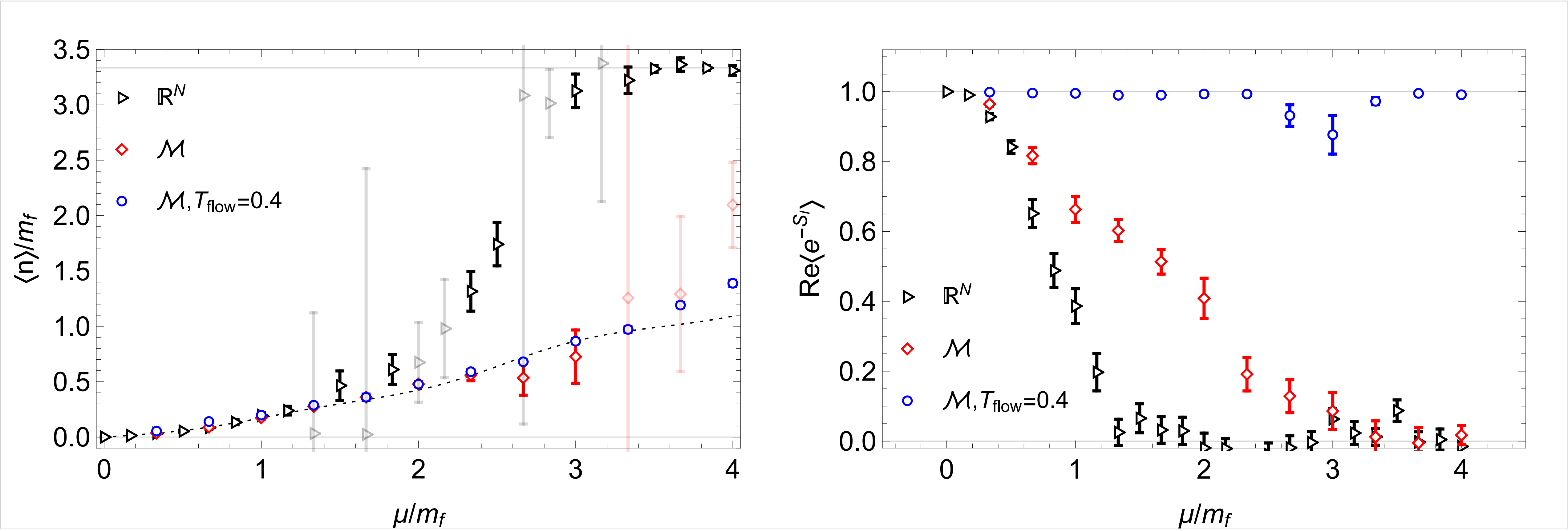
flowed tangent space

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

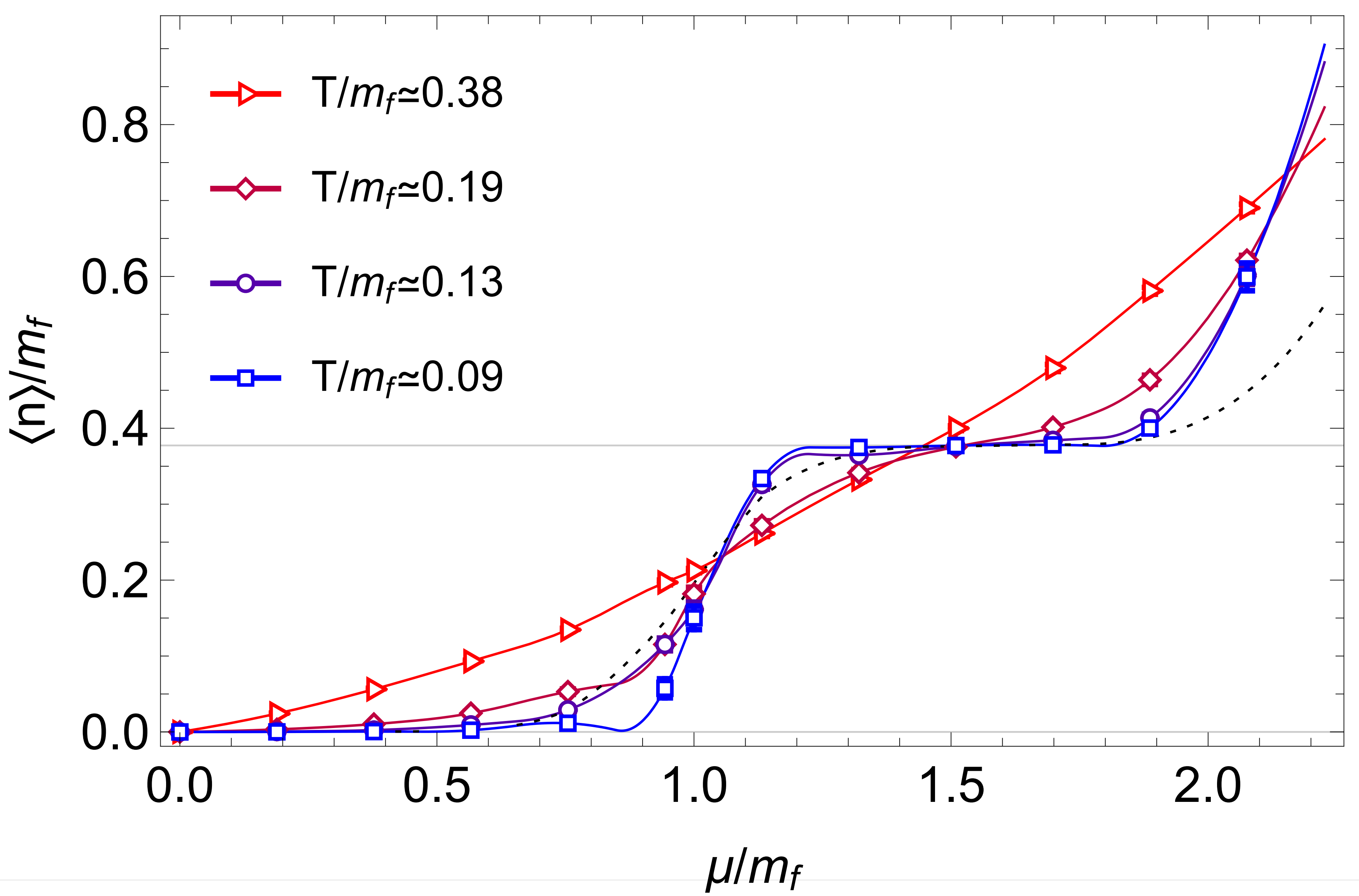


flowed tangent space

Sign problem

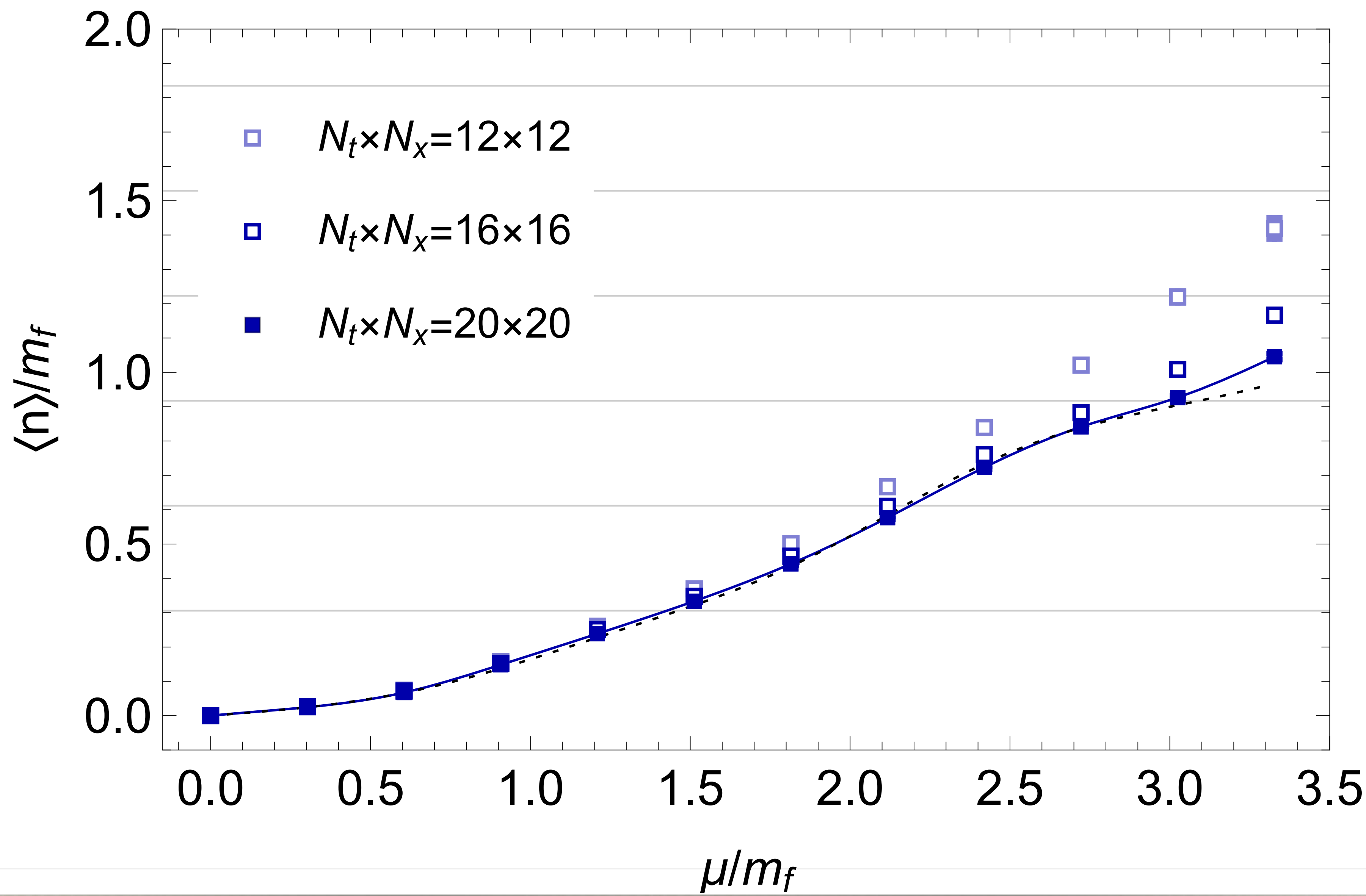


Silver blaze (cold limit)

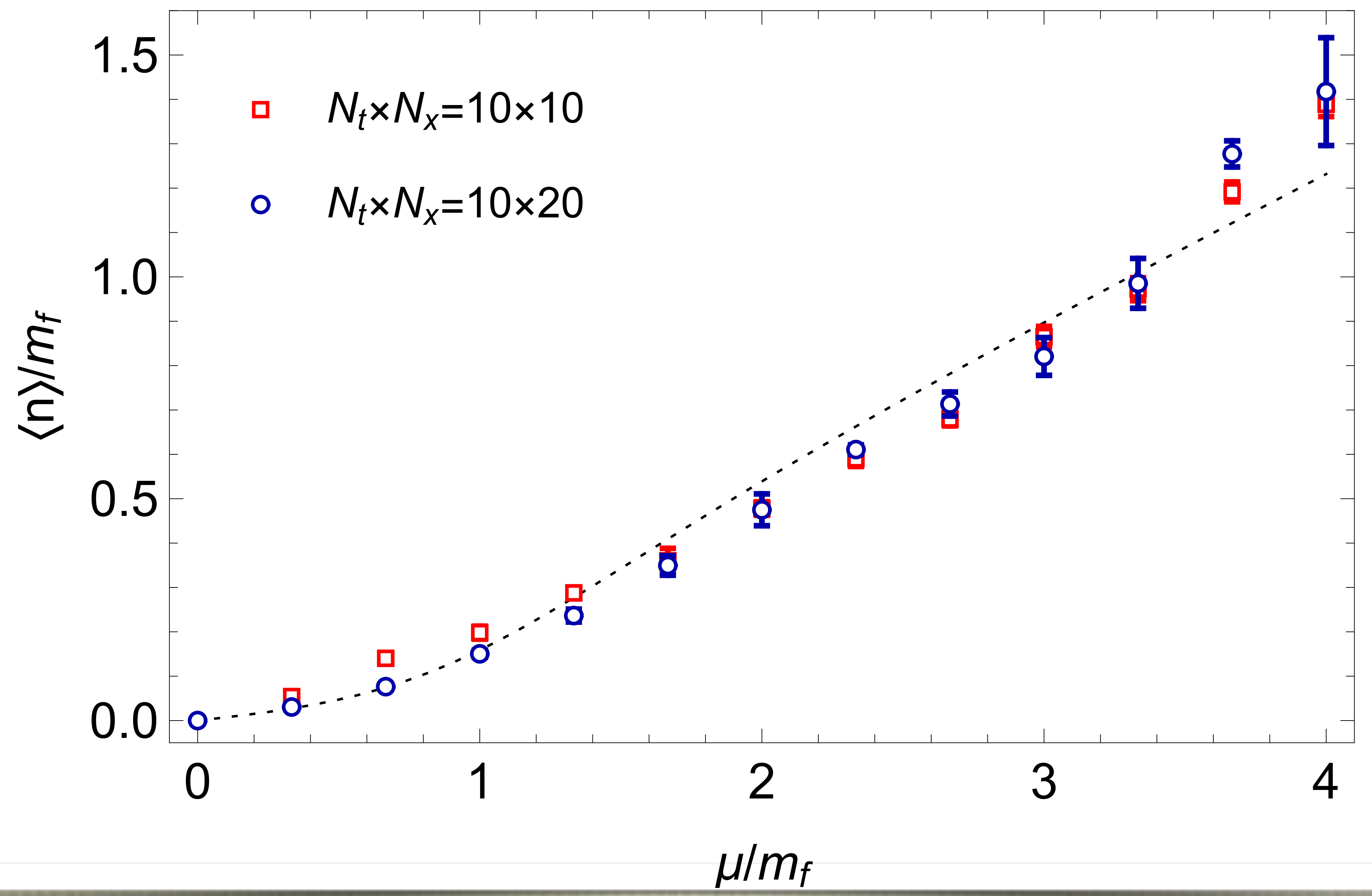


step is missed in a one thimble calculation

Continuum limit



Thermodynamic limit



Case study: real time physics

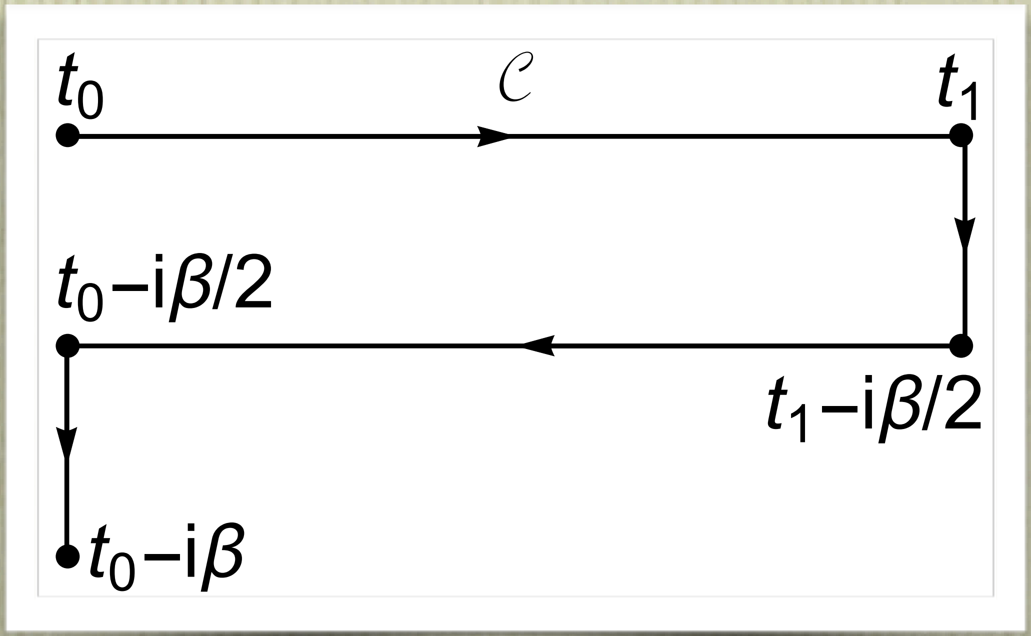
- Motivation: compute out-of-equilibrium correlators, transport coefficients non-perturbatively from first principles

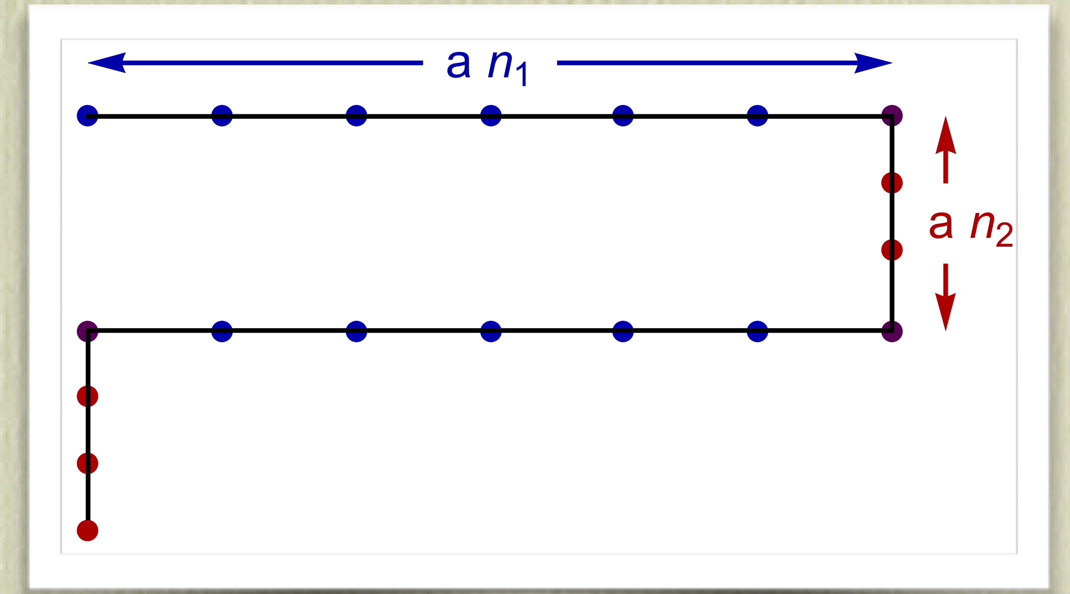
- Observables of interest are transport coefficient such as shear viscosity, conductivity, etc.

- At 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

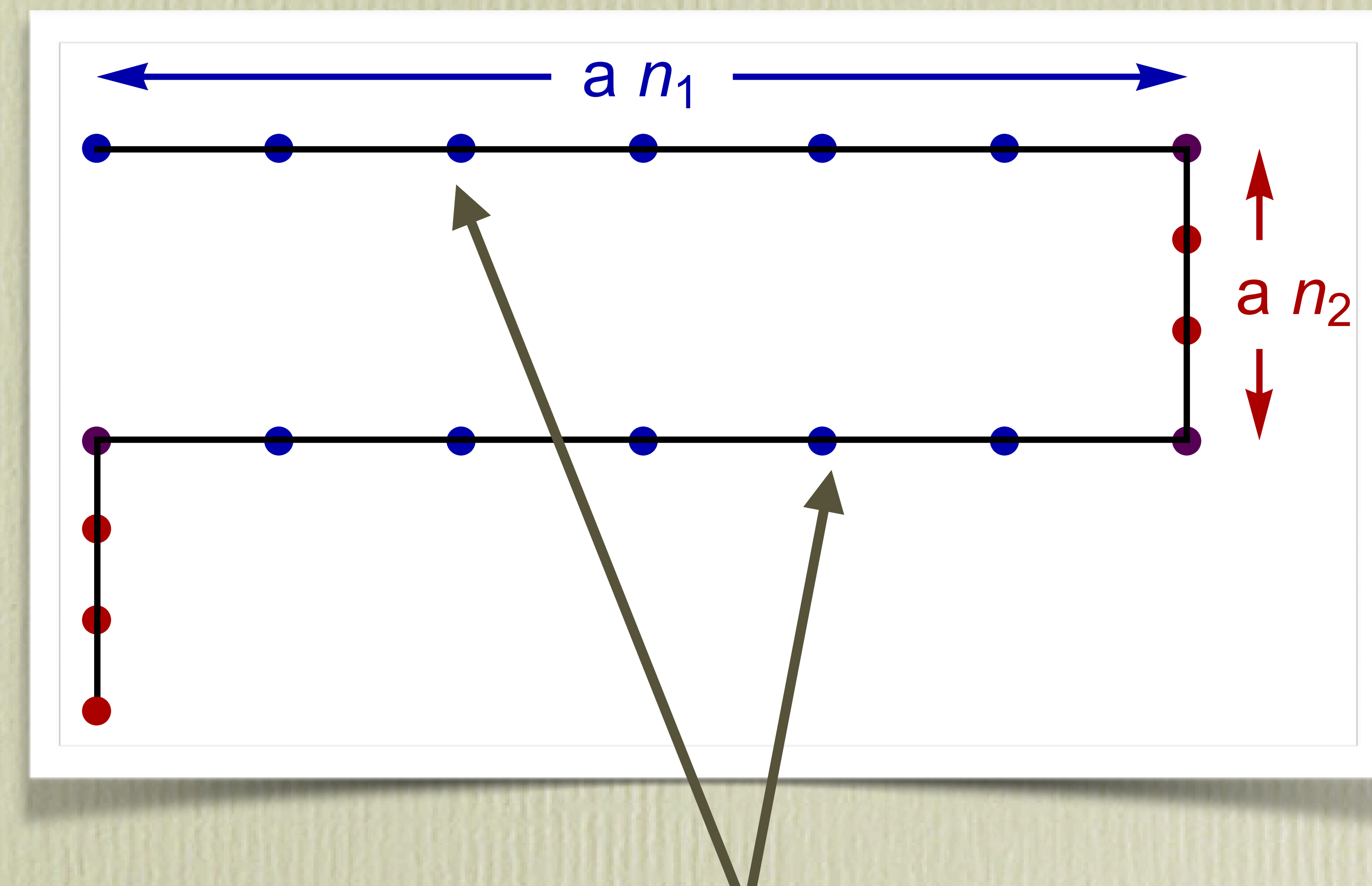




$$S_{SK}[\phi] = iS[\phi] = \int_{\mathcal{C}} dt\, L[\phi] \qquad \langle \mathcal{O}_1(t)\mathcal{O}_2(t')\rangle = \frac{1}{Z}\int \mathcal{D}\phi\, e^{-S[\phi]}\mathcal{O}_1(t)\mathcal{O}_2(t')$$

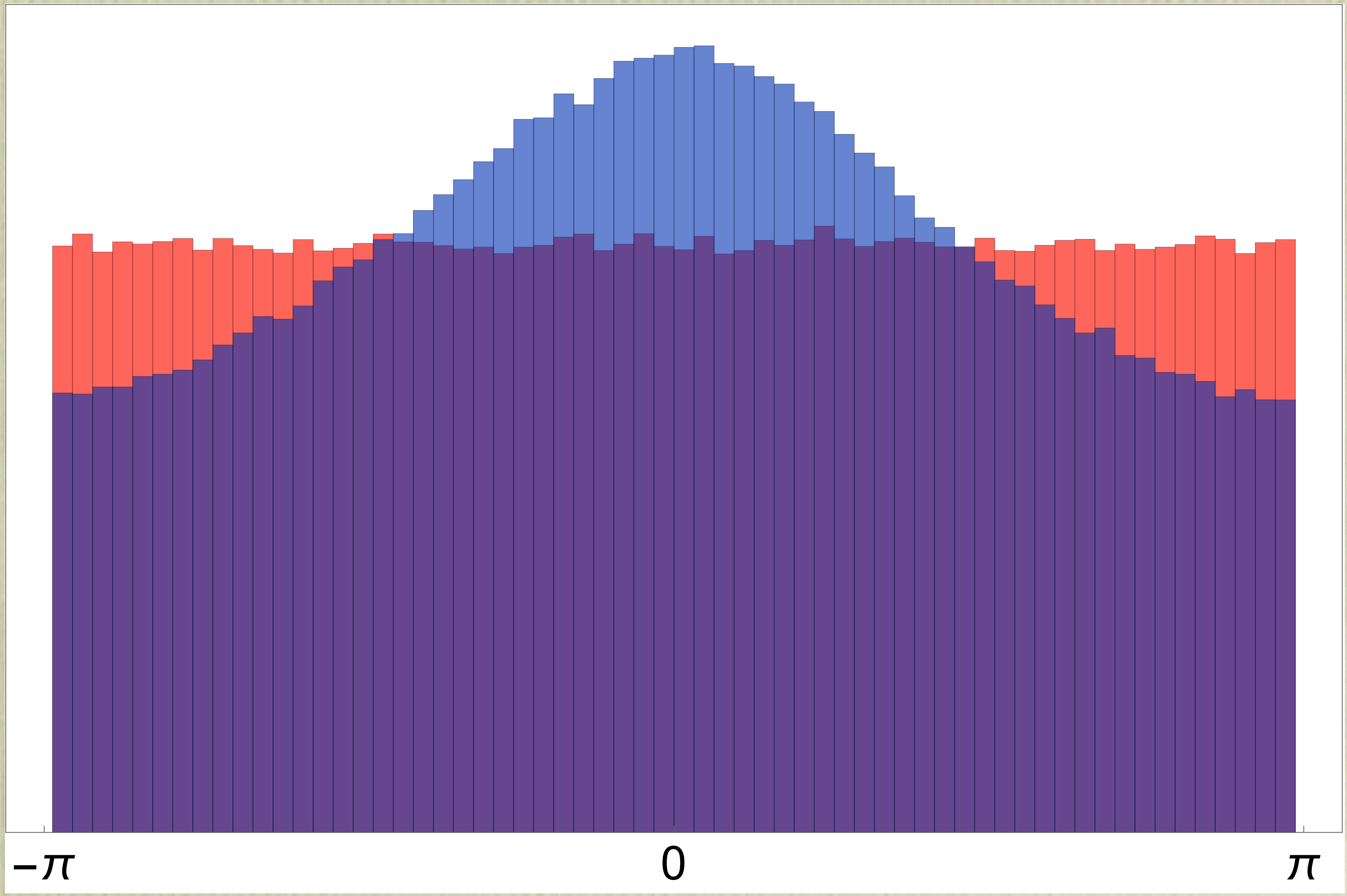
$$S[\phi] = \sum_{t,n} a_t a \left[\frac{(\phi_{t+1,n} - \phi_{t,n})^2}{2a_t^2} + \frac{1}{2}\left(\frac{(\phi_{t+1,n+1} - \phi_{t+1,n})^2}{2a^2} + \frac{(\phi_{t,n+1} - \phi_{t,n})^2}{2a^2} \right) + \frac{1}{2}m^2 \frac{\phi_{t,n}^2 + \phi_{t+1,n}^2}{2} + \frac{\lambda}{4!}\frac{\phi_{t+1,n}^4 + \phi_{t,n}^4}{2}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

The worst sign problem



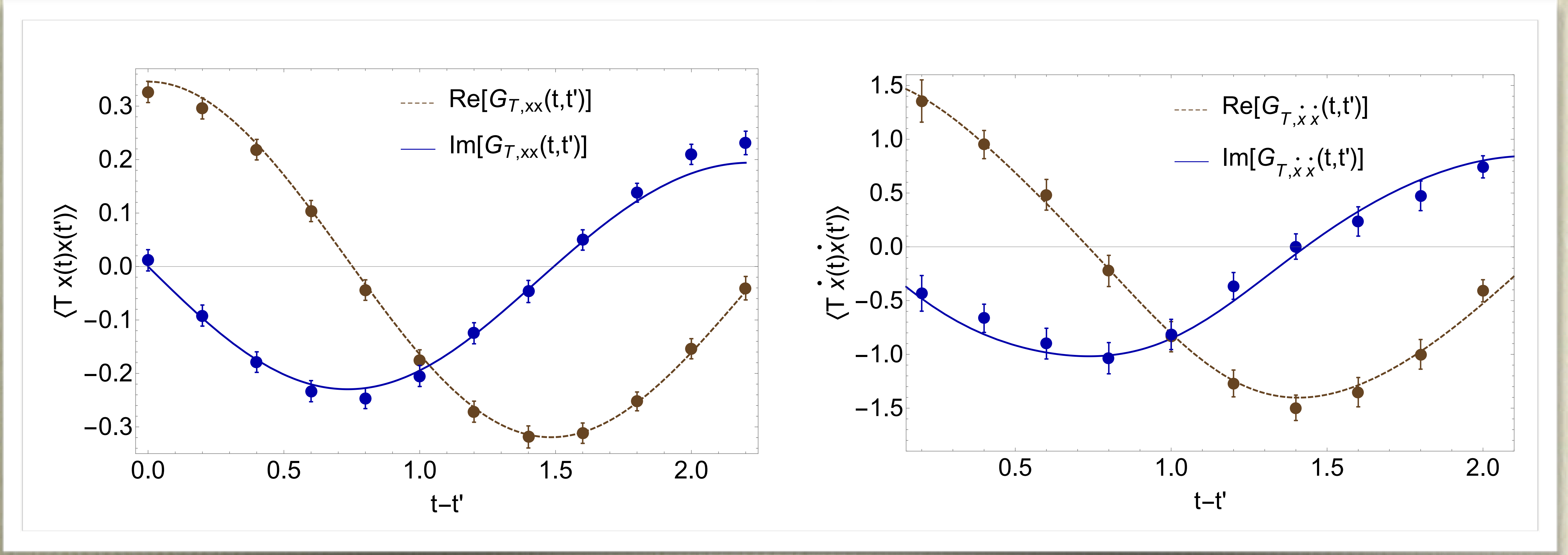
The field variables attached to real time legs contribute a purely imaginary factor to the action because $\exp(-aS_n) = \langle \phi_{n+1} | \exp(-iaH) | \phi_n \rangle$ produces a contribution to the action S_n that is purely imaginary.

The worst sign problem



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

Real time physics (0+1D)



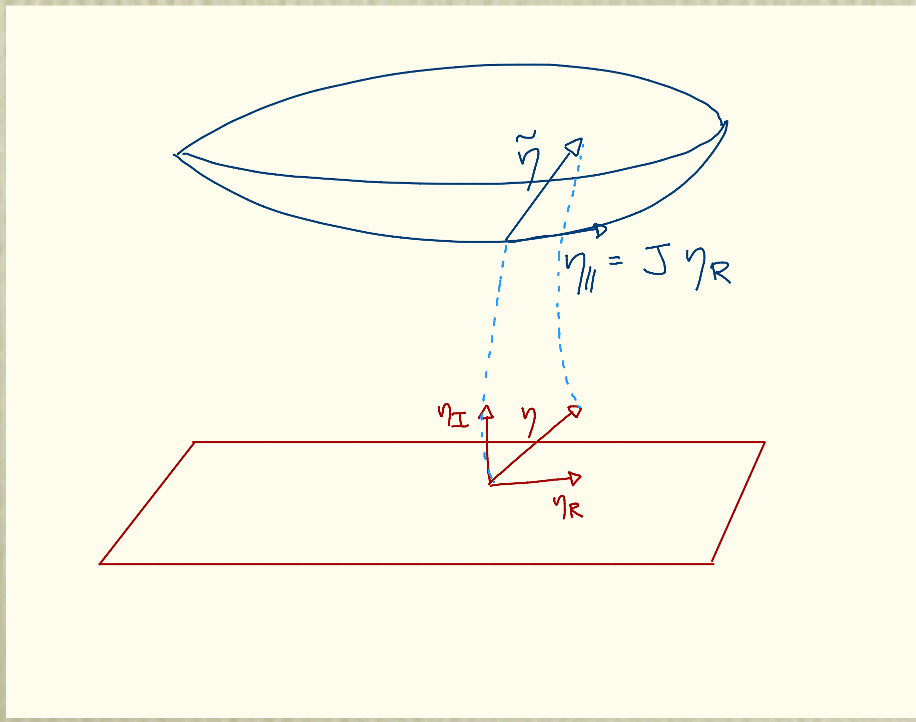
$$L = \frac{1}{2}\dot{x}^2 + \frac{1}{2}x^2 + \frac{\lambda}{4!}x^4$$

Real time physics

Problems

- large flow needed (from R^N)
- jacobian expensive
- anisotropic proposals
- tangent space in wrong homology class

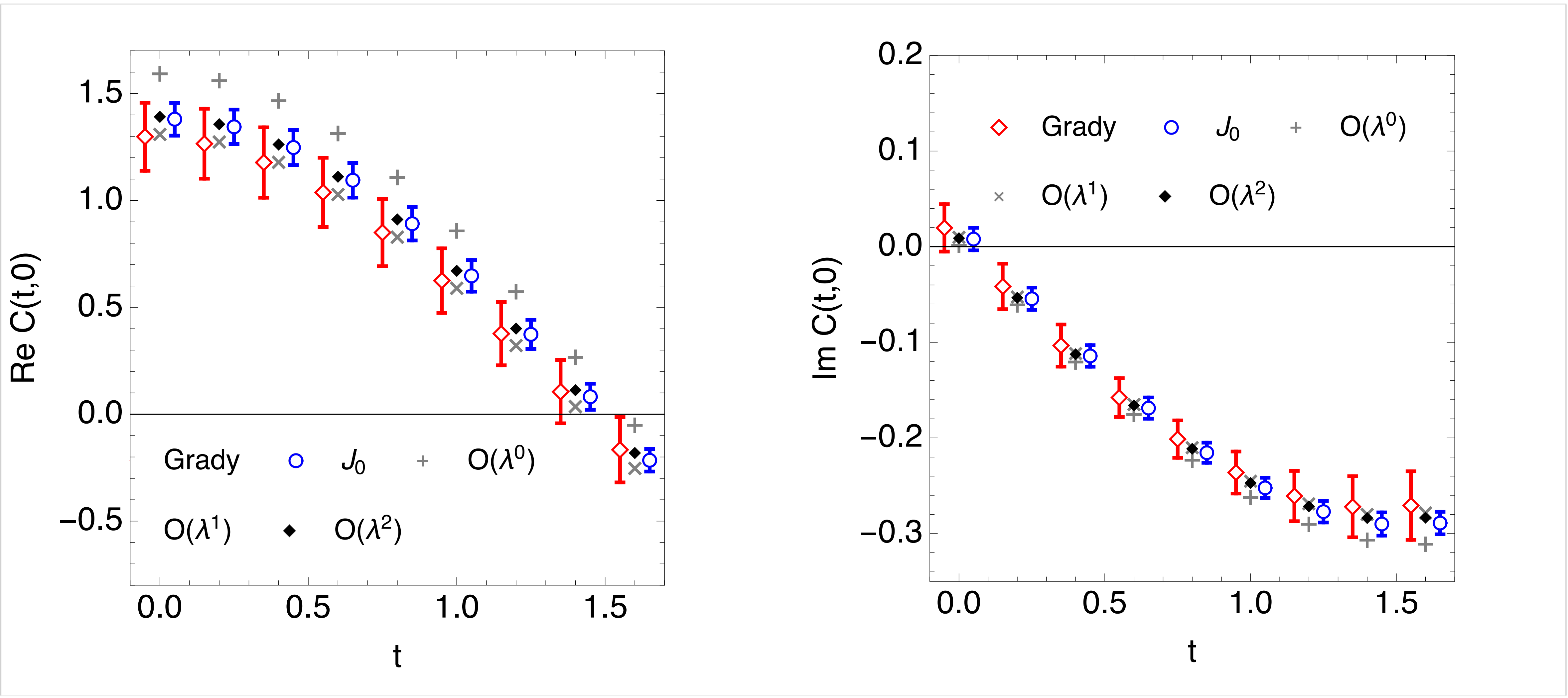
Grady method for the jacobian



$$J\eta = \tilde{\eta} \qquad \eta_{||} = J\,\mathrm{Re}\,\eta$$

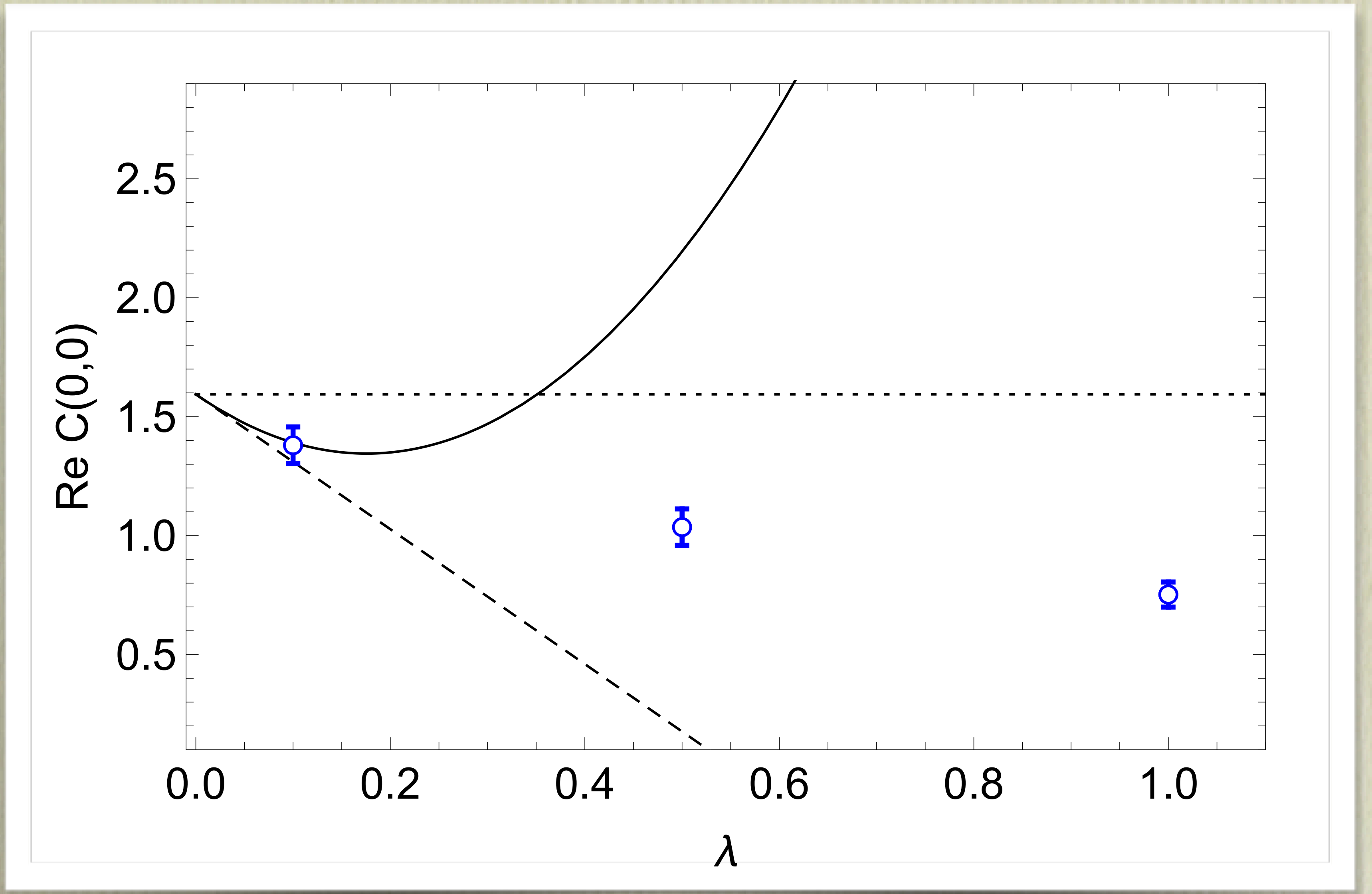
- isotropic proposal
- no need to compute det(J)

Real time physics (1+1D) weak coupling

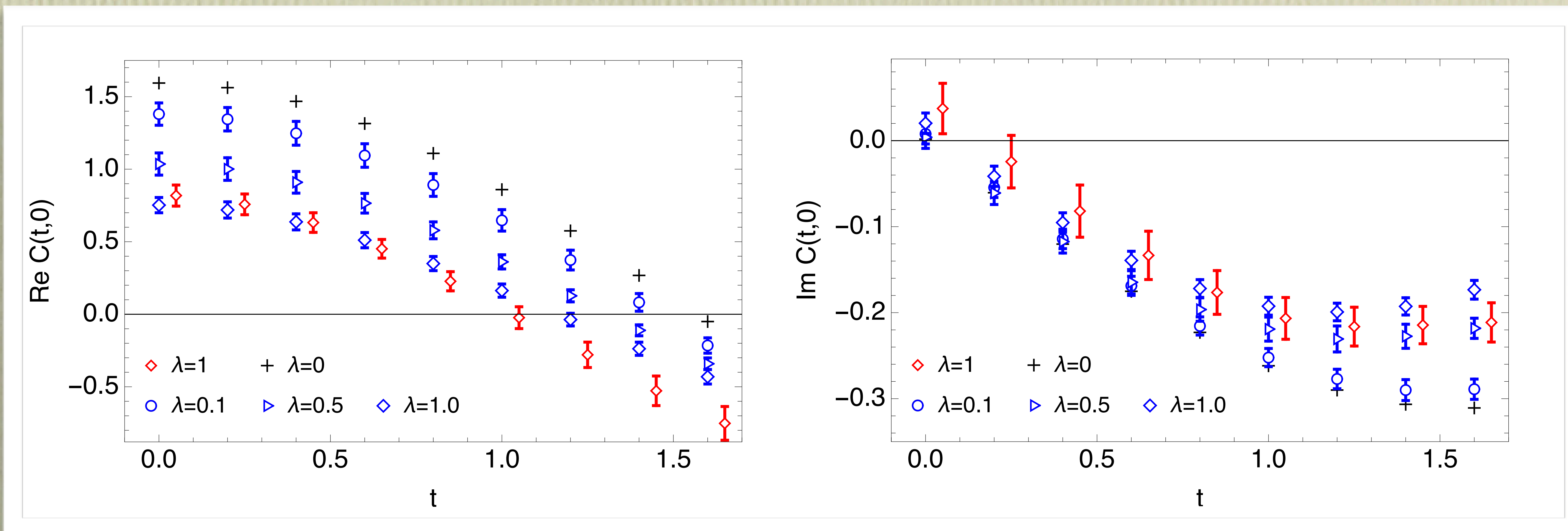


1+1D ϕ^4: n_t=8, n_x=8, n_β=2, λ=0.1

Real time physics (1+1D) perturbation theory

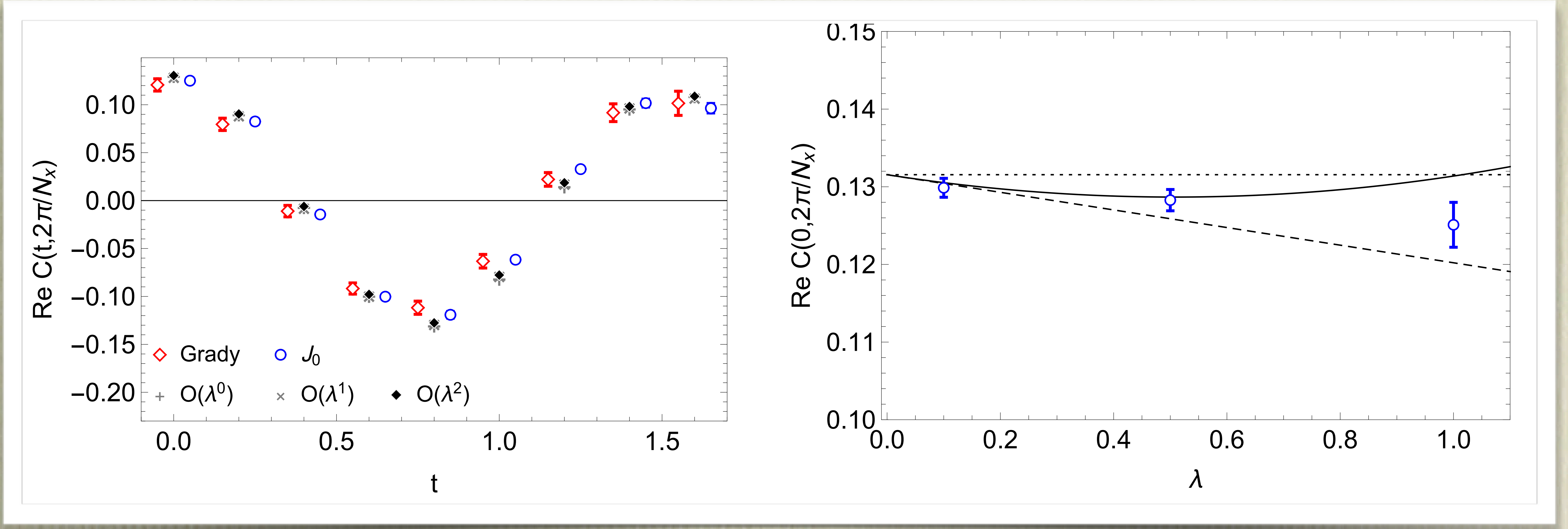


Real time physics (1+1D) strong coupling



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

Real time physics (1+1D) higher momenta



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

Conclusions

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

Outlook

- A number of challenges need to be overcome to attack large systems
  - hessian diagonalization for tangent manifolds — possible matrix-function projection.
  - fermion determinant and Jacobian evaluation — variants of pseudo-fermion algorithms.
  - sampling multi-modal distributions — tempered transition algorithm (Fukuma&Masafumi `17, Alexandru et al. `17)
  - flow integration for fermionic systems.

ECT* workshop

“**Simulating QCD on Lefschetz thimbles**”

Trento, Italy, June 28-30, 2017

Extra slides

The algorithm

$$P_{\text{acc}} = \min\{1, e^{-[S_R(z_{\text{new}}) - S_R(z_{\text{old}})]}\} \quad \text{(basic Metropolis)}$$

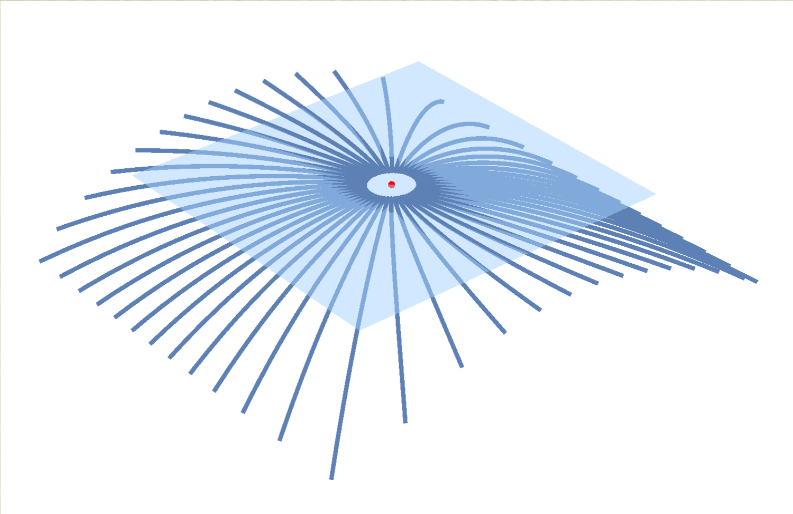
$$P(z_{\text{old}} \to z_{\text{new}}) = P(z_{\text{new}} \to z_{\text{old}})$$

How to stay on the thimble?

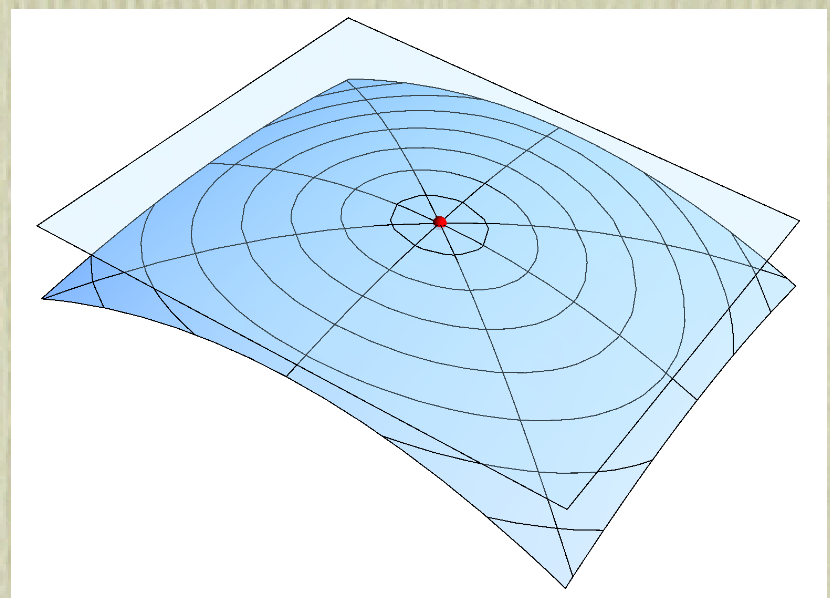
- assume thimble to be Gaussian
- do complicated to and fro integration (HMC, Aurora, etc)
- use a map

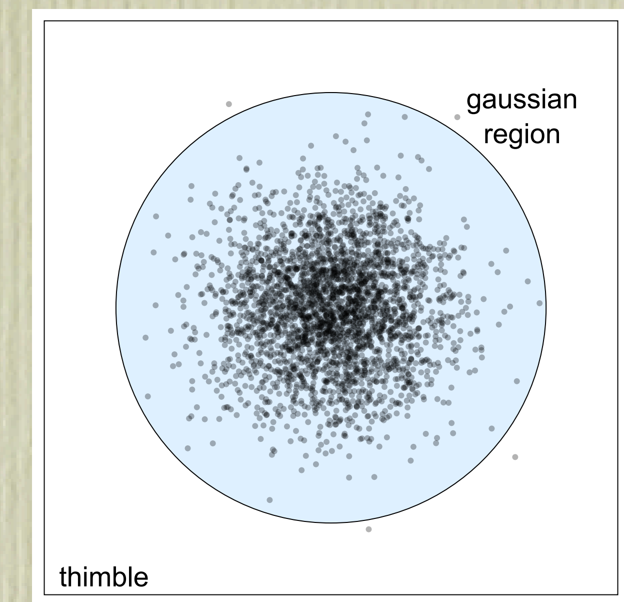
$$\frac{dz}{d\tau} = \overline{\frac{dS}{dz}} \quad \text{(upward flow – stable)}$$

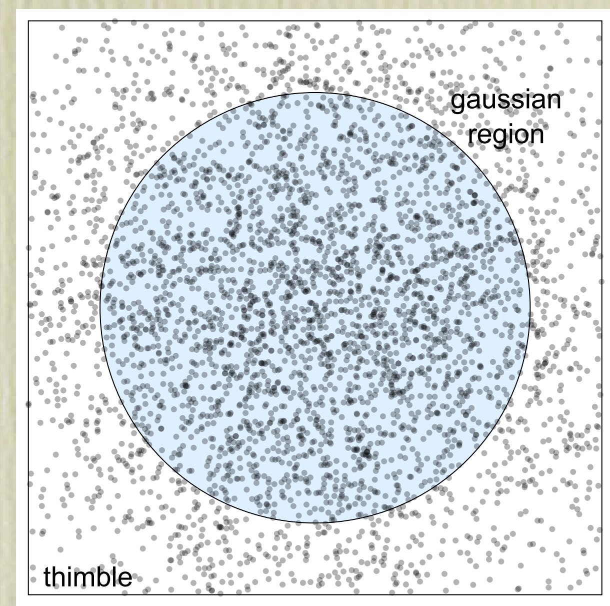
$$\frac{dz}{d\tau} = -\overline{\frac{dS}{dz}} \quad \text{(downward flow – unstable)}$$



The algorithm

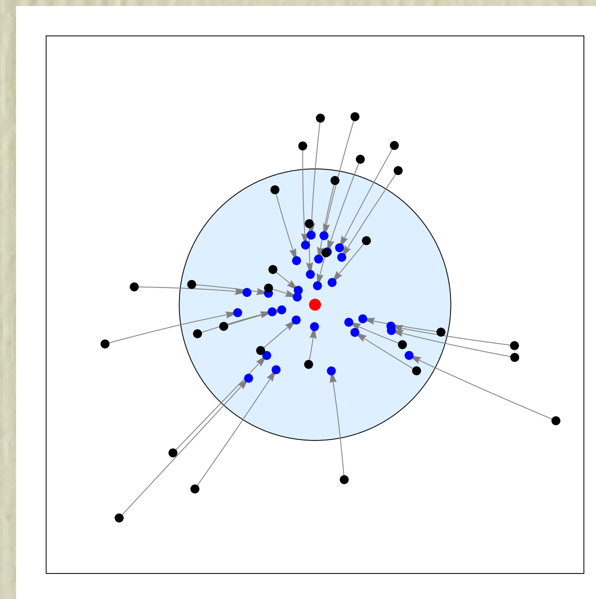


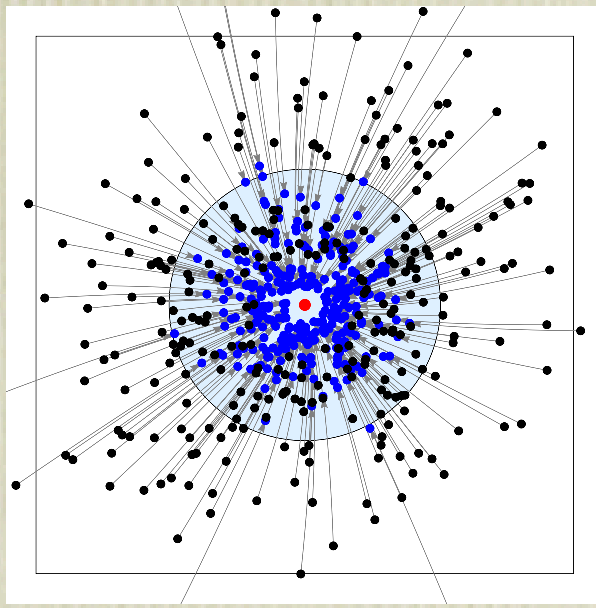




good

bad





f is a contraction map

f : thimble $\to$ thimble

$z_{\text{far}} \to z_{\text{near}} = f(z_{\text{far}})$

$P(z_{\text{far}})(\text{bad}) \to \tilde{P}(z_{\text{near}})(\text{good})$

The algorithm

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

$$z_n = f(z_f) \,, \quad z_f = f^{-1}(z_n)$$

$$\left\| \frac{dz_f}{dz_n} \right\| = \det \frac{\partial (f^{-1})_i}{\partial (z_n)_j}$$

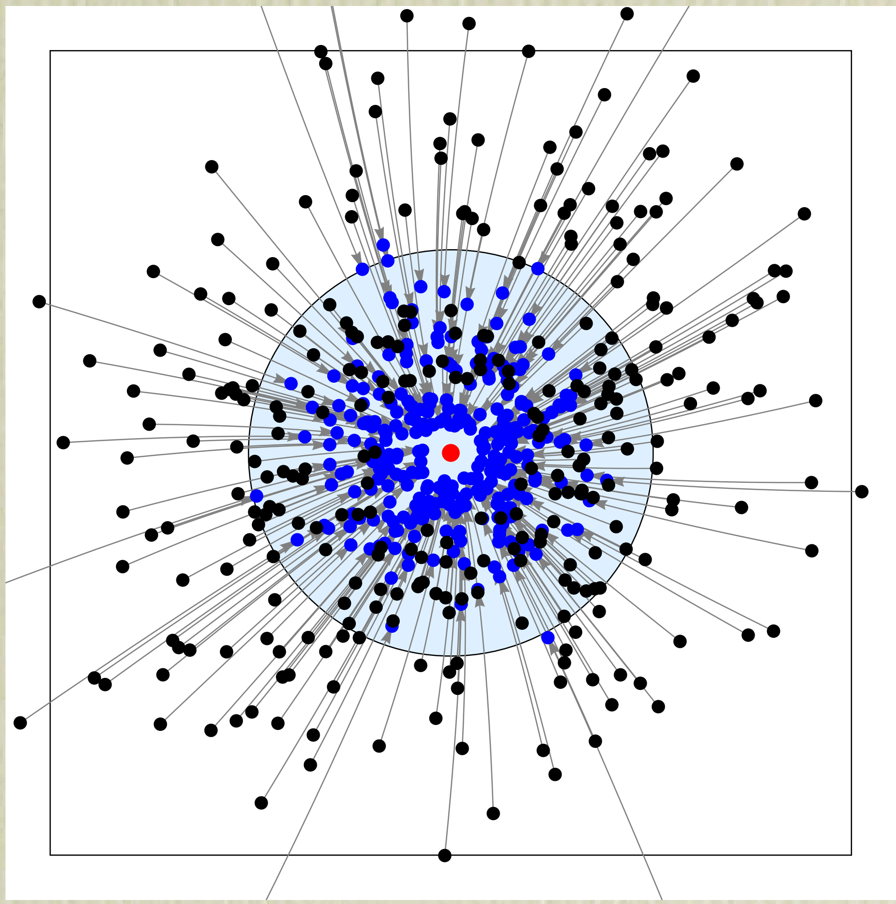
f is the downward flow

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

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

f^{-1} is the upward flow

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



The algorithm

Basic Metropolis

- Propose new config such that $P(z_{\text{old}} \to z_{\text{new}}) = P(z_{\text{new}} \to z_{\text{old}})$
- Accept/reject using $P_{\text{acc}} = \min\{1, \exp(-\Delta S_{\text{eff}})\}$
- The effective action includes the Jacobian of the map

$$S_{\text{eff}}(z_n) = S_R(z_f) - \log\det J \quad \text{with} \quad z_f = f^{-1}(z_n)\,.$$

- Both z_f and J are computed using the upward (stable) flow

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

A. Mukherjee, M. Cristoforetti, and L. Scorzato, *Metropolis Monte Carlo integration on the Lefschetz thimble*, Phys. Rev. D88 (2013)

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

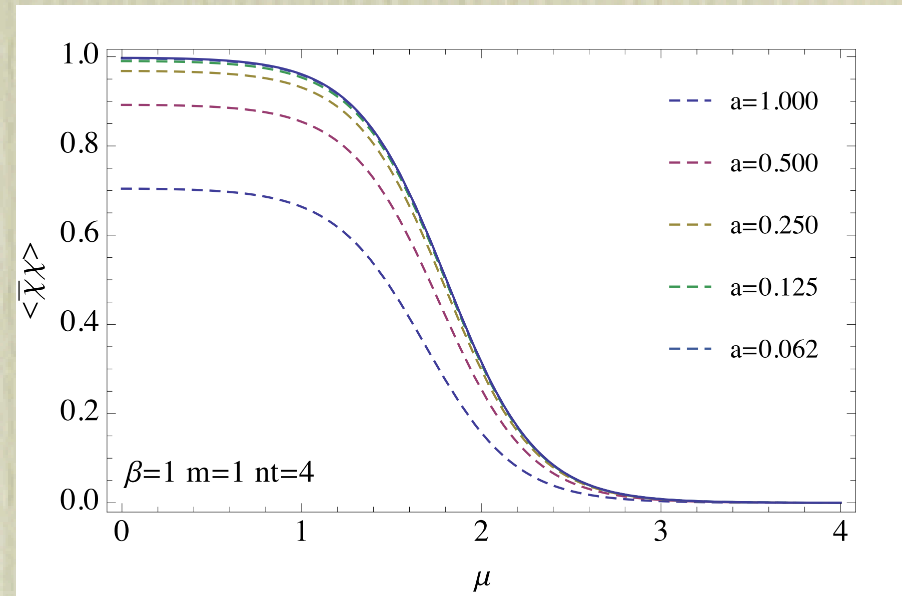
Thirring model 0+1

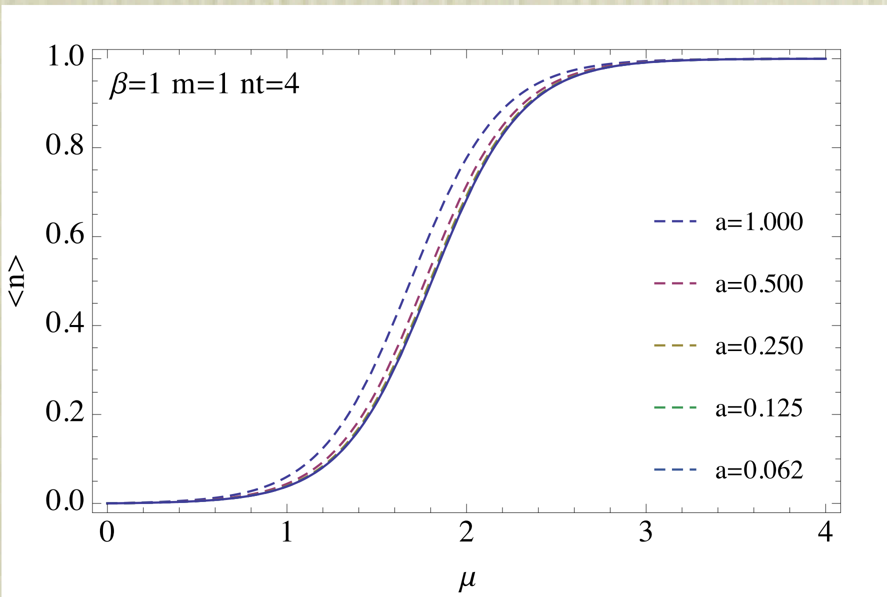
- The action can be computed analytically and the condensate is:

$$\langle \bar{\chi}\chi \rangle = \frac{1}{N}\frac{\partial Z}{\partial m}$$

- Staggered fermions imply that the model represents a system with 2 species of fermions at one site.

- Reverse engineering the action allows you to determine the energy of the four levels and define a continuum limit for the system.





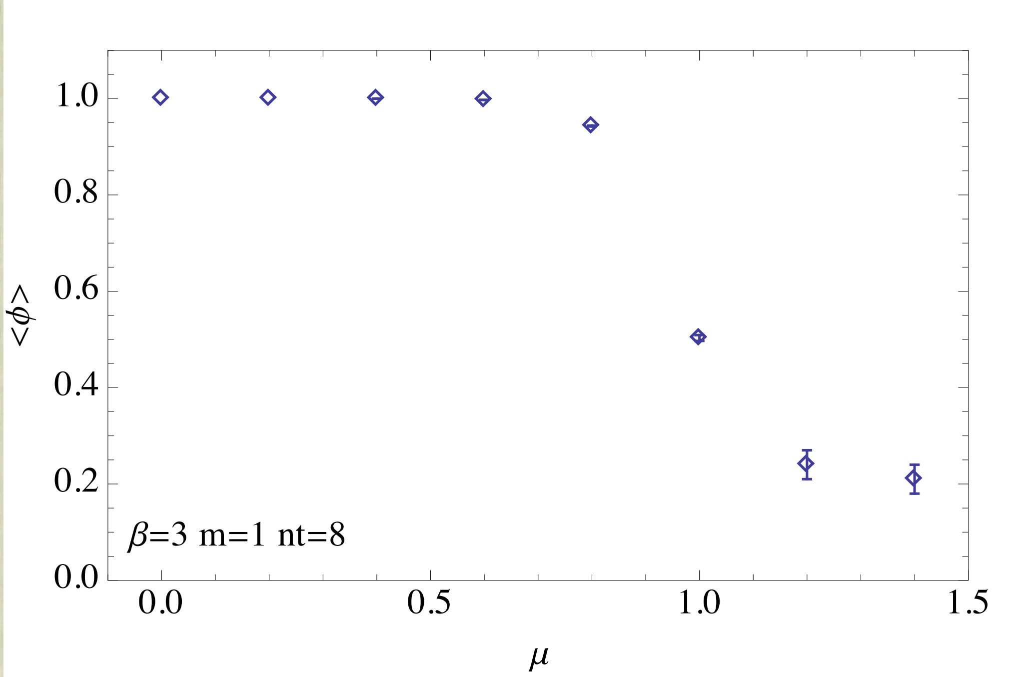
Thirring model 0+1

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

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

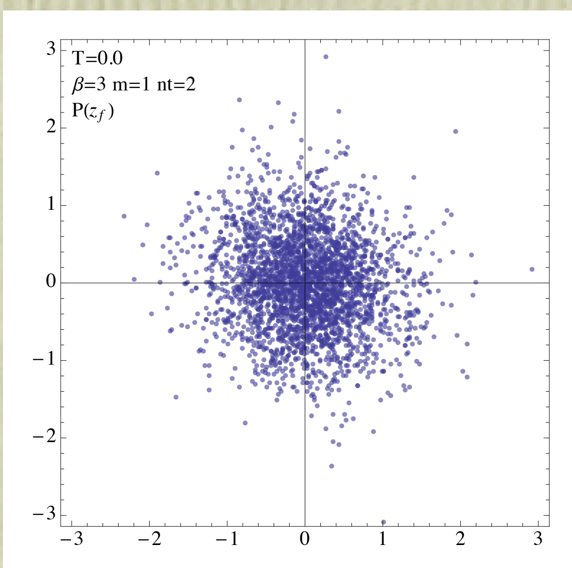
$$\langle O \rangle = \frac{\langle O\phi \rangle_0}{\langle \phi \rangle_0}$$

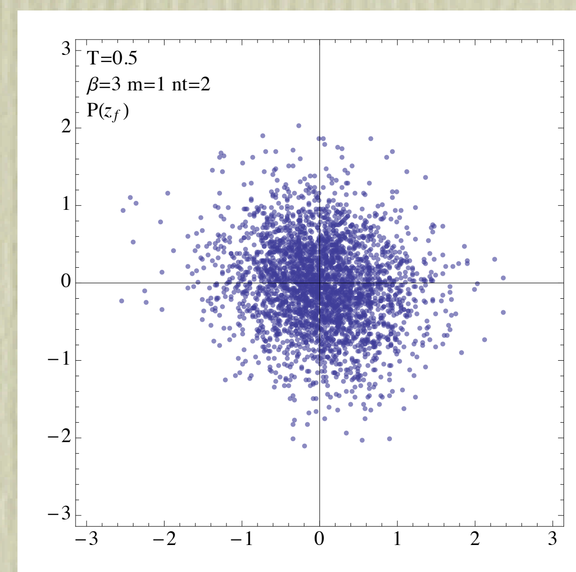
$$\langle \cdot \rangle_0 \propto e^{-S_g} |\det K| \quad \phi = \frac{\det K}{|\det K|}$$

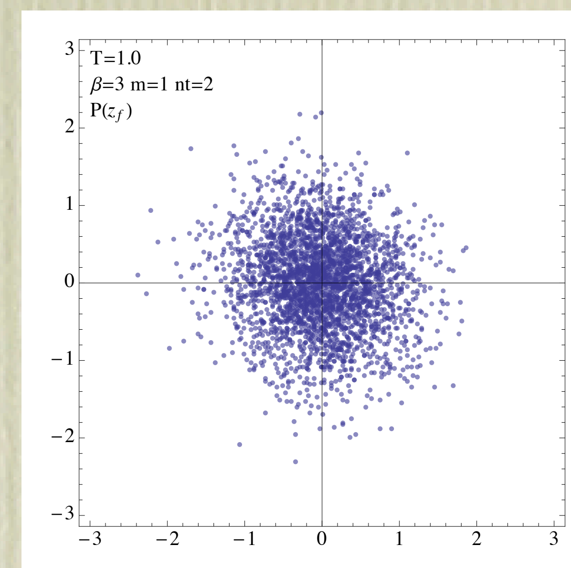


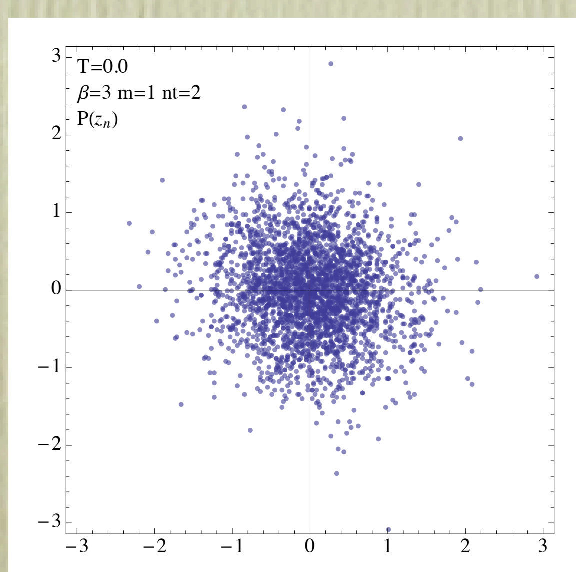
Numerical results

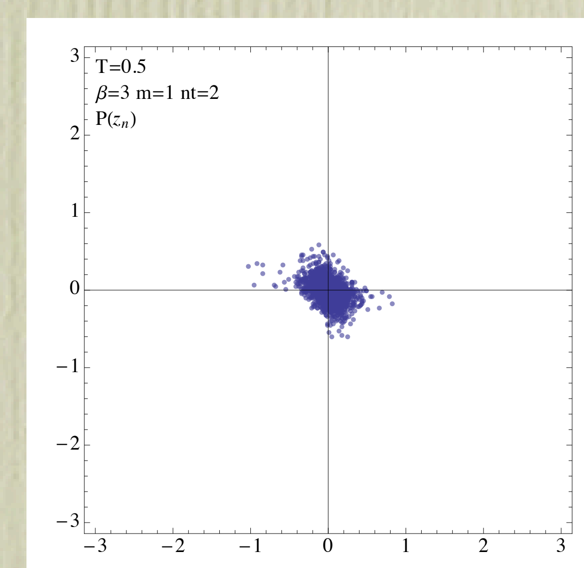
Algorithm check

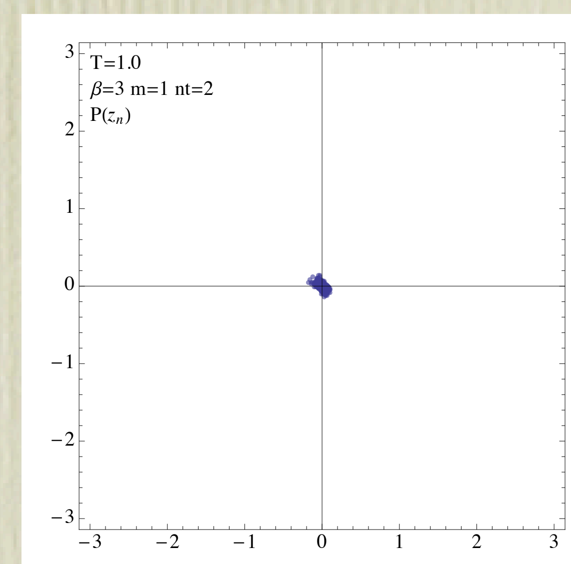




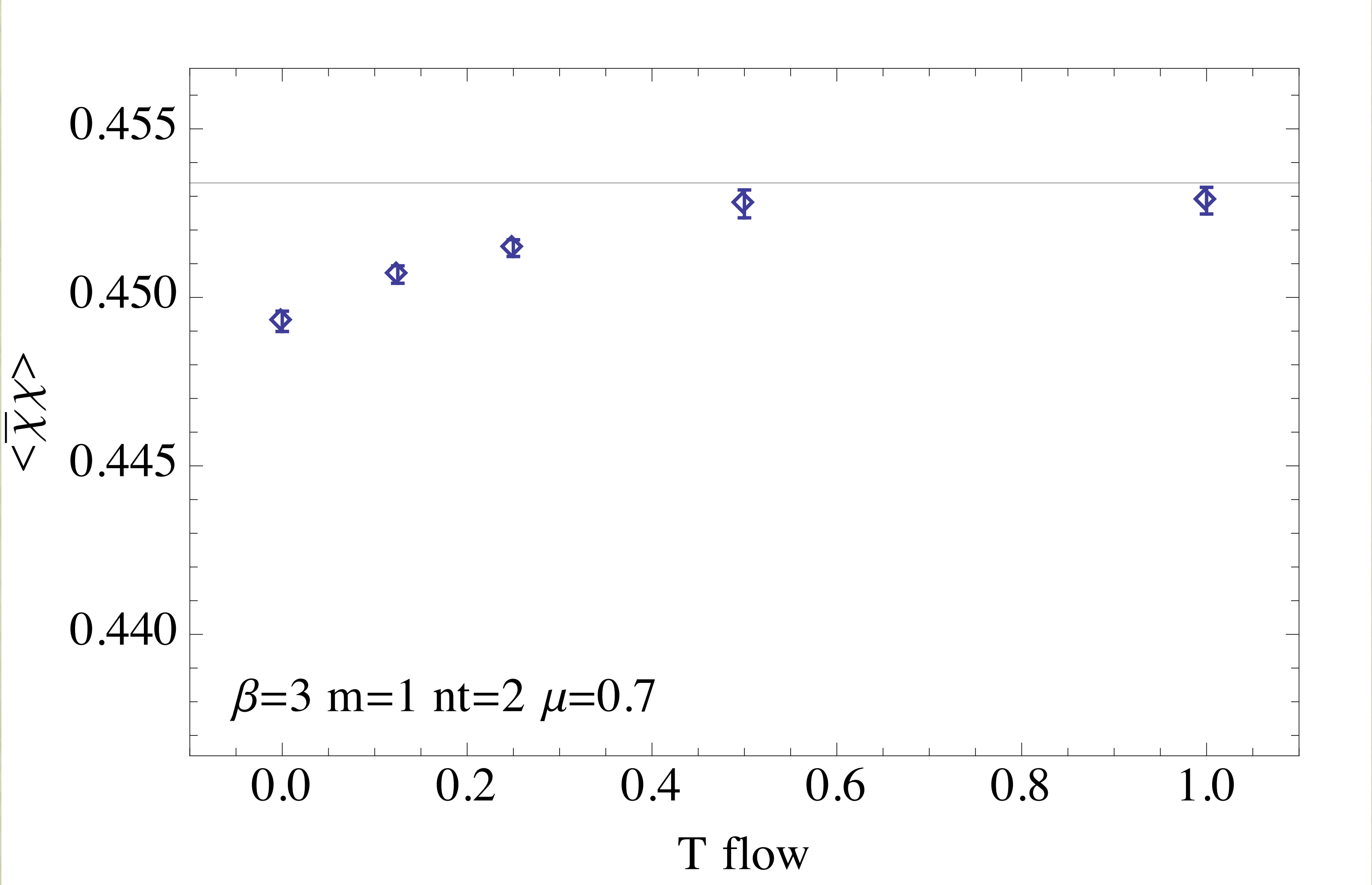




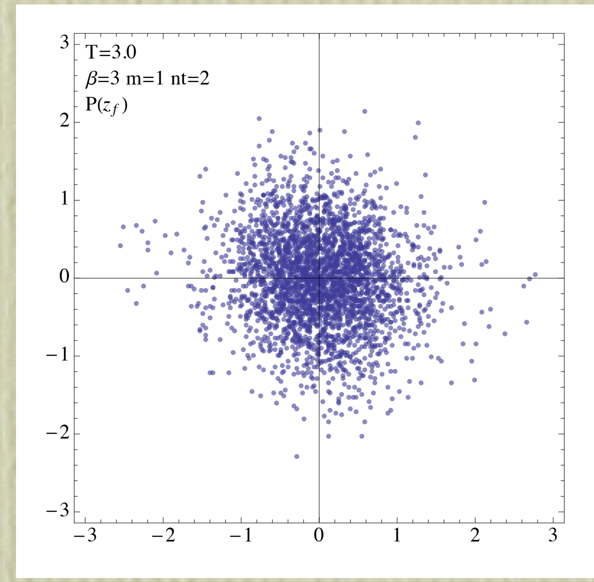


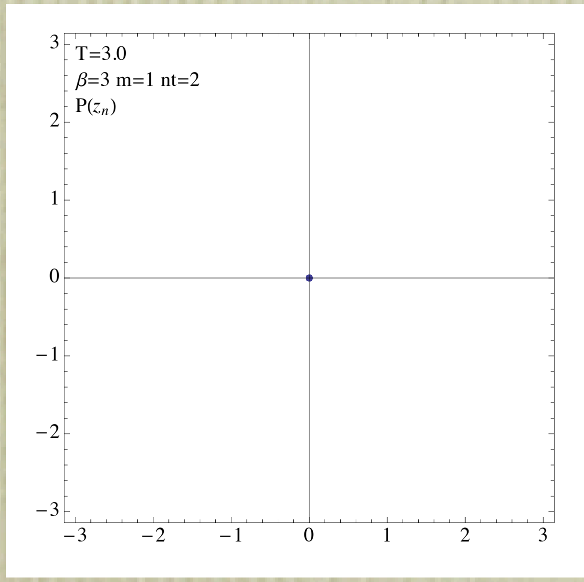


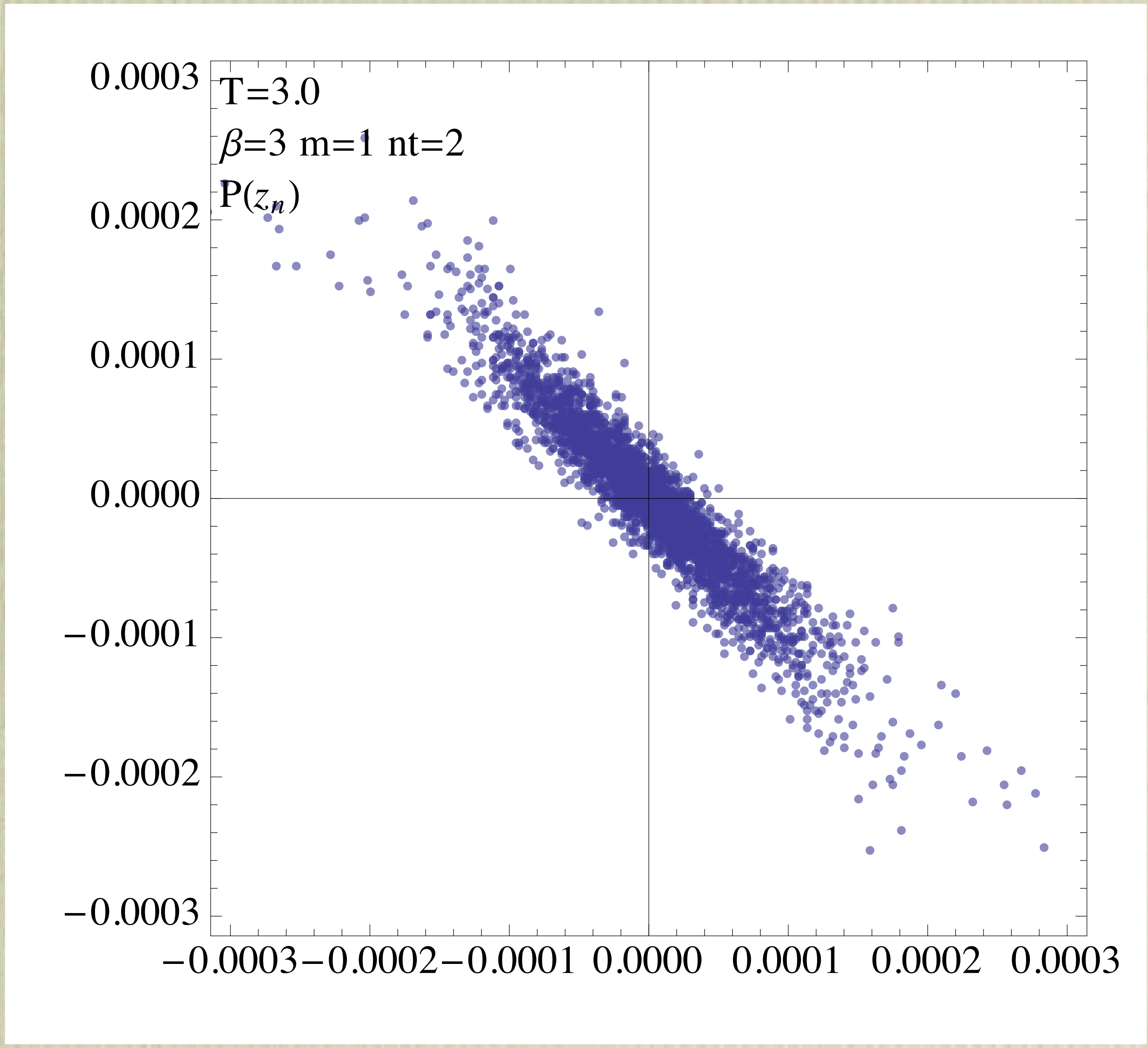
Algorithm check



Anisotropic proposals





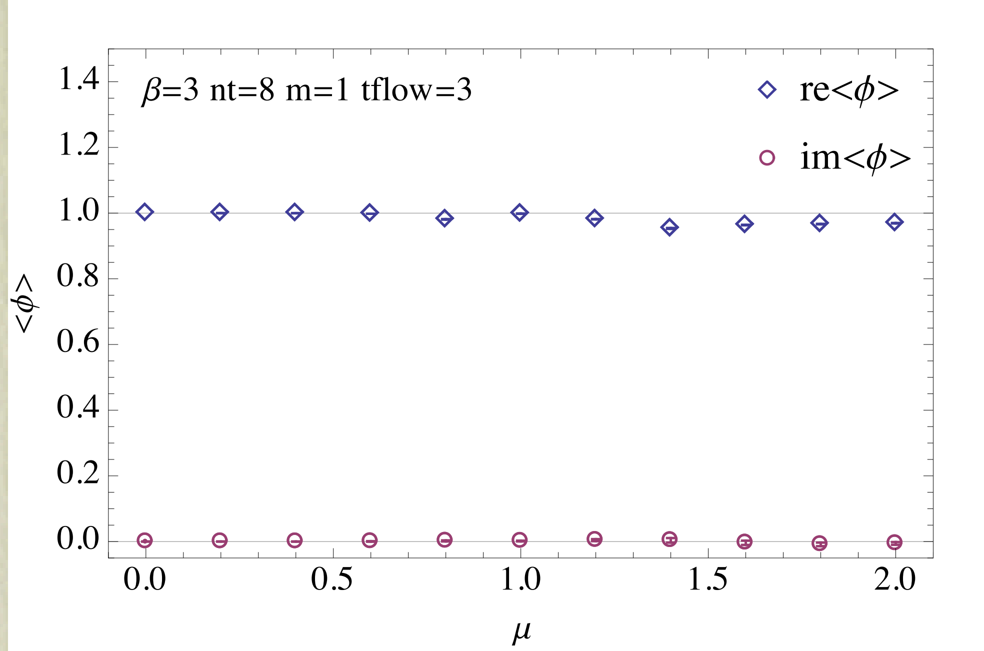


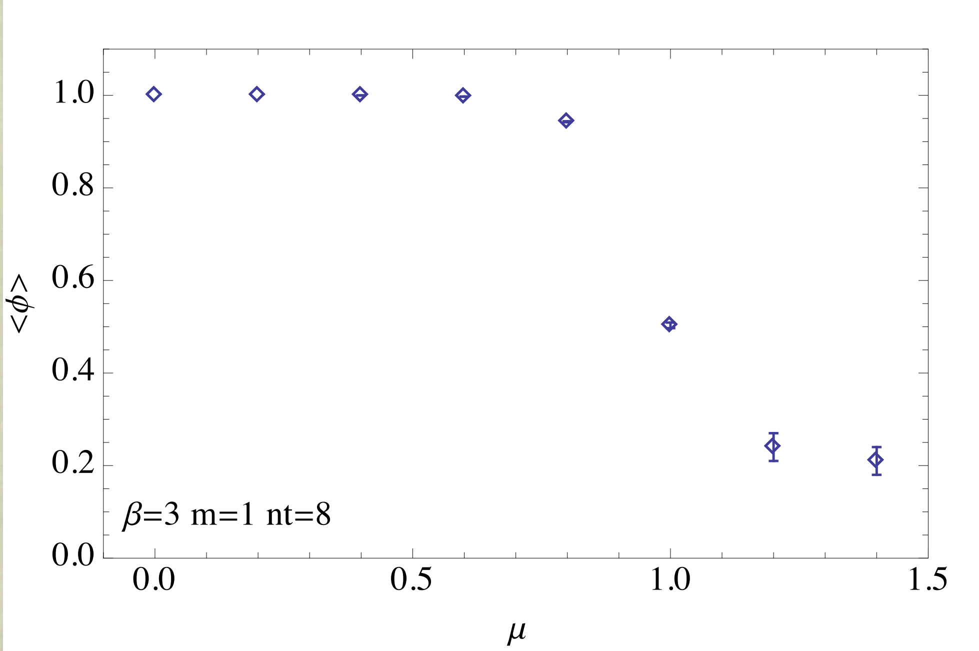
Residual phase

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

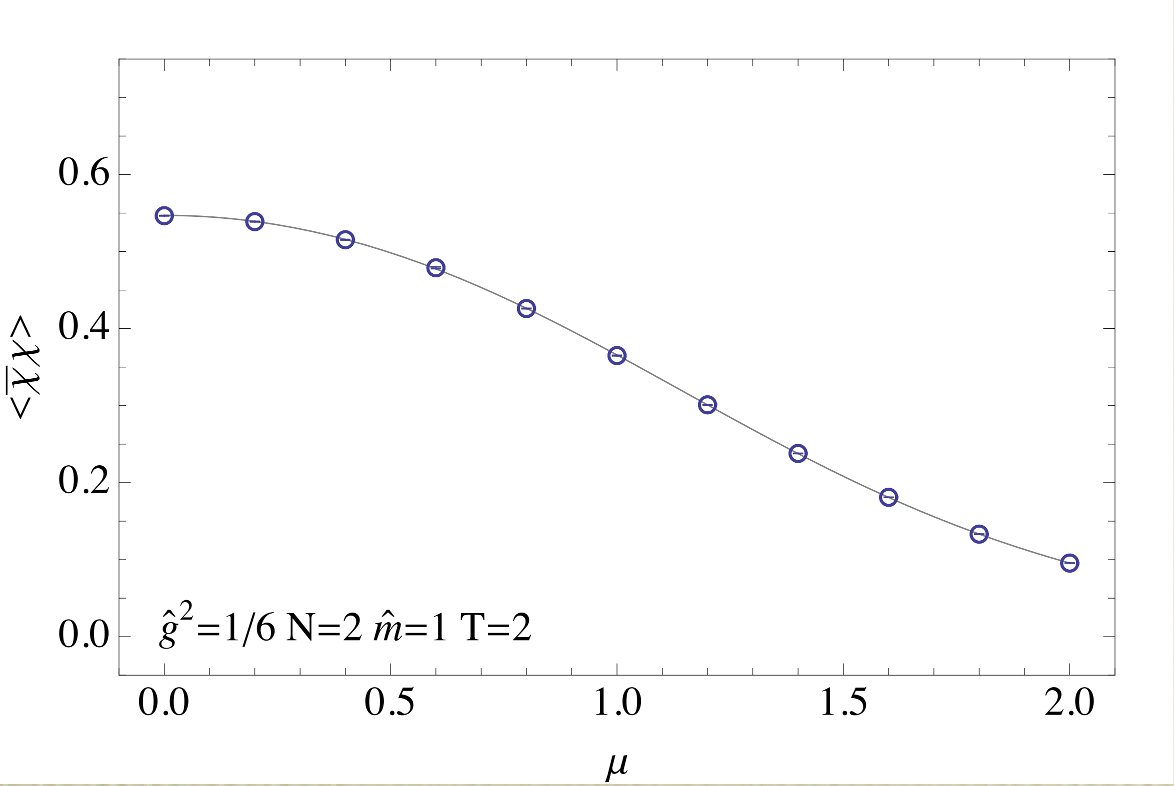
$$S_{\text{eff}} = S_R - \log|\det J|\,.$$

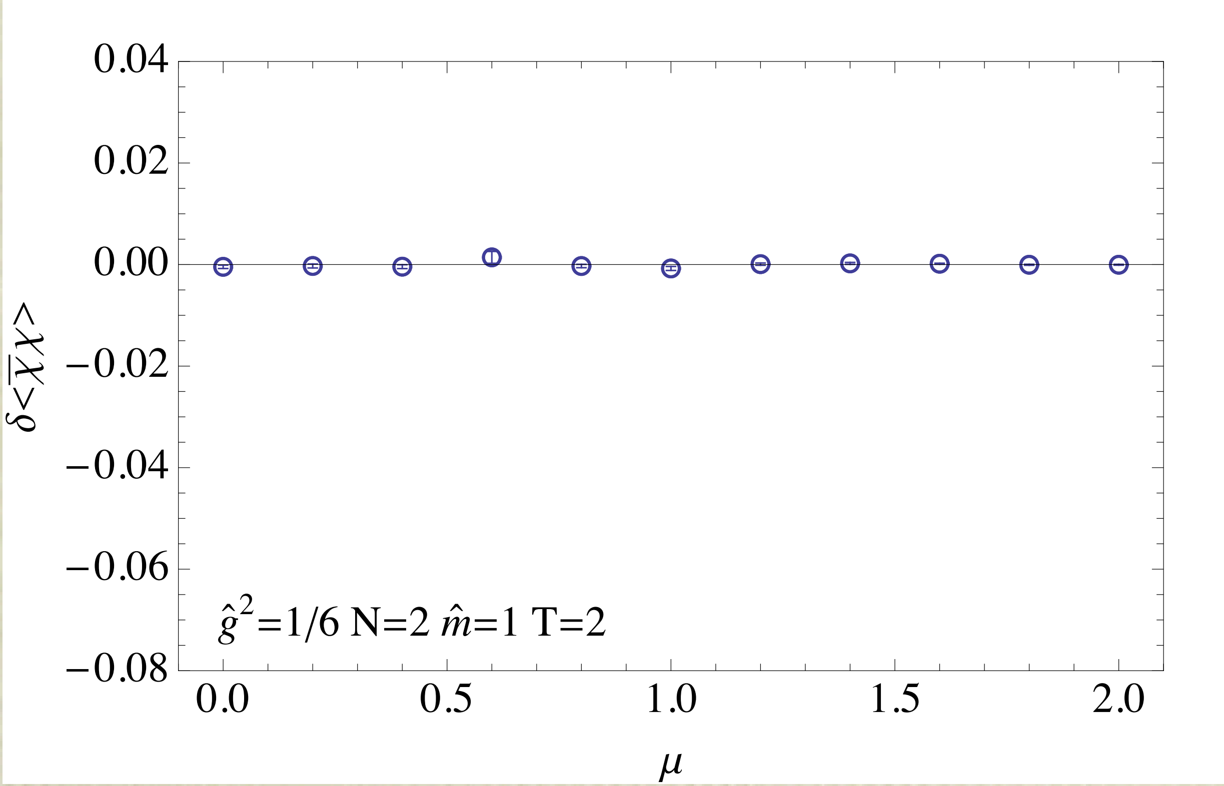
- The residual phase $\phi = \det J/|\det J|$ is folded in the observable.
- This is *not* the same phase as in the phase quenched theory.
- The sign fluctuations of the residual phase are observable but mild in our model.



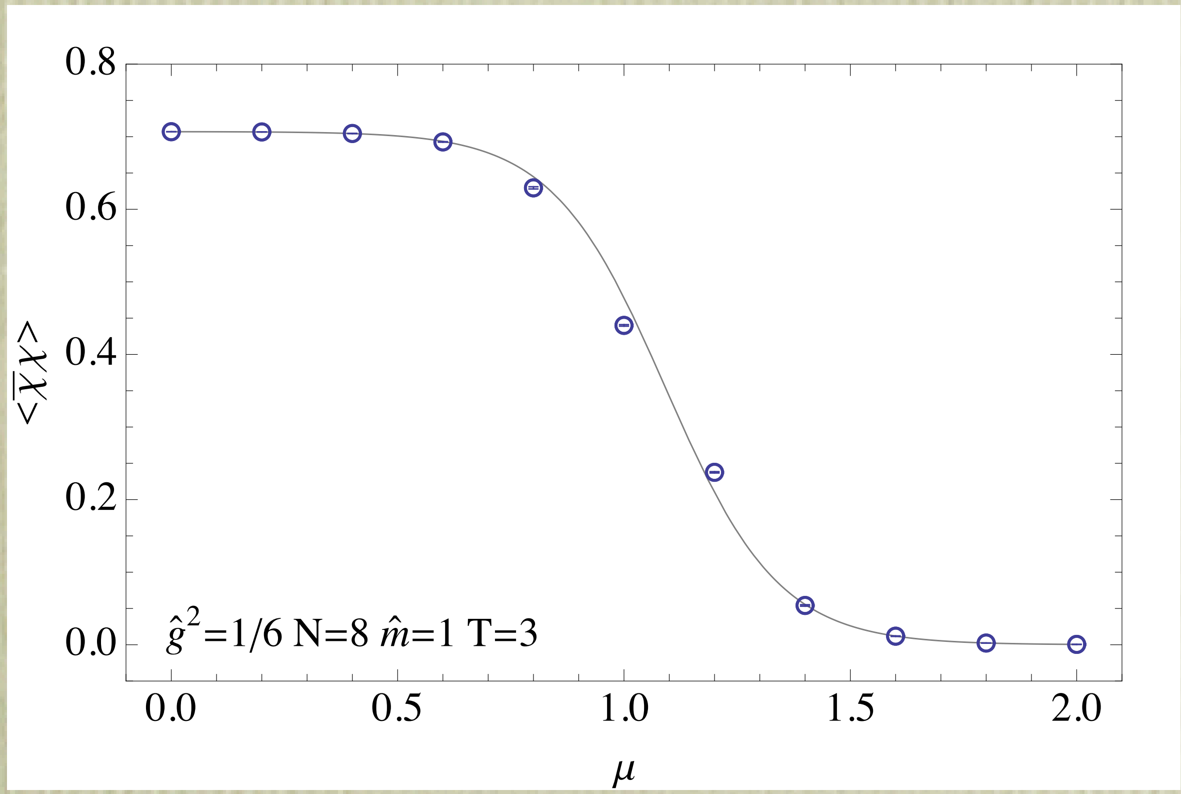


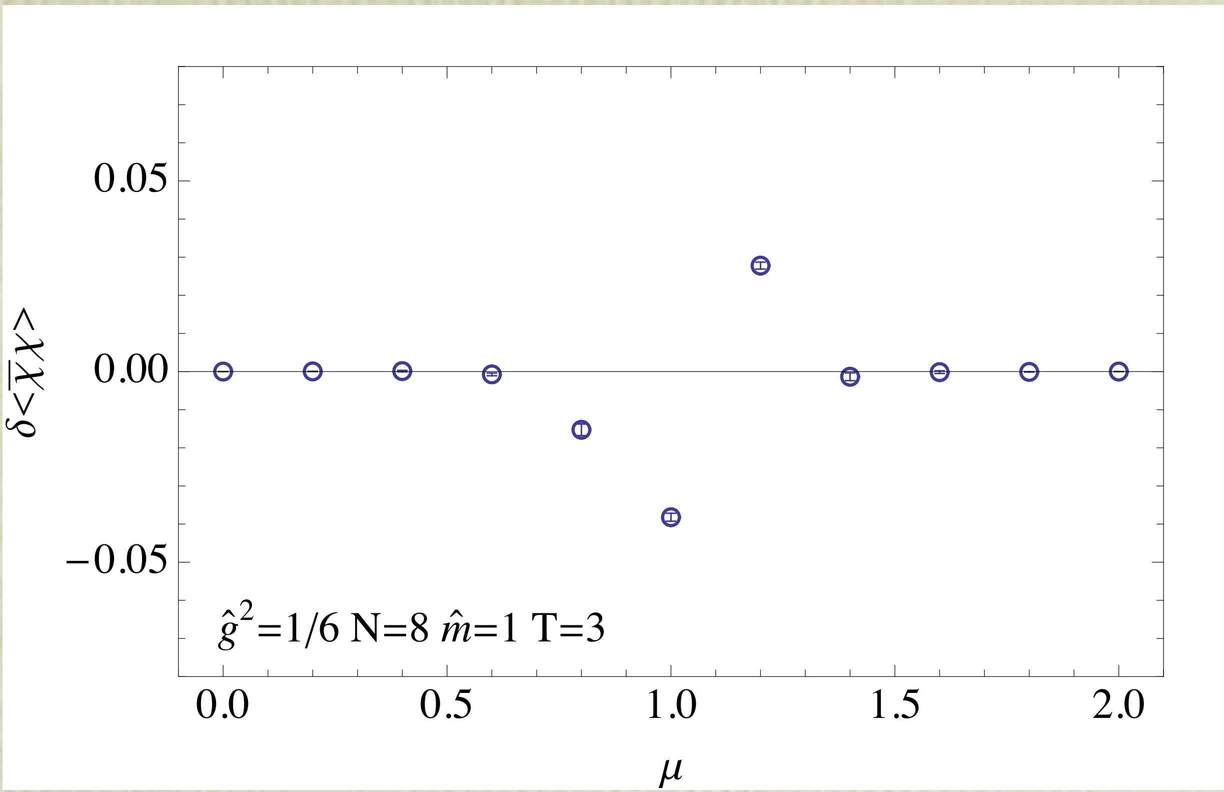
Weak coupling



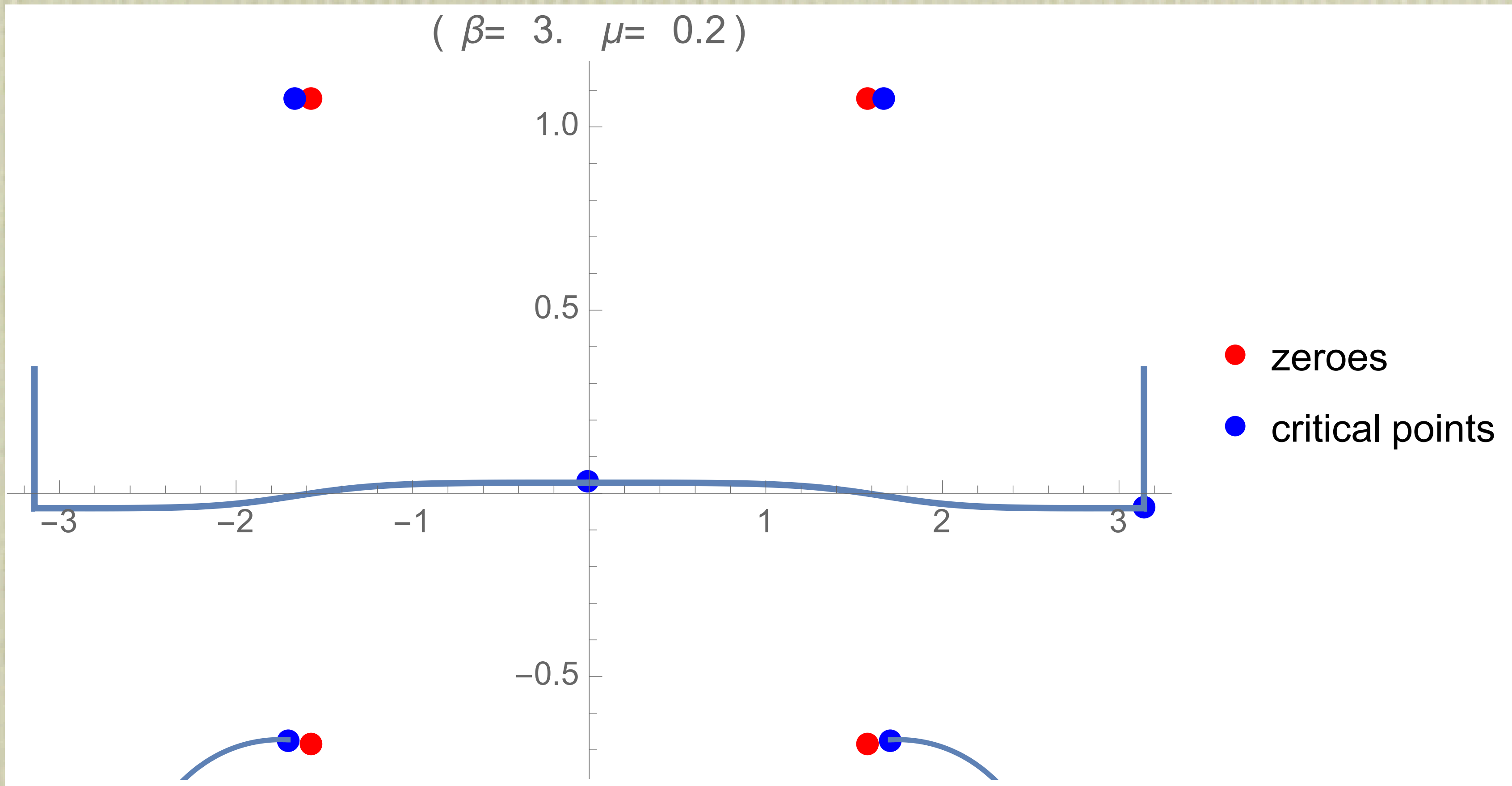


Weak coupling (low temp)

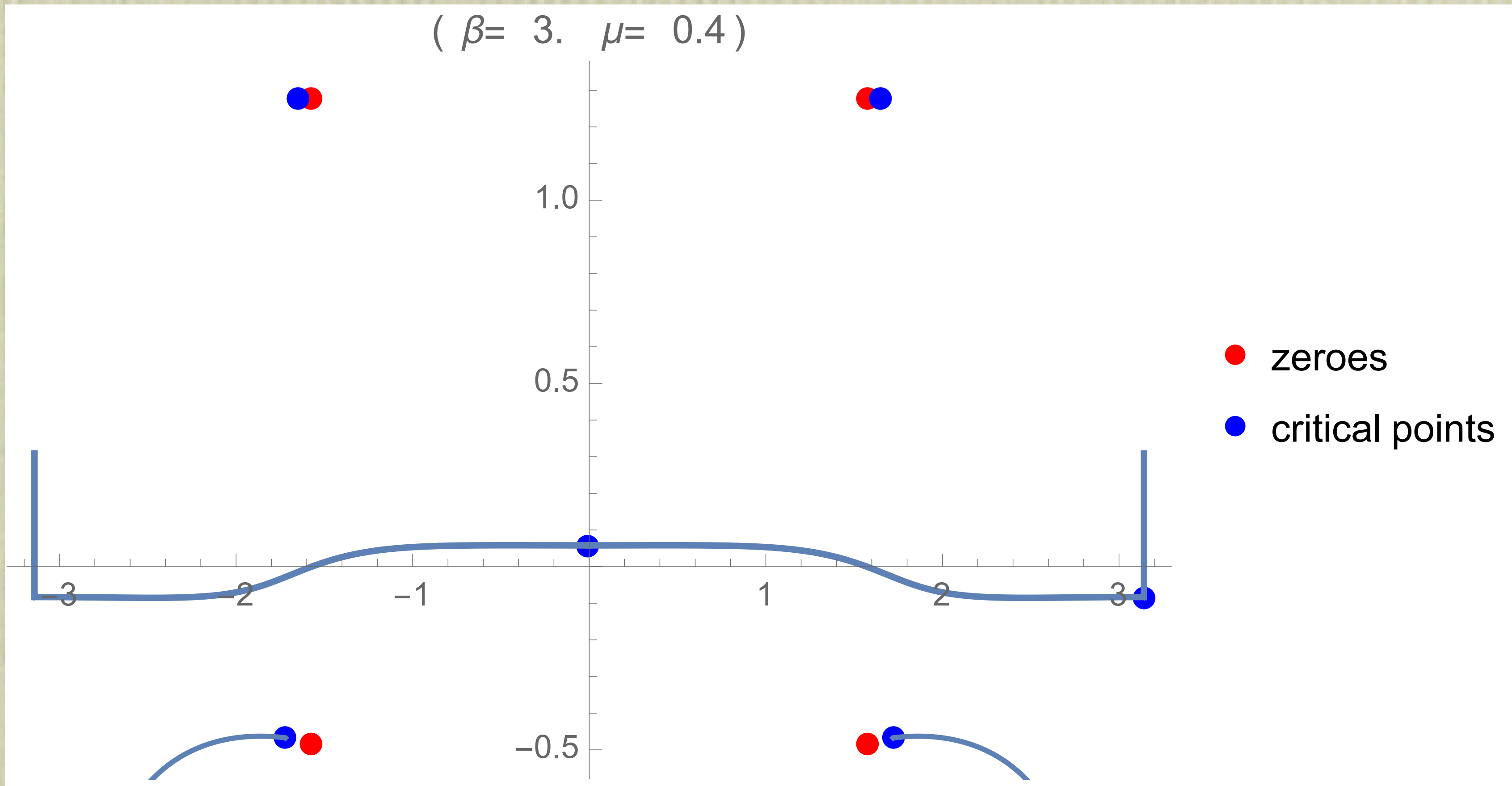




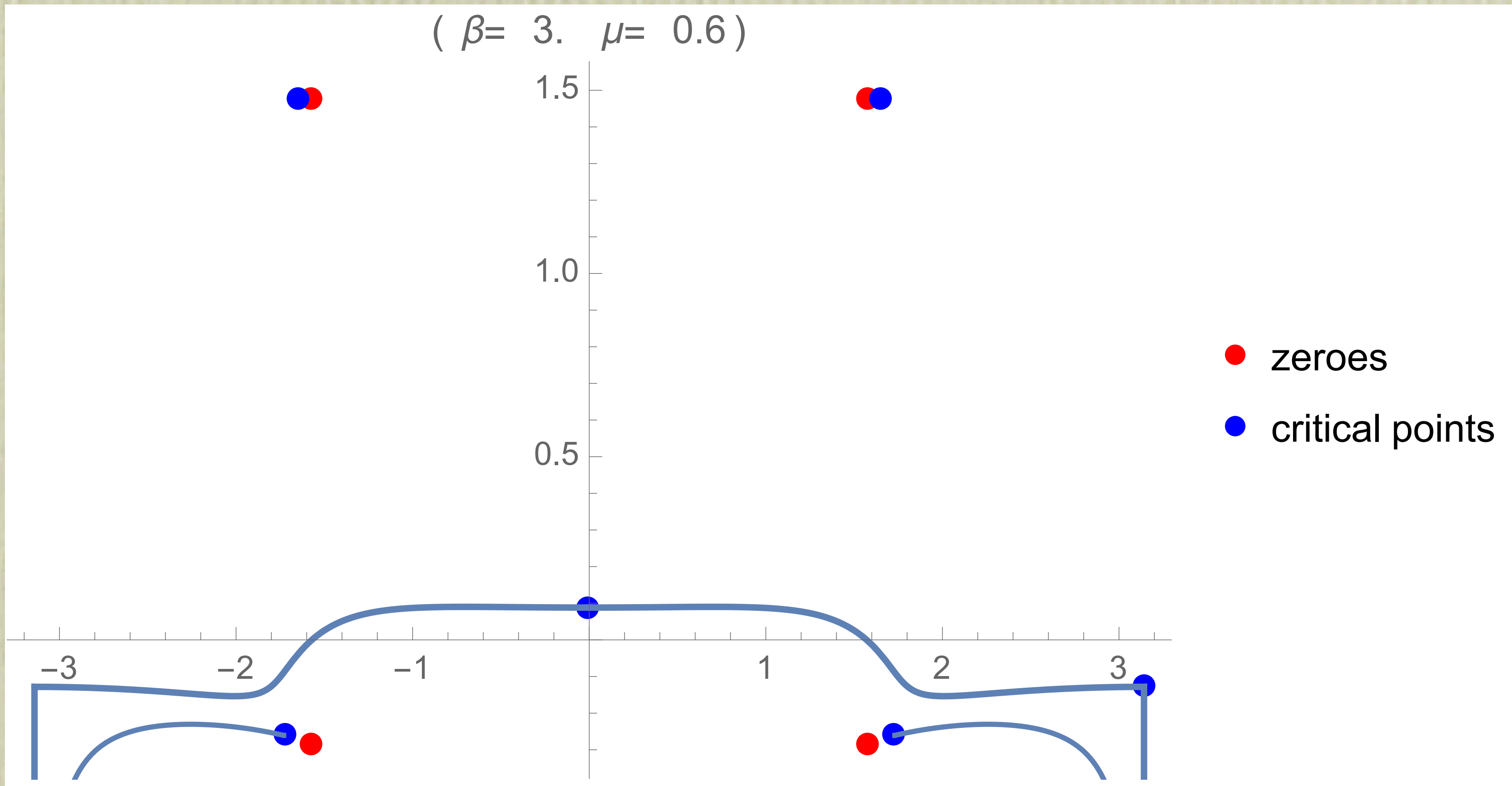
Thimble contributions



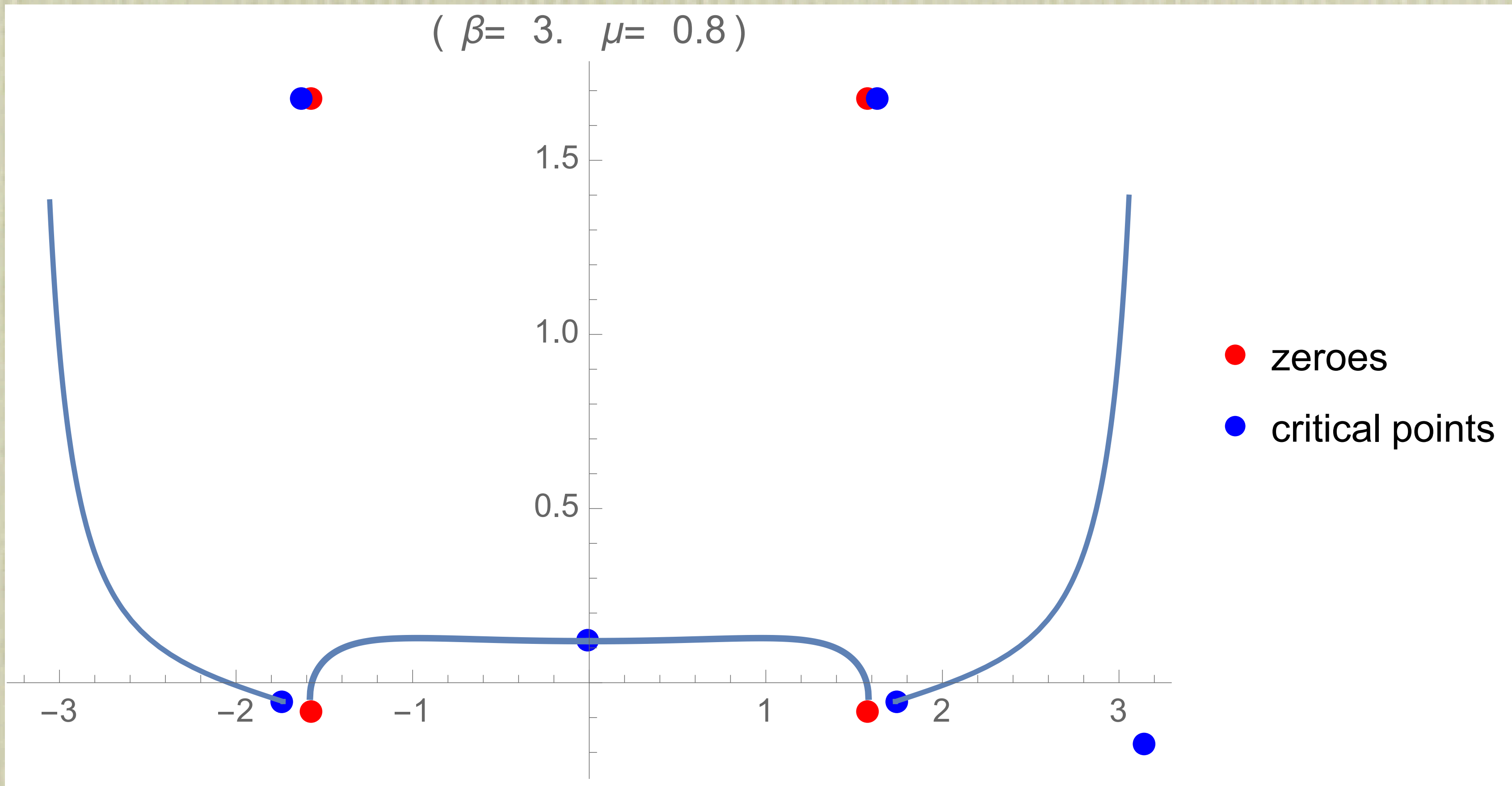
Thimble contributions



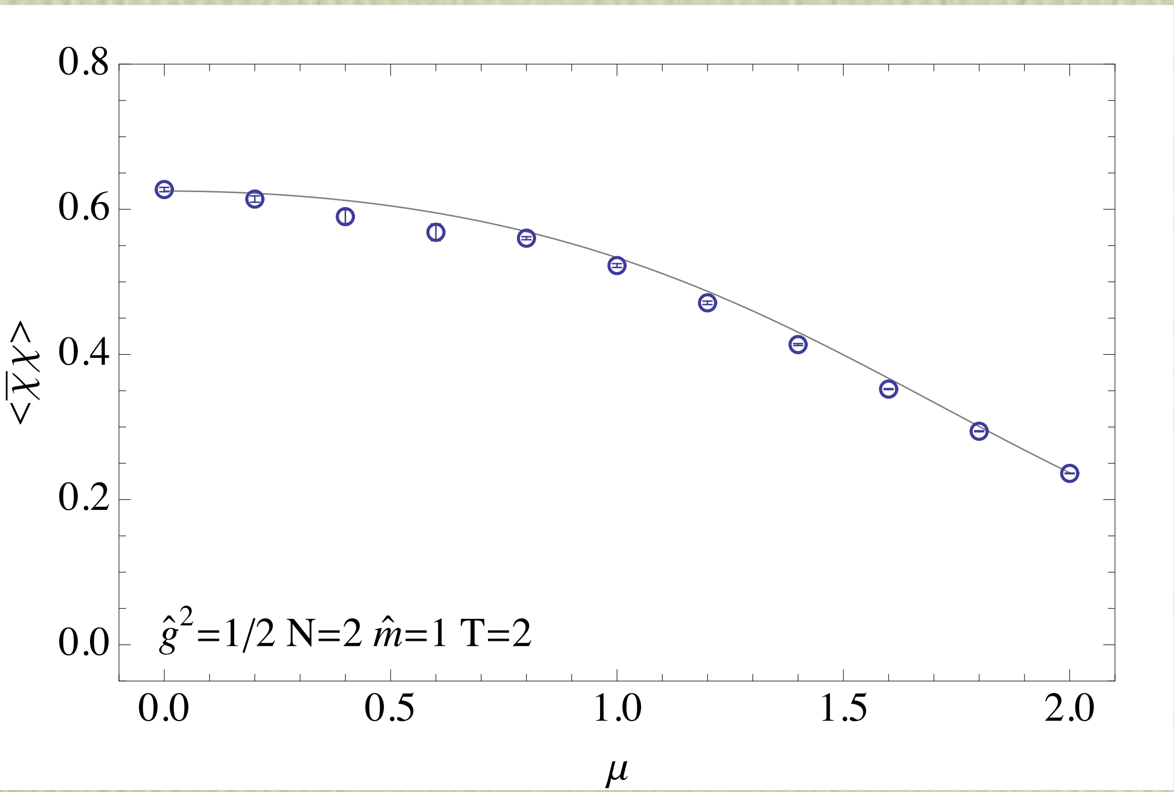
Thimble contributions

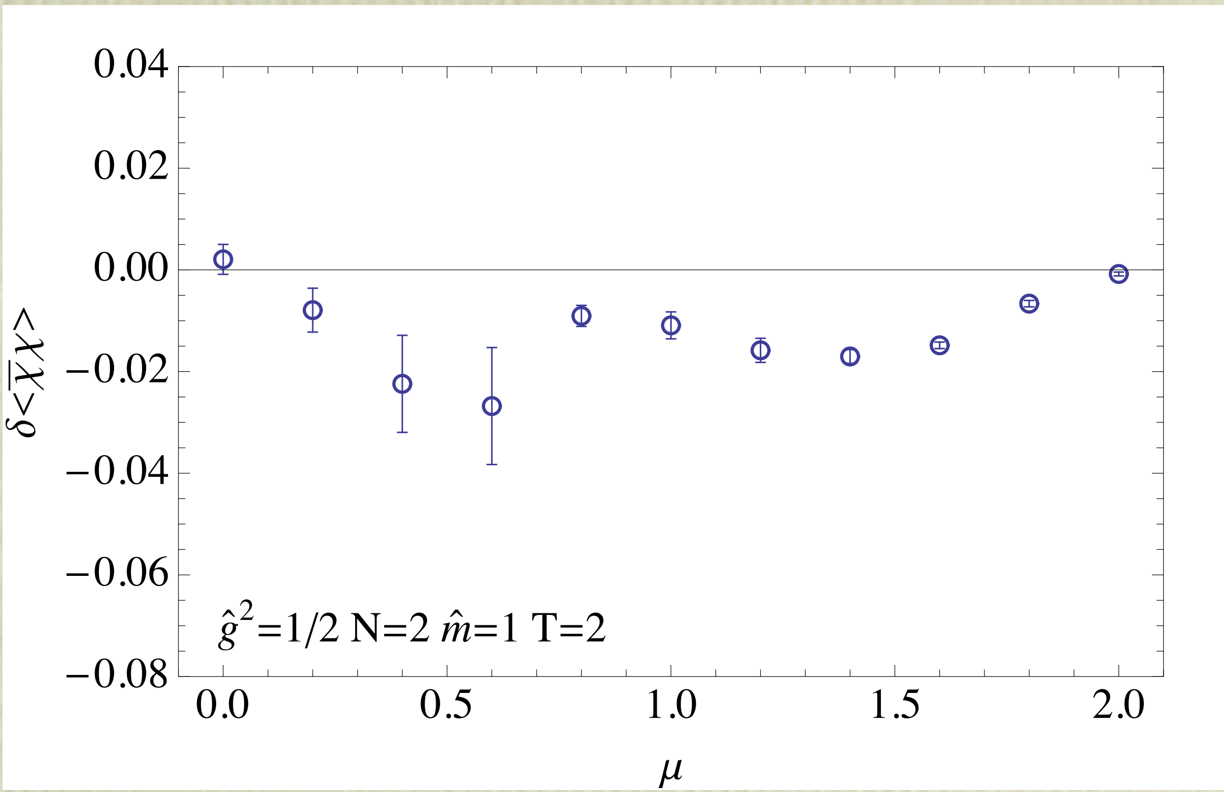


Thimble contributions

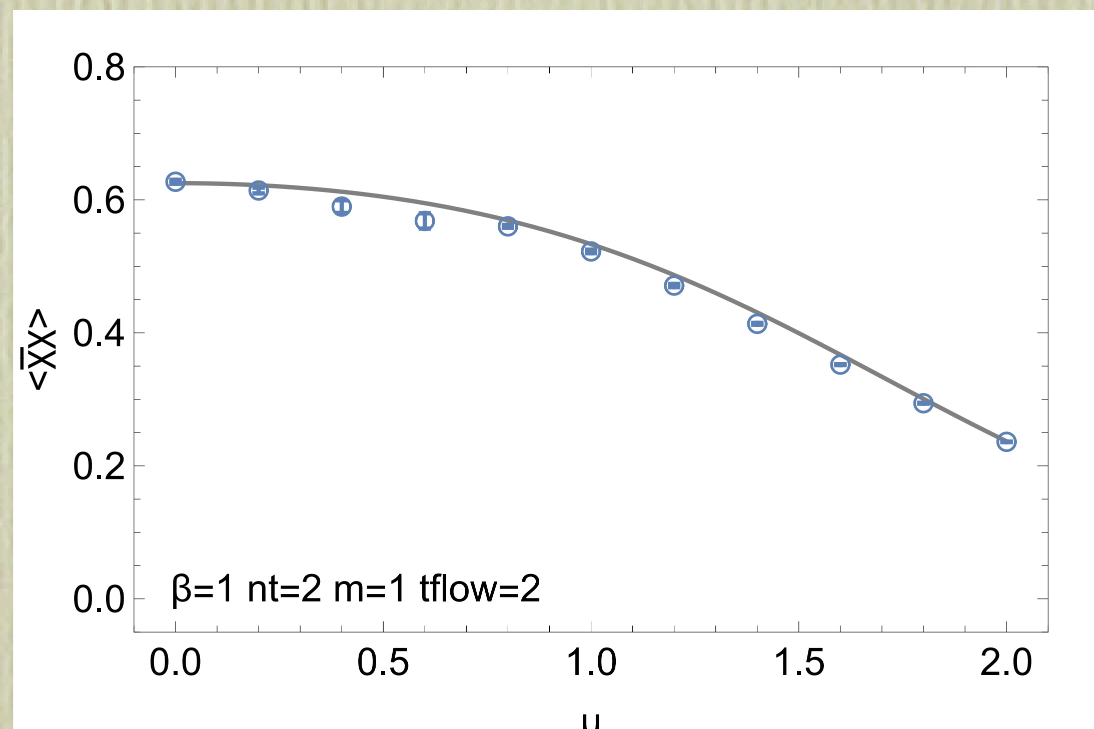


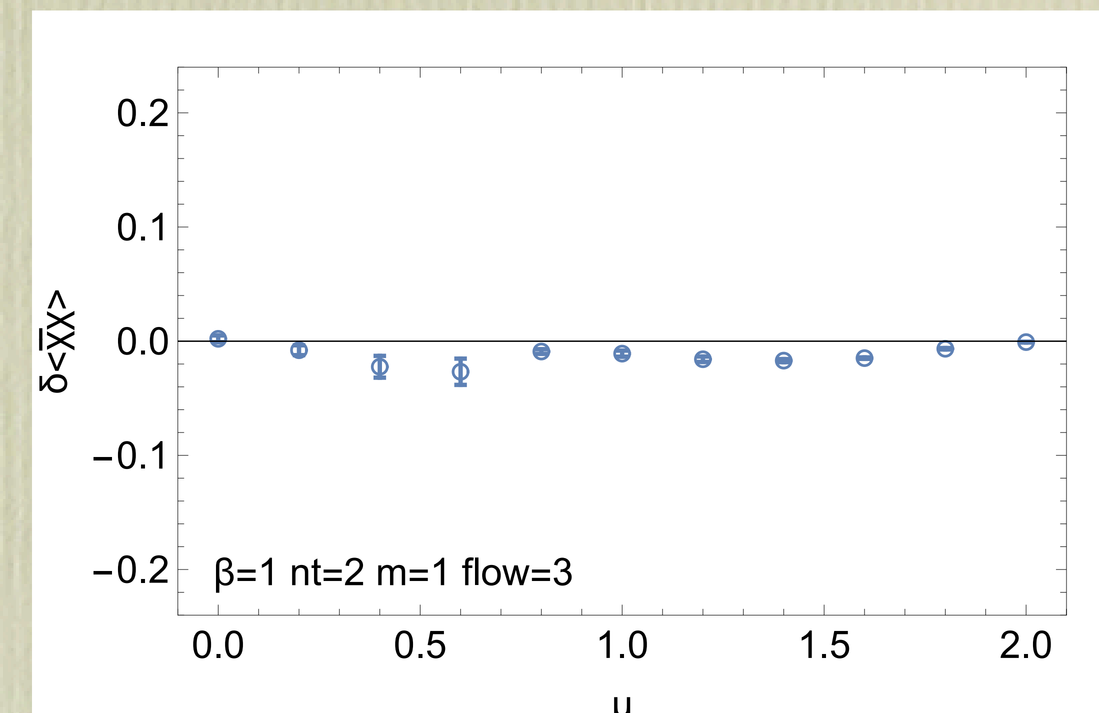
Strong coupling

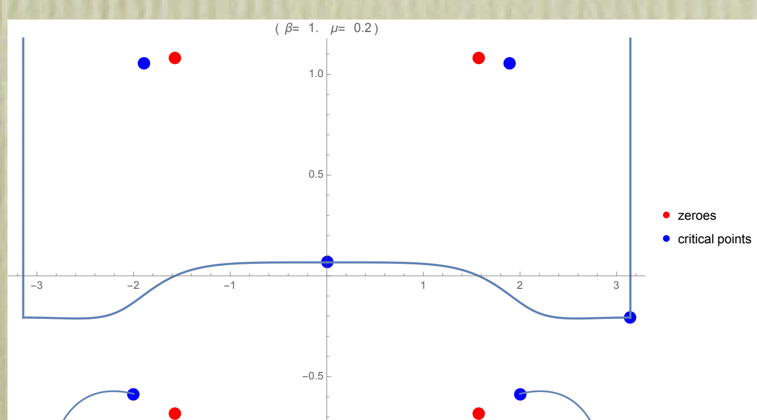


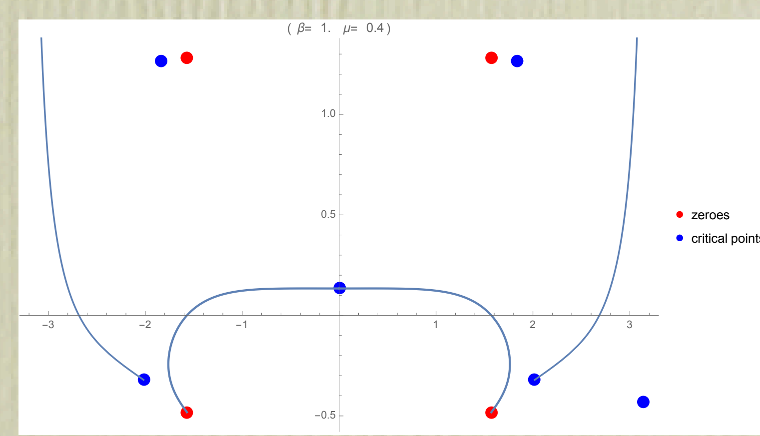


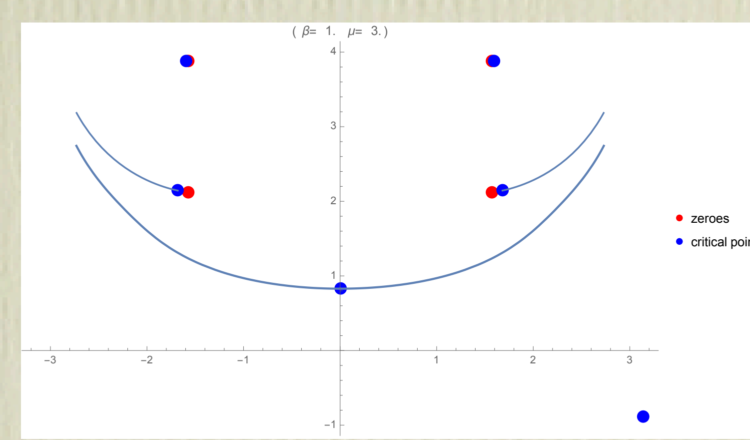
Contributing thimbles



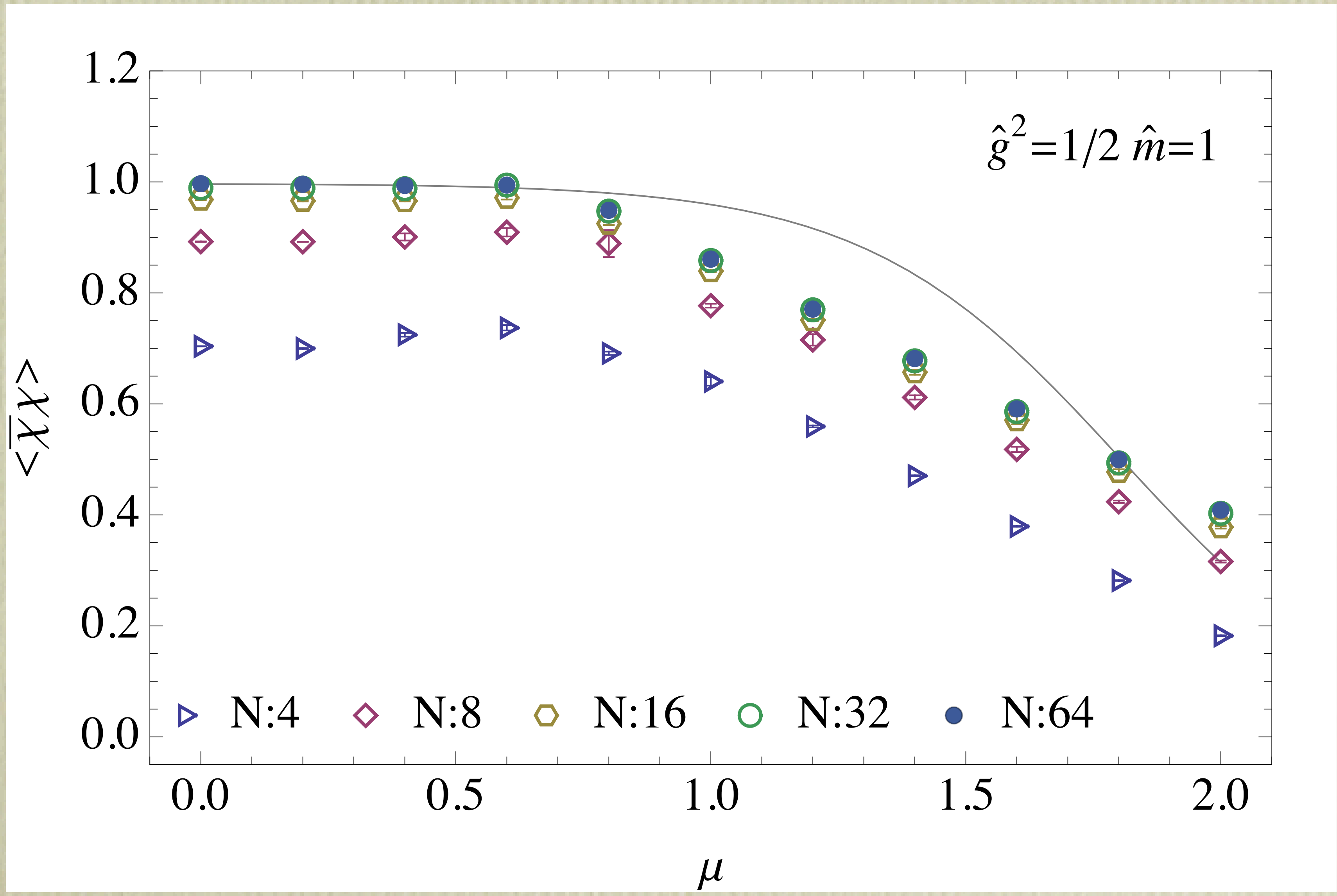






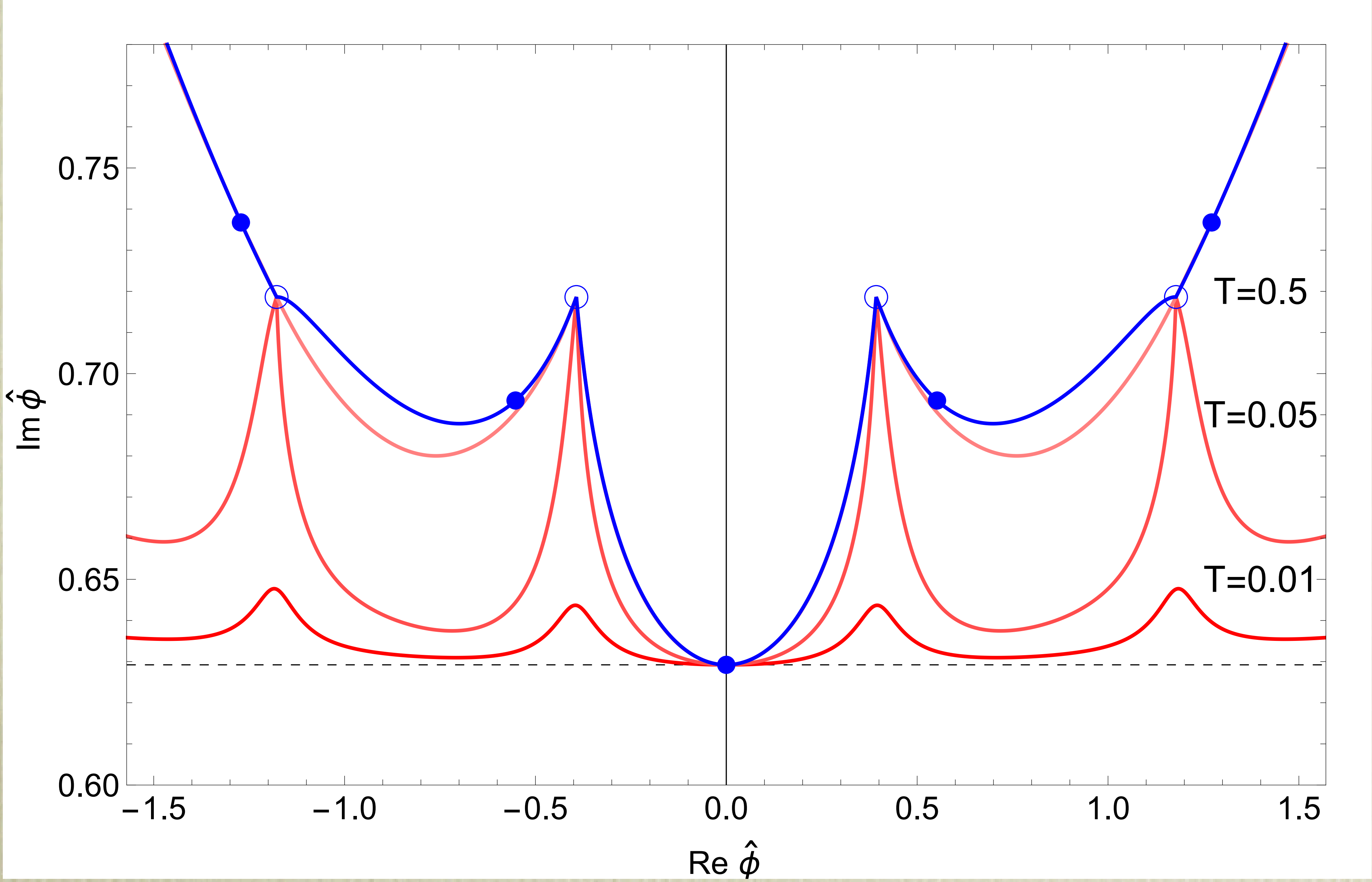


Strong coupling (cont limit)

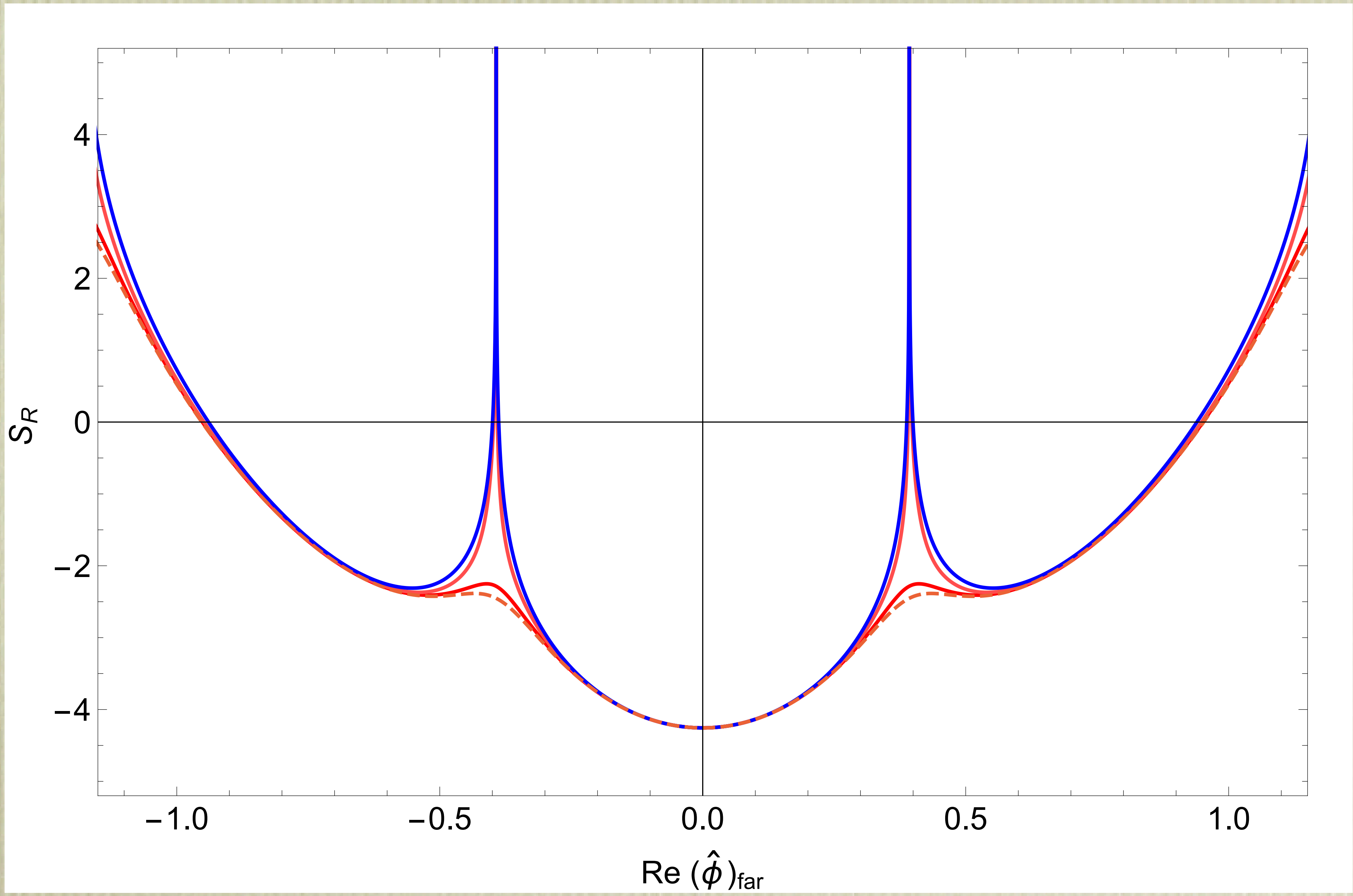


Beyond thimbles

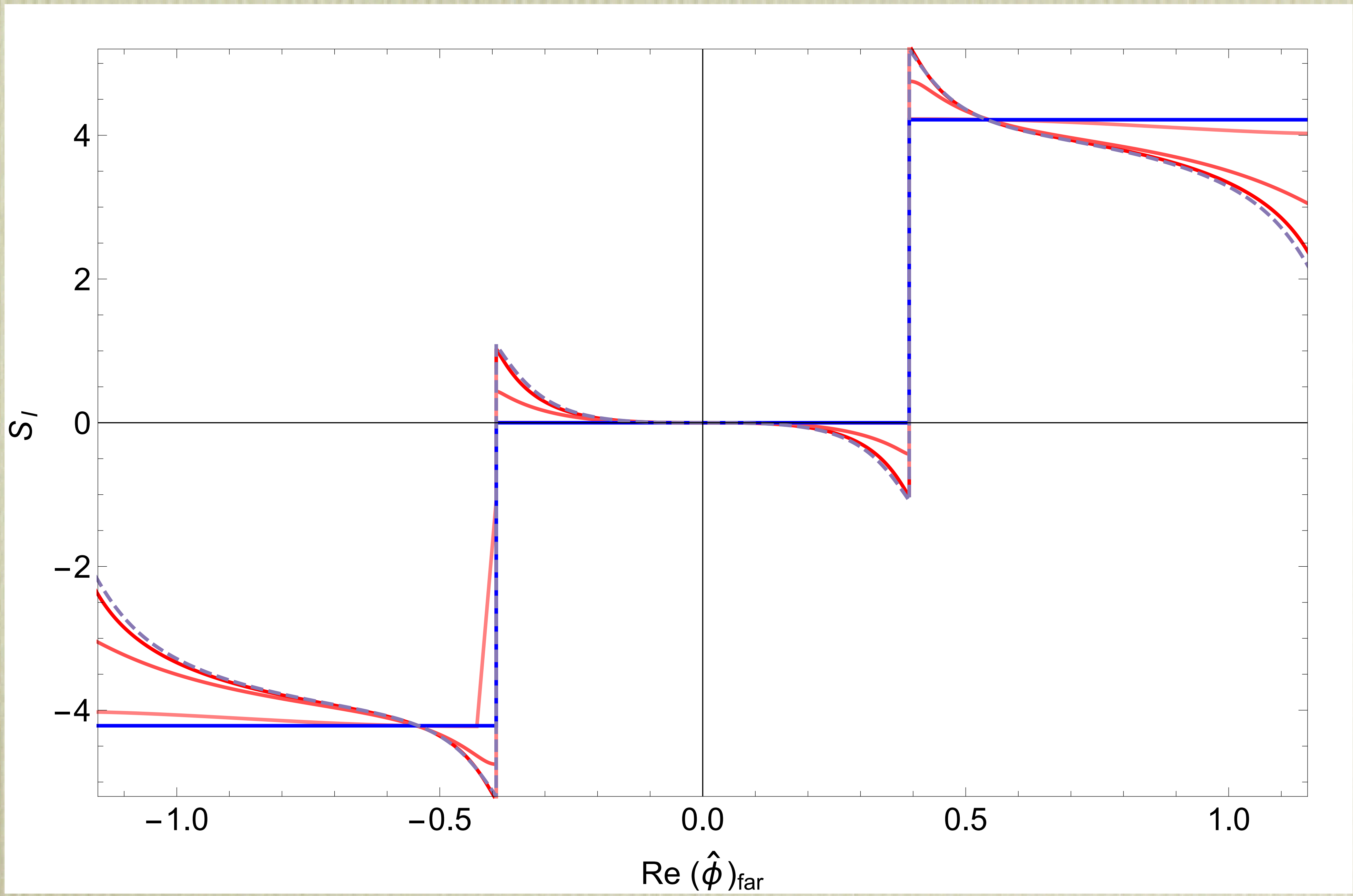
Thimble approximations



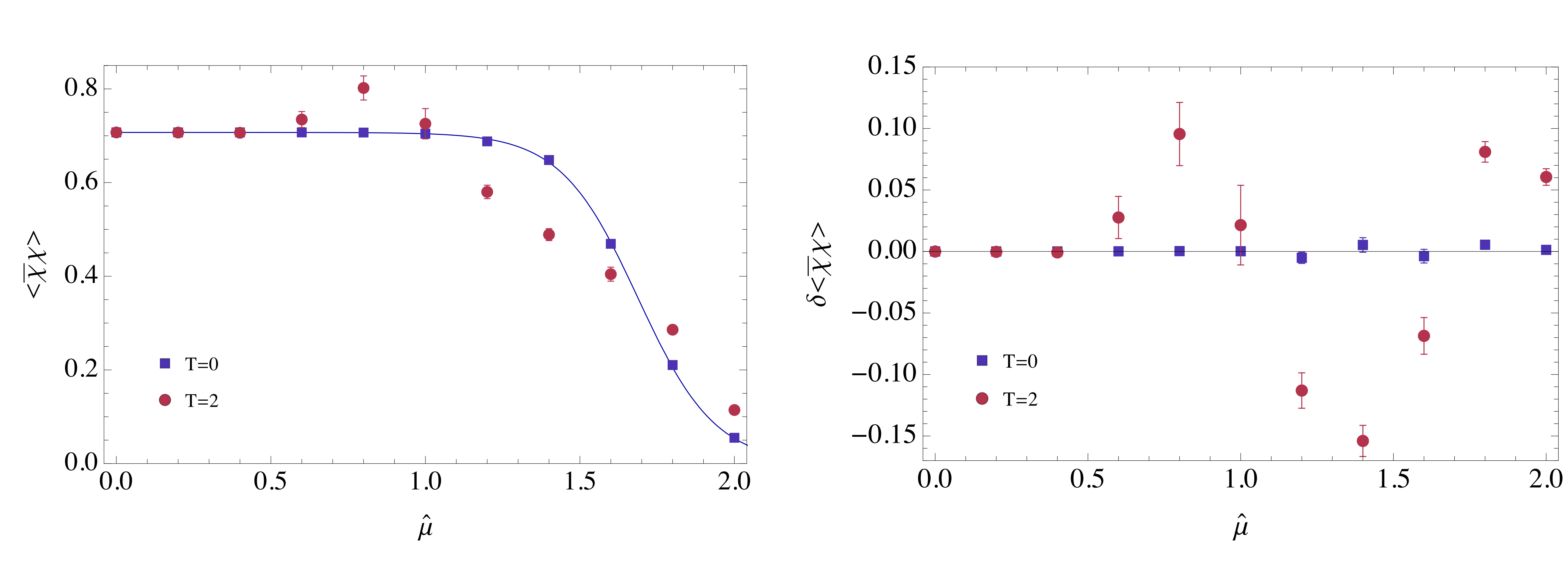
Action on thimbles



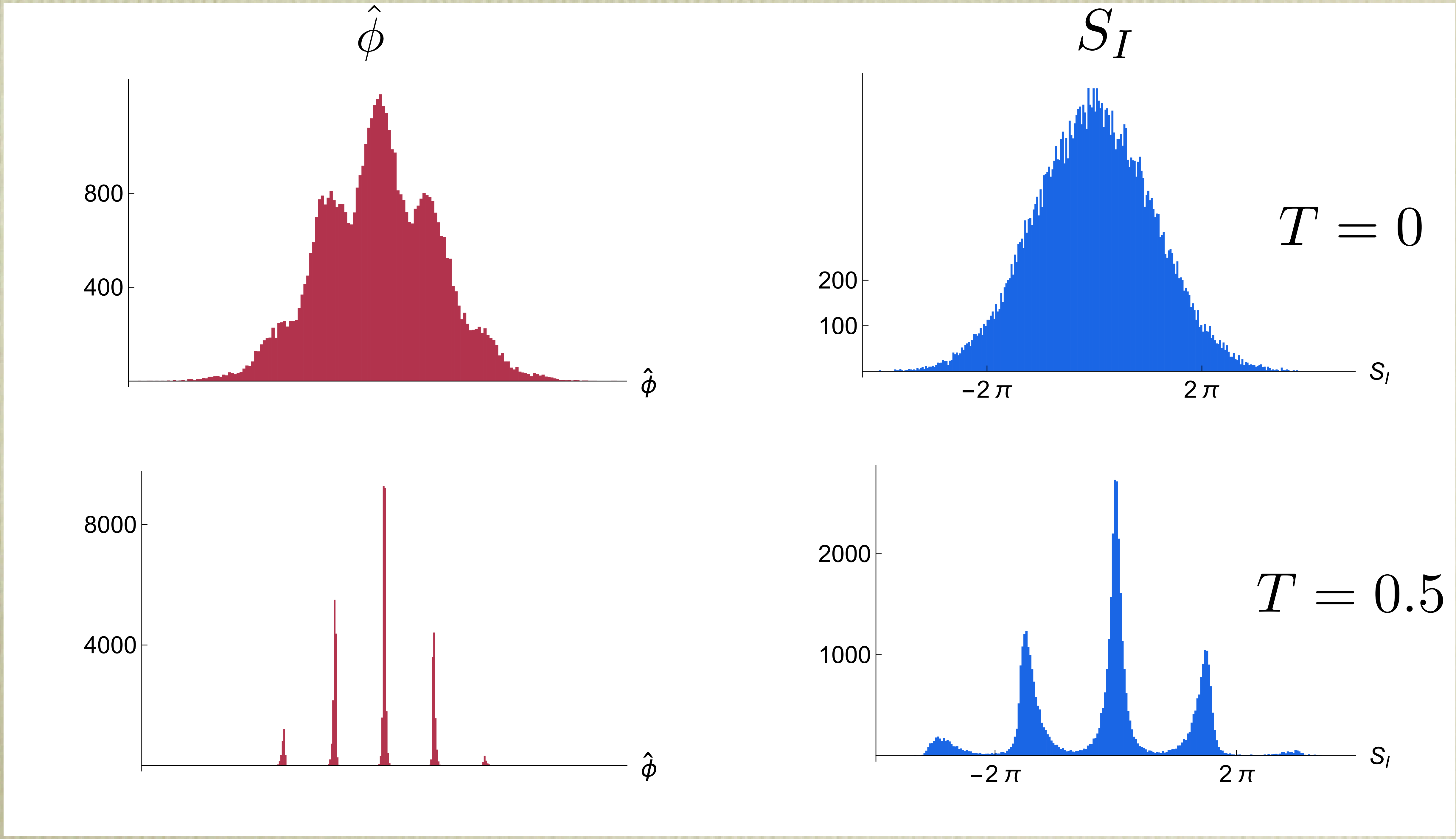
Action on thimbles



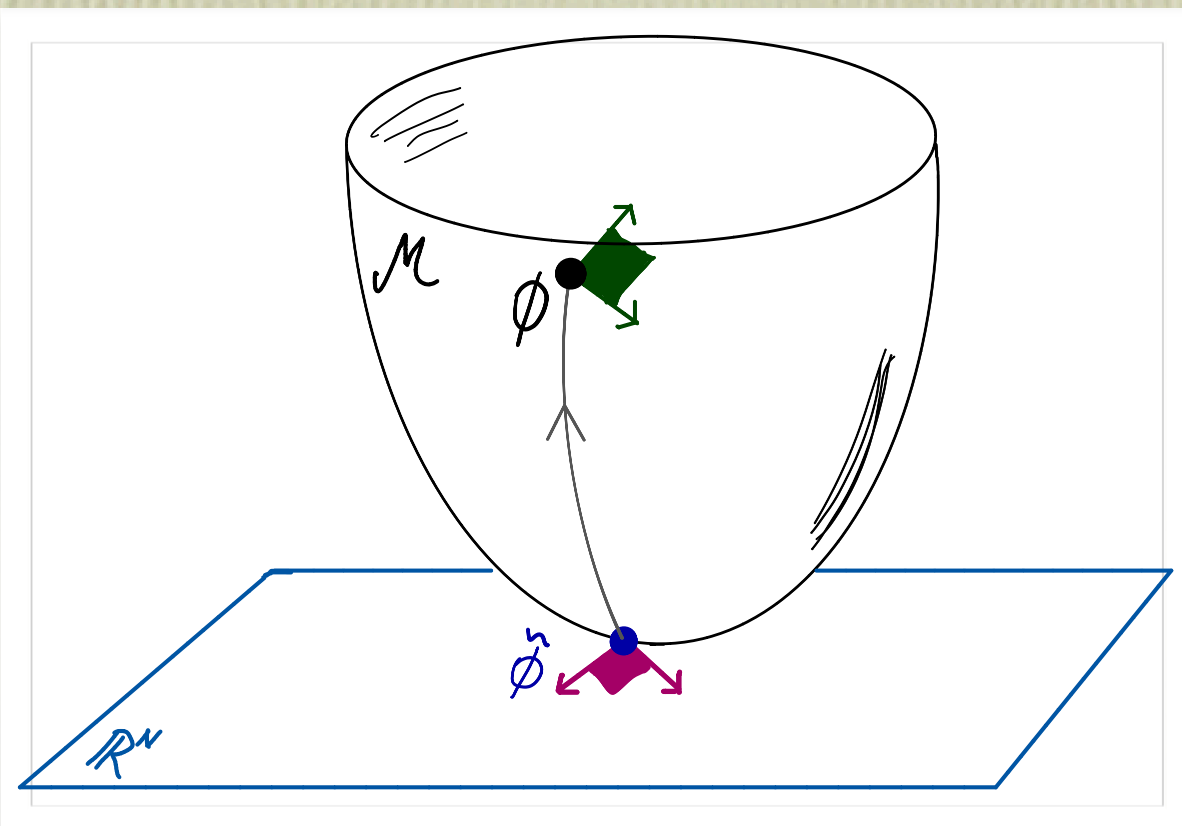
Strong coupling (revisited)



Taming the sign fluctuations



Manifolds generated by holomorphic gradient flow

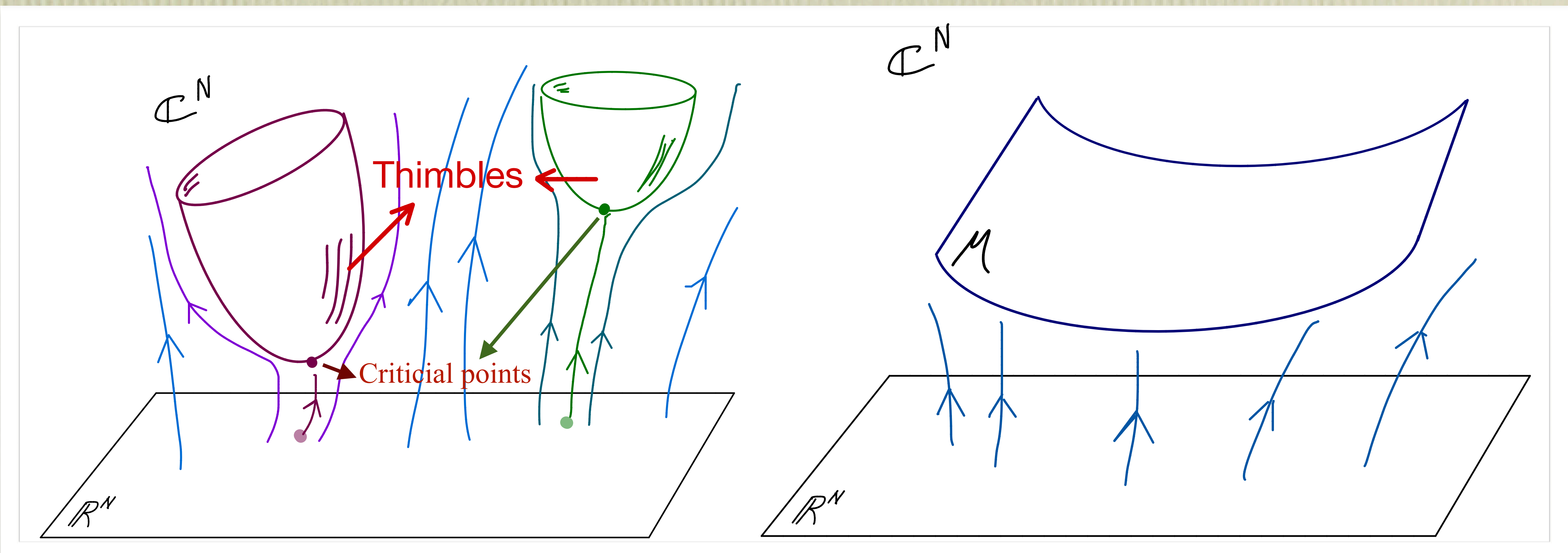


$$\frac{d\phi_a}{d\tau} = \overline{\frac{\partial S}{\partial \phi_a}}, \qquad \phi_a \equiv x_a + i y_a$$

$$\begin{cases} \dfrac{dx_a}{d\tau} = \dfrac{\partial S_R}{\partial x_a} = \dfrac{\partial S_I}{\partial y_a} \\ \dfrac{dy_a}{d\tau} = \dfrac{\partial S_R}{\partial y_a} = -\dfrac{\partial S_I}{\partial x_a} \end{cases}$$

$$\langle \mathcal{O} \rangle = \frac{\int d\tilde{\phi}_i\, \mathcal{O} e^{-i\,\mathbb{Im}(S - \log\det J)} e^{\overbrace{-\mathbb{Re}\,(S + \log\det J)}^{S_{\text{eff}}}}}{\int d\tilde{\phi}_i\, e^{-i\,\mathbb{Im}(S-\log\det J)}\, e^{-S_{\text{eff}}}}$$

Manifolds generated by holomorphic gradient flow



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