Monte Carlo calculations on Lefschetz thimbles and beyond

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arXiv:1604.00956

Delta Workshop
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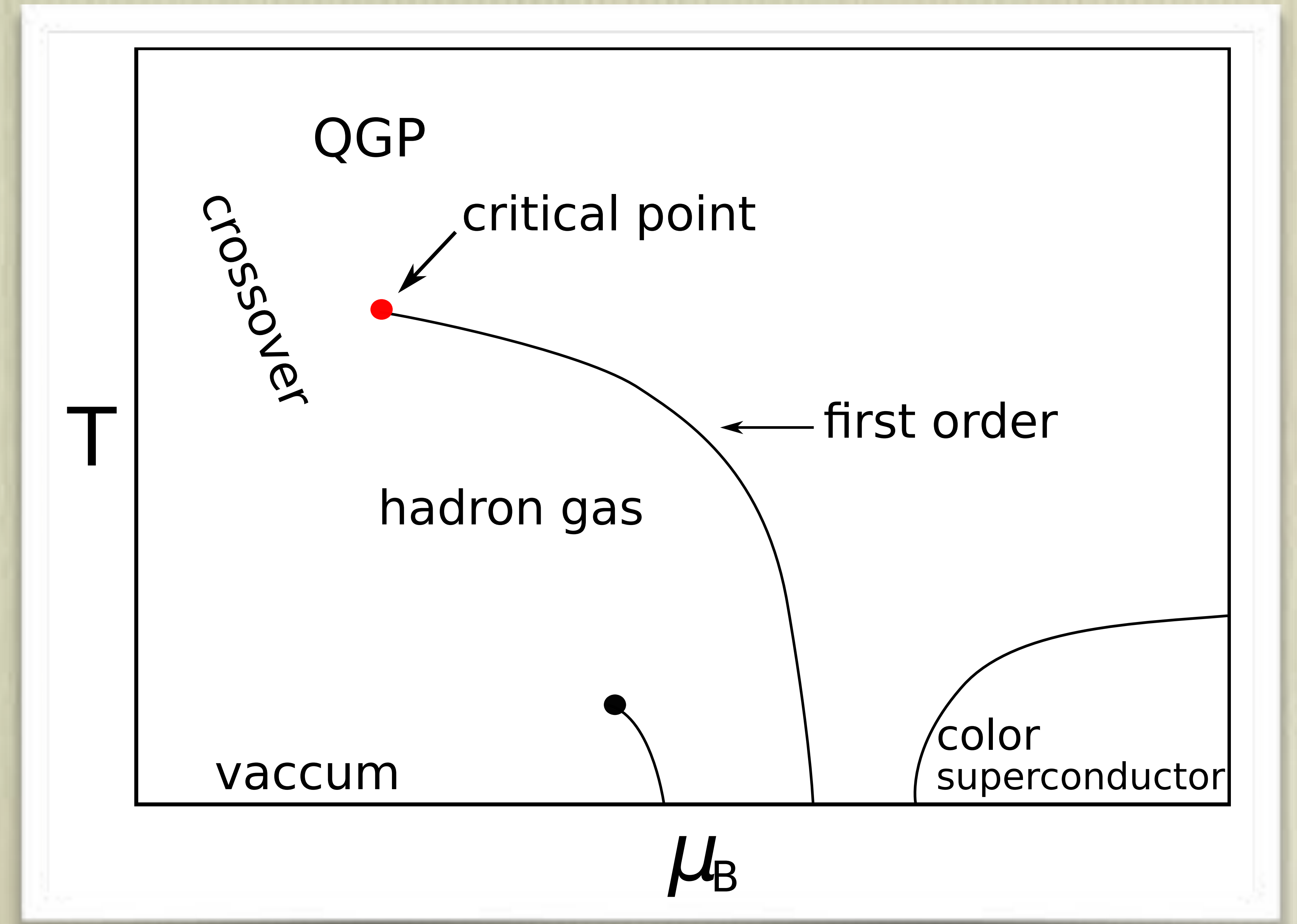
THE GEORGE WASHINGTON UNIVERSITY
WASHINGTON, DC

Motivation



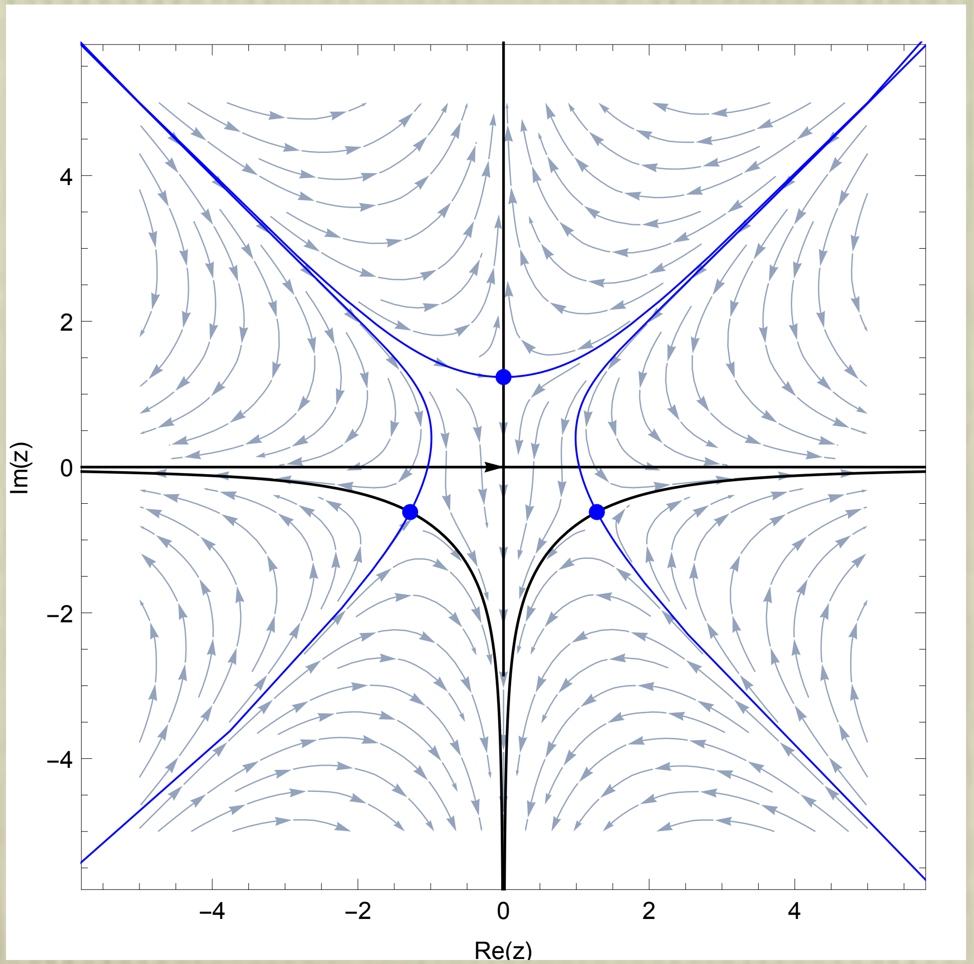
complex

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

The plan

- Lefschetz thimble
- A simple (Metropolis) algorithm
- Toy fermionic model
- Numerical results
- Beyond thimbles

Lefschetz thimble



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

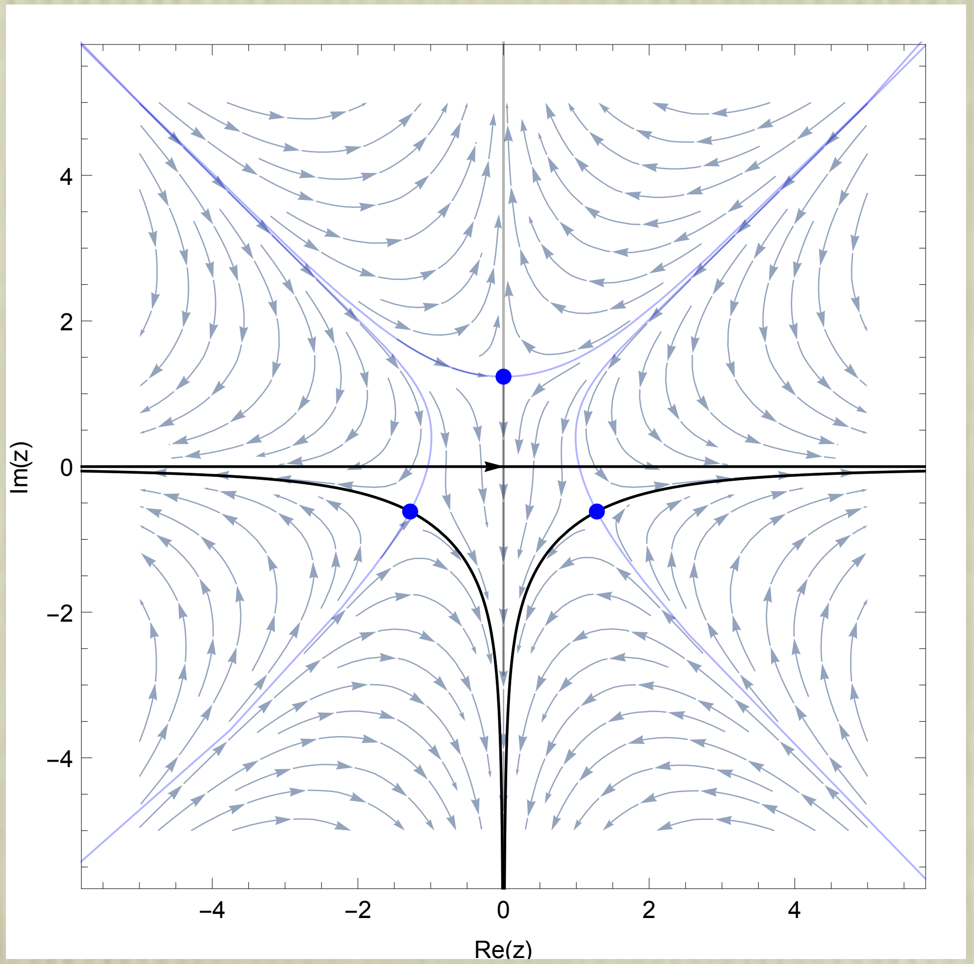
$$\frac{dS}{dz} = 0 \quad \text{(critical points)}$$

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

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

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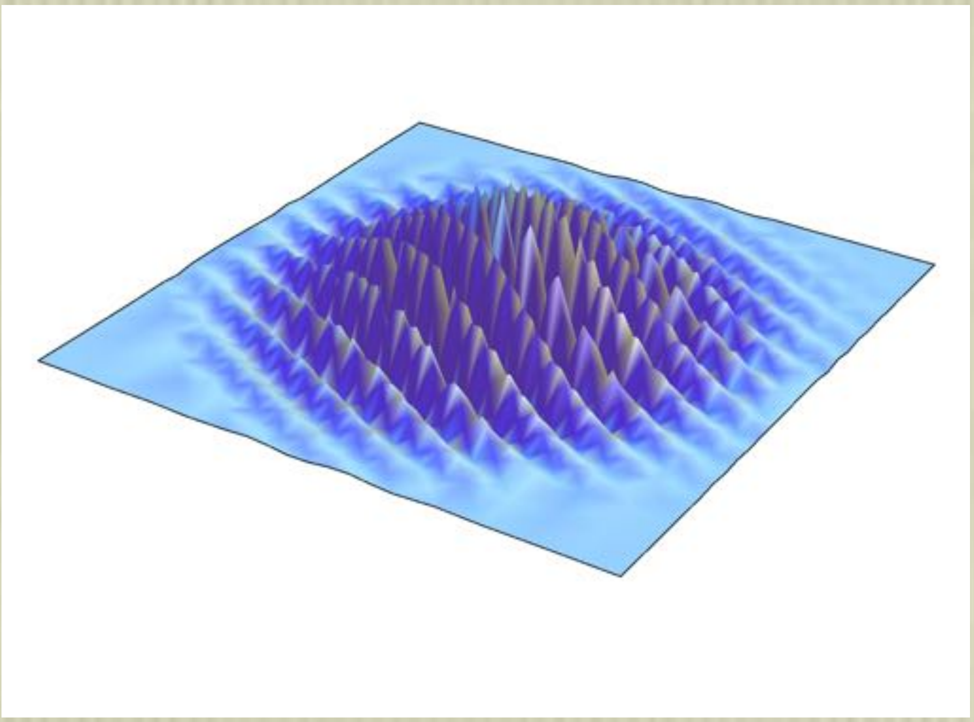
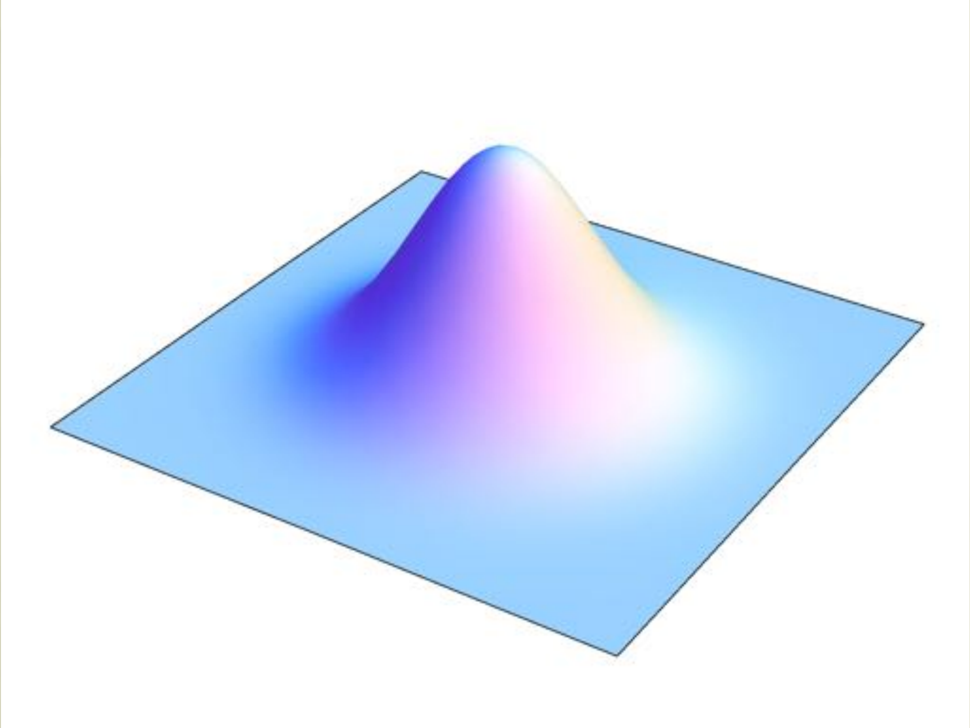
$$Z = \sum_{\sigma} n_{\sigma} \int_{J_{\sigma}} dz \, e^{-S(z)}$$

Lefschetz thimble



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



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

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

Lefschetz thimble

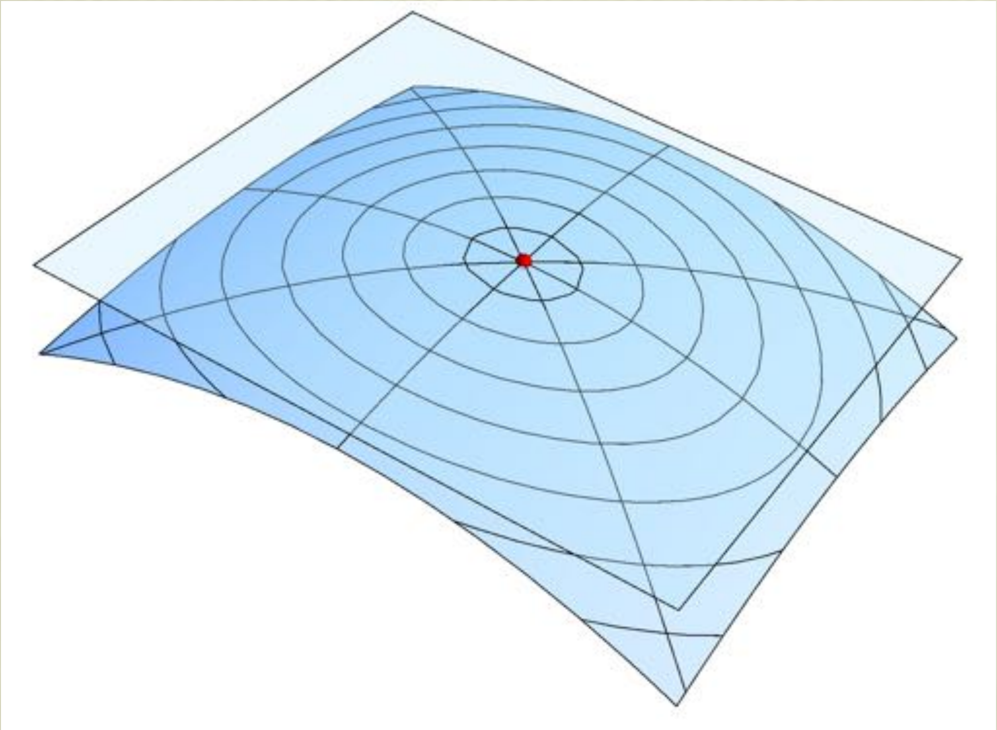
$$\langle O \rangle = \frac{1}{Z} \int \mathrm{d}x\, e^{-S(x)} O(x) = \frac{1}{Z} \sum_{\sigma} n_\sigma e^{-S_I(\sigma)} \int_{J_\sigma} \mathrm{d}z\, e^{-S_R(z)} O(z)$$

$$\langle O \rangle = \frac{1}{Z_R} \int_{J_\sigma} \mathrm{d}z\, e^{-S_R(z)} O(z) \quad Z_R = \int_{J_\sigma} \mathrm{d}z\, e^{-S_R(z)} \quad \text{(single thimble)}$$

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

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

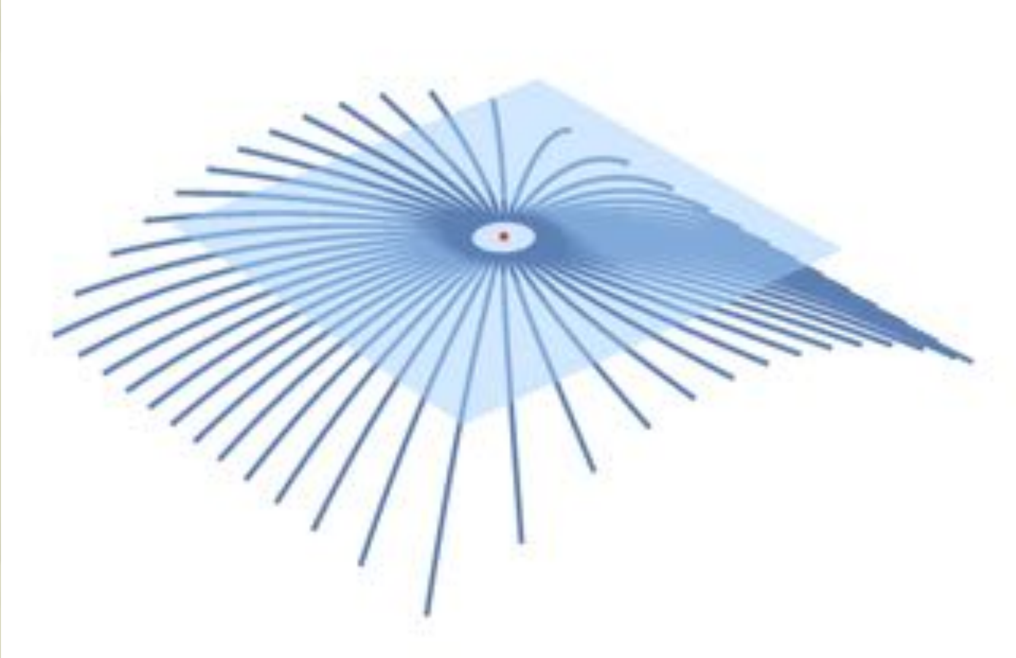
$$\phi = \frac{|\mathrm{d}z|}{\mathrm{d}z} \quad \text{(residual phase)}$$



Lefschetz thimble

$$S \approx S(z_{\rm cr}) + (z - z_{\rm cr})_i \left. \frac{\partial^2 S}{\partial z_i \partial z_j} \right|_{z_{\rm cr}} (z - z_{\rm cr})_j$$

$$S_R \approx S_R(z_{\rm cr}) + (x - x_{\rm cr})_i H_R (x - x_{\rm cr})_j$$



$$H_R = \begin{pmatrix} \mathrm{Re}\, H & -\mathrm{Im}\, H \\ -\mathrm{Im}\, H & -\mathrm{Re}\, H \end{pmatrix}$$

$$H_R\, x_\lambda = \lambda\, x_\lambda \quad \text{with } \lambda > 0 \text{ (stable)}$$

$$H_R\, x_\lambda = \lambda\, x_\lambda \quad \text{with } \lambda < 0 \text{ (unstable)}$$

$$\frac{dz}{d\tau} = \overline{\frac{dS}{dz}} \qquad z(\tau = 0) = z_0$$

$$z_0 = z_{\rm cr} + \sum_{\lambda > 0} c_\lambda x_\lambda \quad \text{with } \| z - z_{\rm cr} \| = r \ll 1$$

The algorithm

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

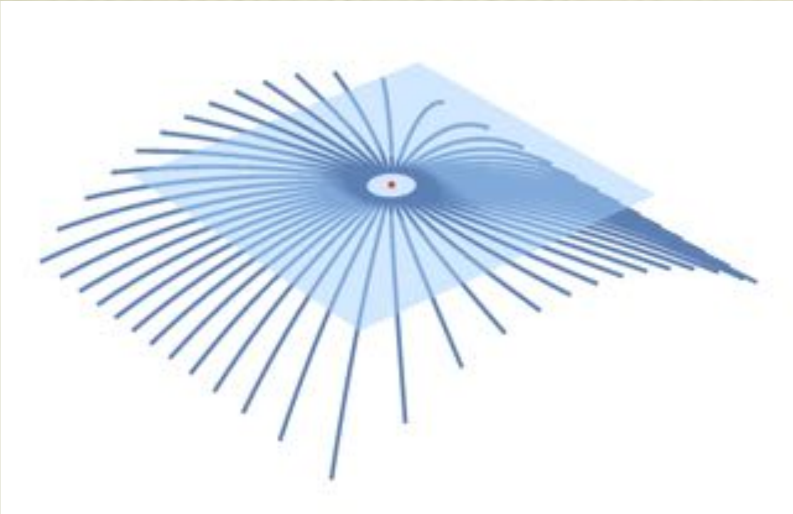
$$P(z_{\text{old}} \to z_{\text{new}}) = P(z_{\text{new}} \to z_{\text{old}})$$

How to stay on the thimble?

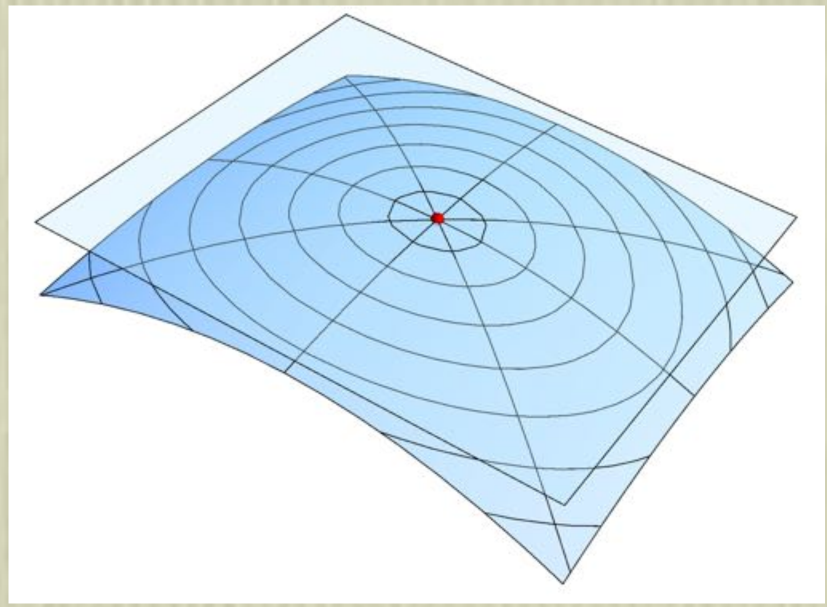
- assume thimble to be Gaussian
- do complicated to and fro integration (HMC, Aurora, etc)
- use a map

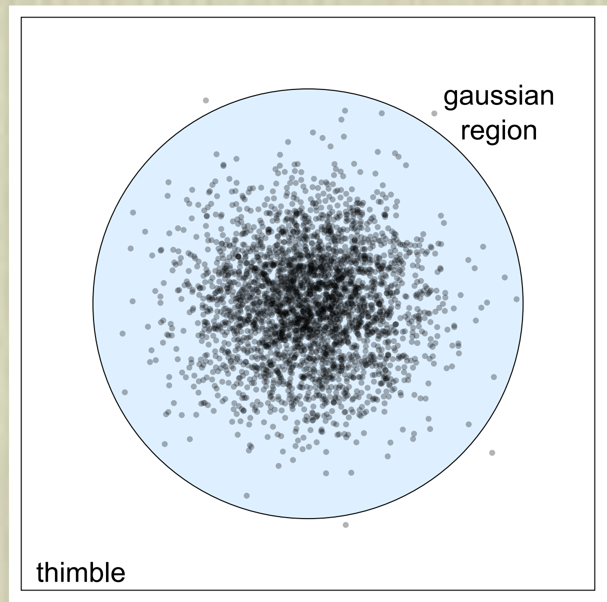
$$\frac{dz}{d\tau} = \overline{\frac{dS}{dz}} \quad \text{(upward flow – stable)}$$

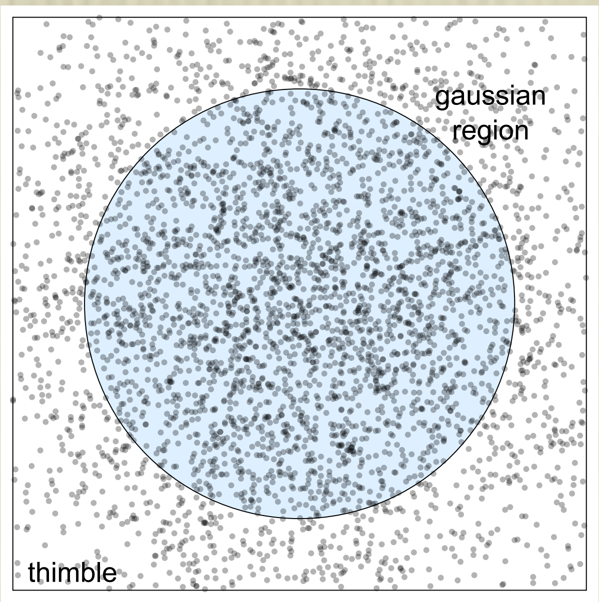
$$\frac{dz}{d\tau} = -\overline{\frac{dS}{dz}} \quad \text{(downward flow – unstable)}$$



The algorithm

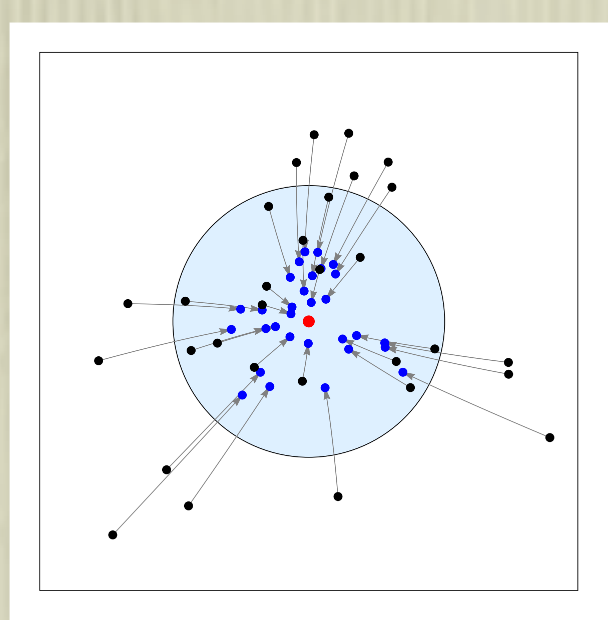


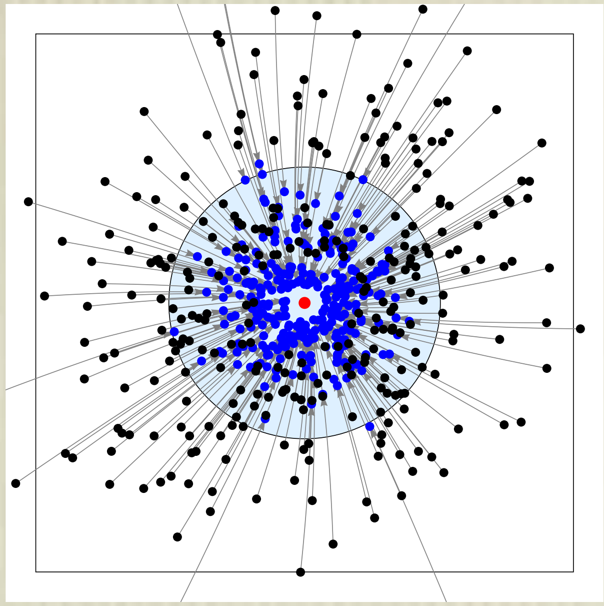




good

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

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

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

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

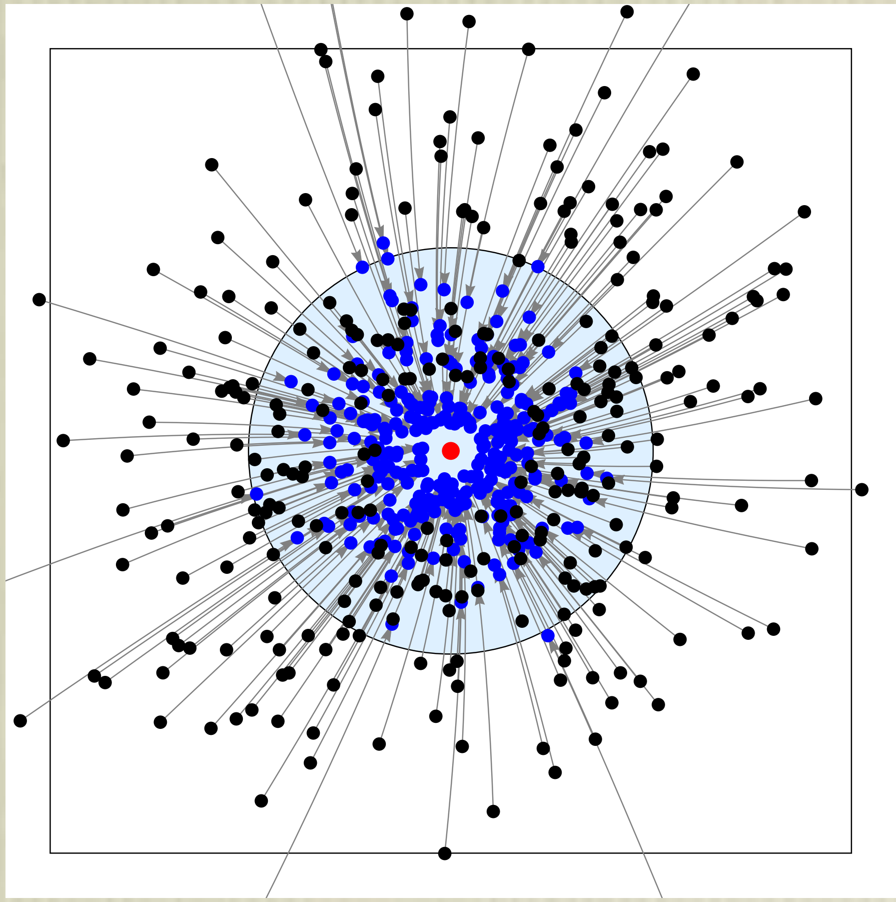
f is the downward flow

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

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

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)

The model

- $0+1$ 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

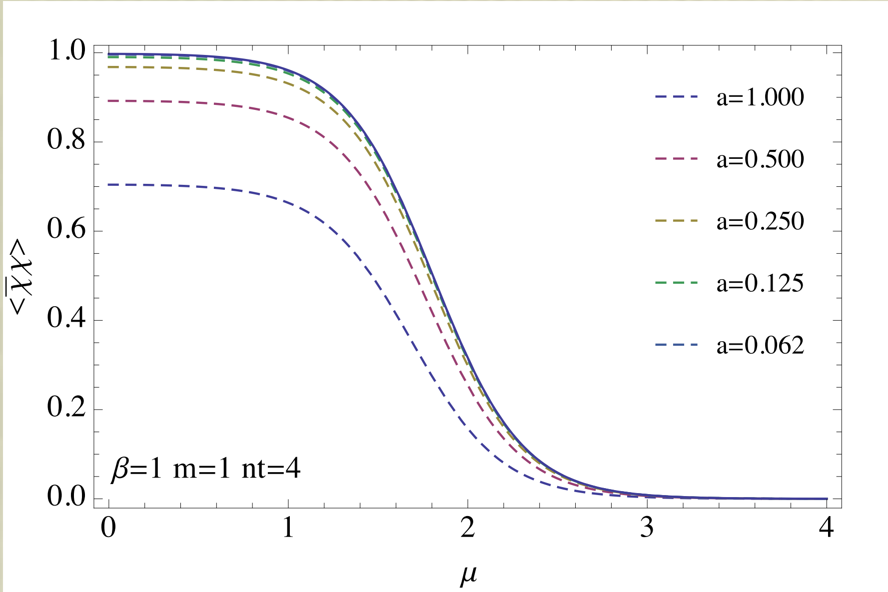
The model

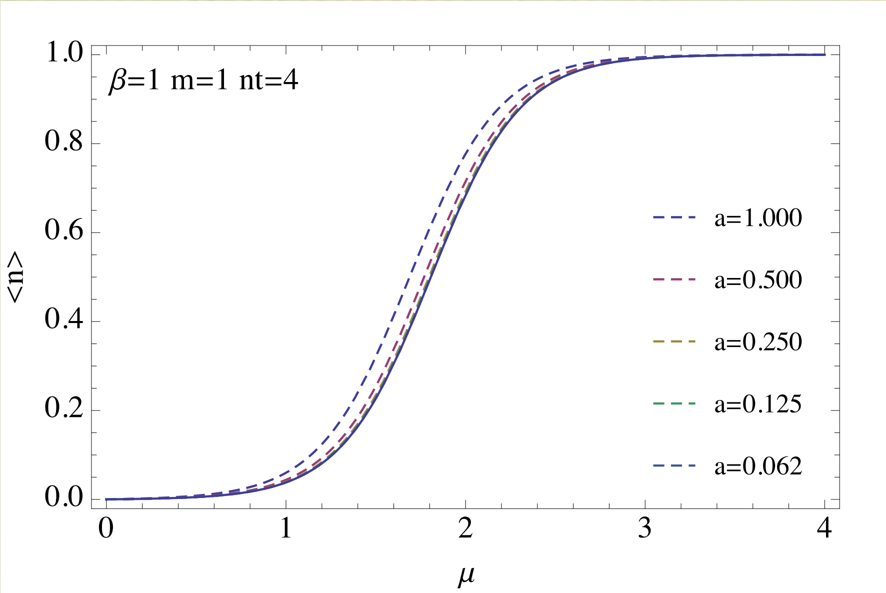
- The action can be computed analytically and the condensate is:

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

- 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.





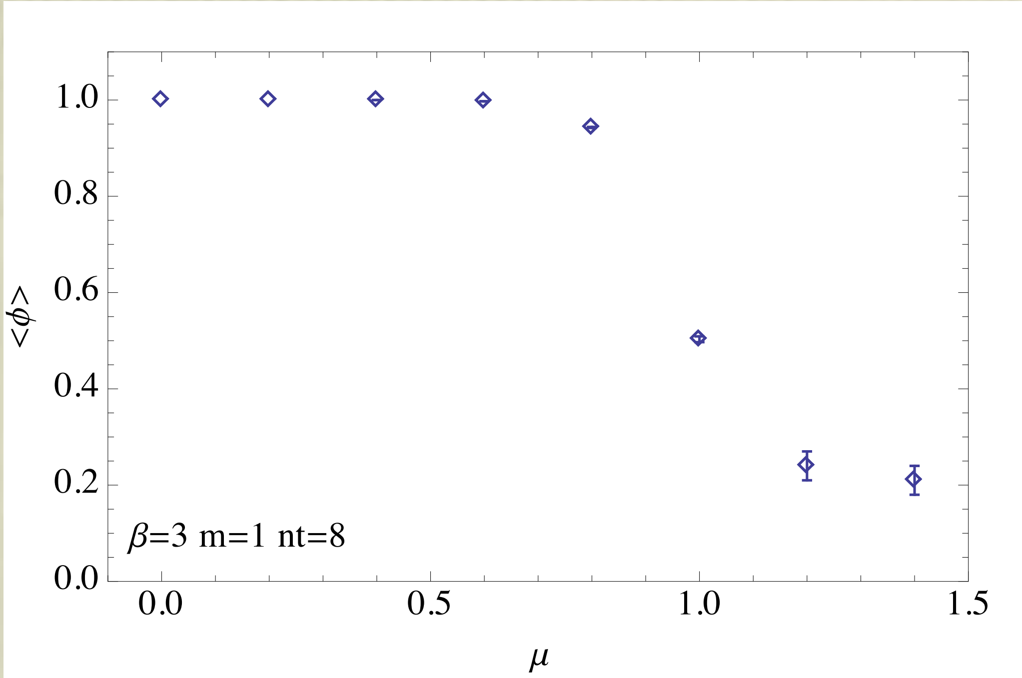
The model

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

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

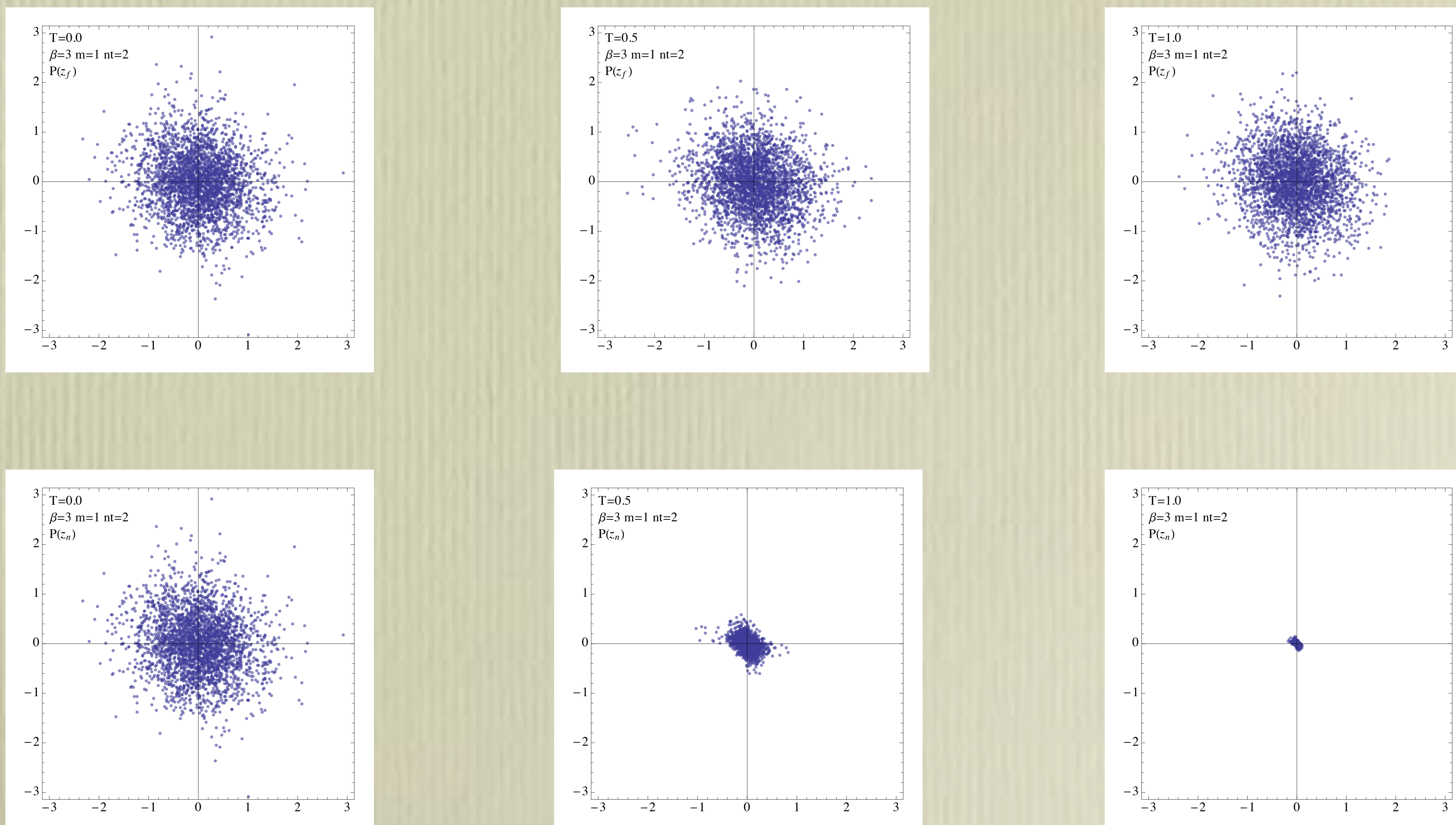
$$\langle O \rangle = \frac{\langle O\phi \rangle_0}{\langle \phi \rangle_0}$$

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



Numerical results

Algorithm check



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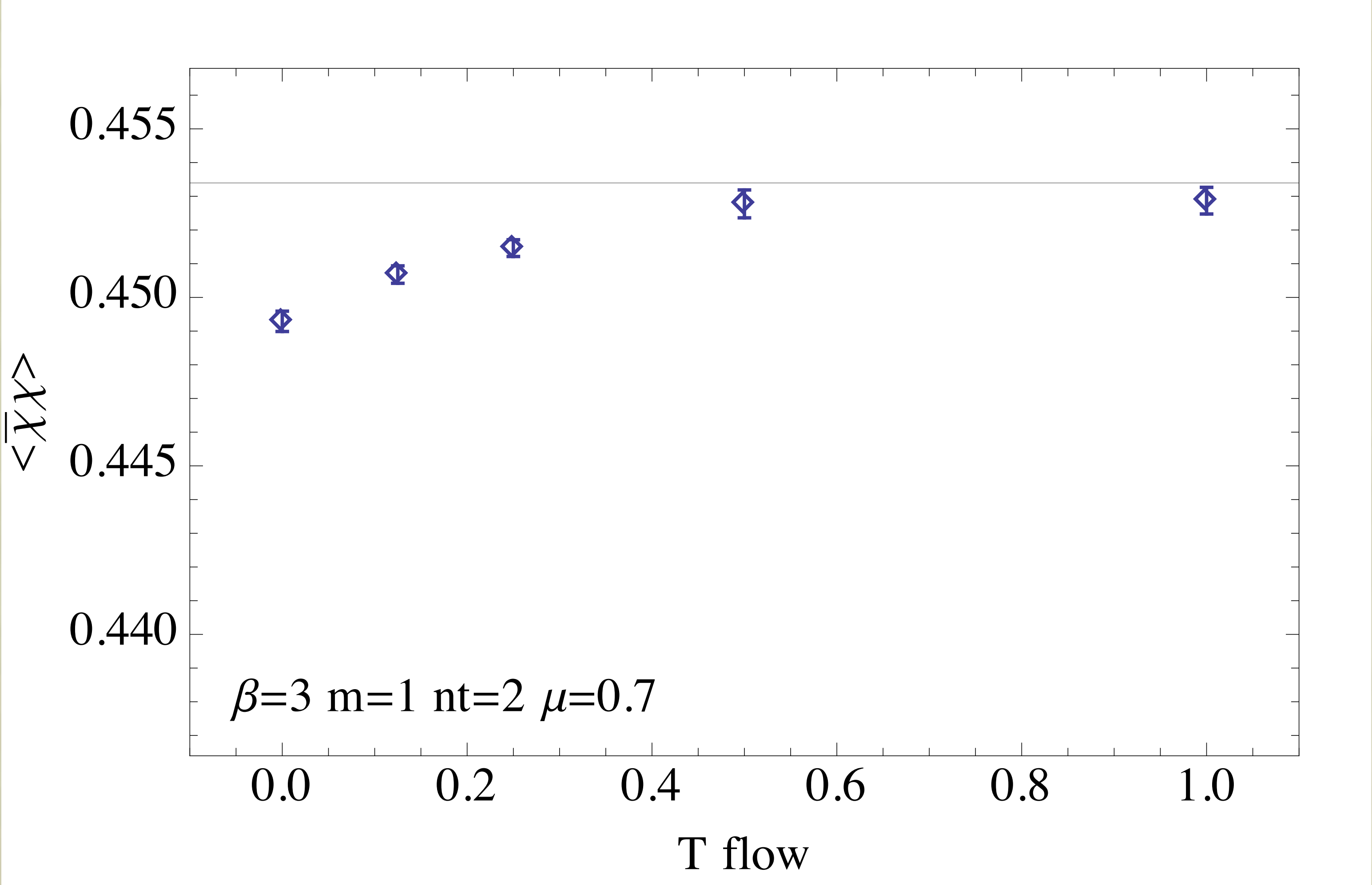
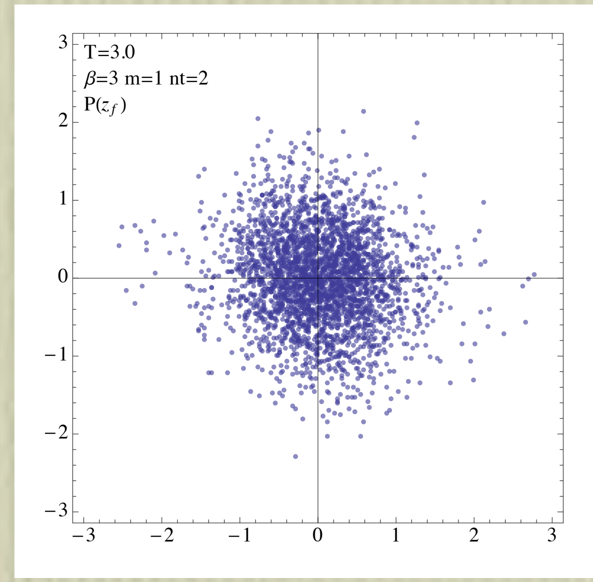
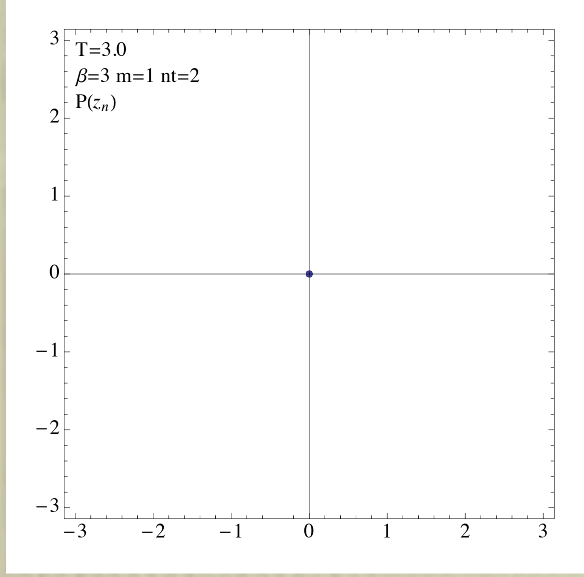
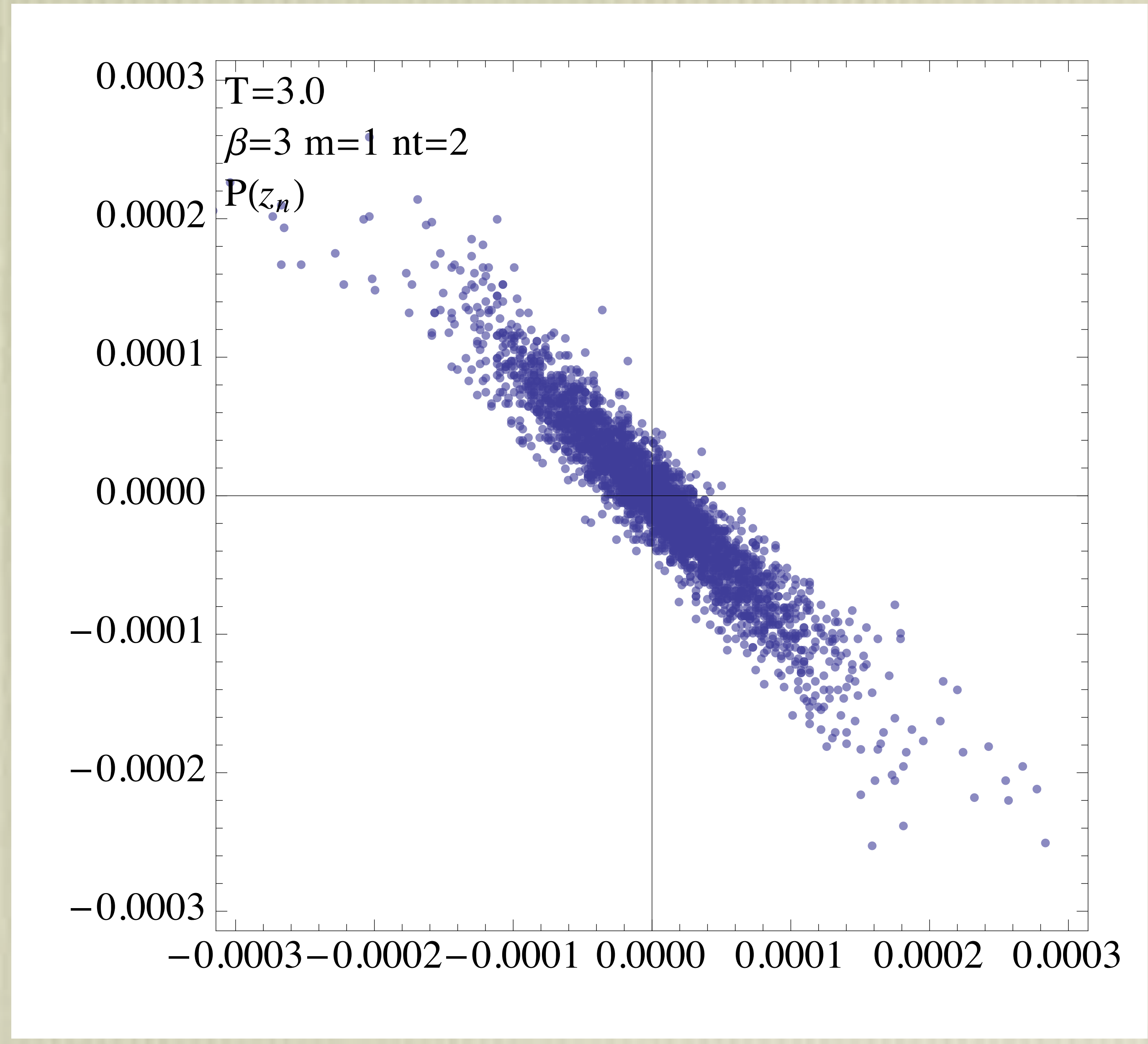


Anisotropic proposals







Residual phase

- The Jacobian of the map function is not real, $\boxed{\det J \notin \mathbb{R}}$

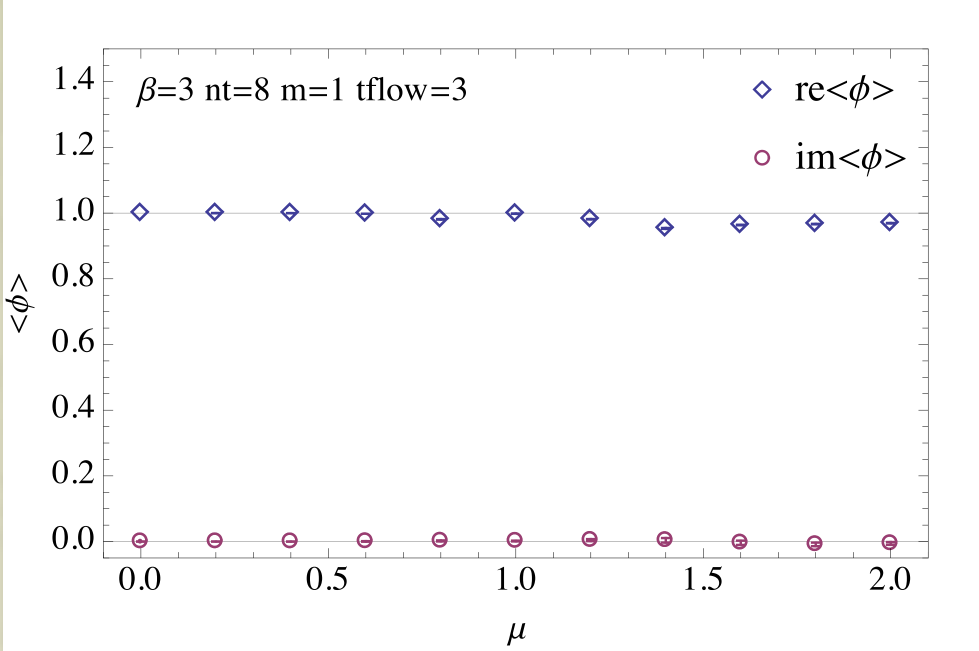
- We use only its magnitude in the updating process

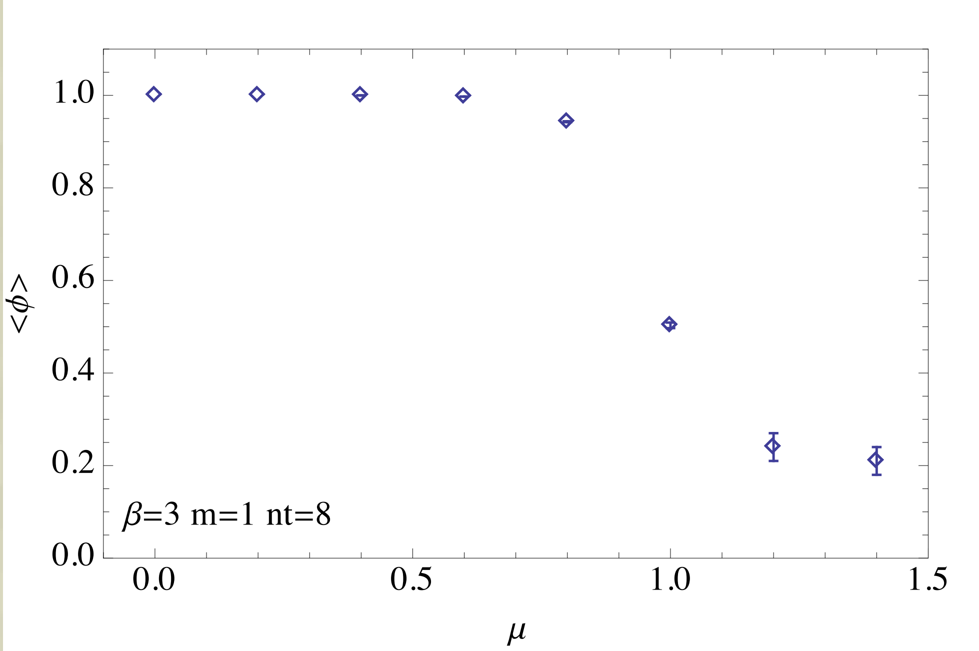
$$S_{\text{eff}} = S_R - \log|\det J|\,.$$

- The residual phase $\phi = \det J / |\det J|$ is folded in the observable.

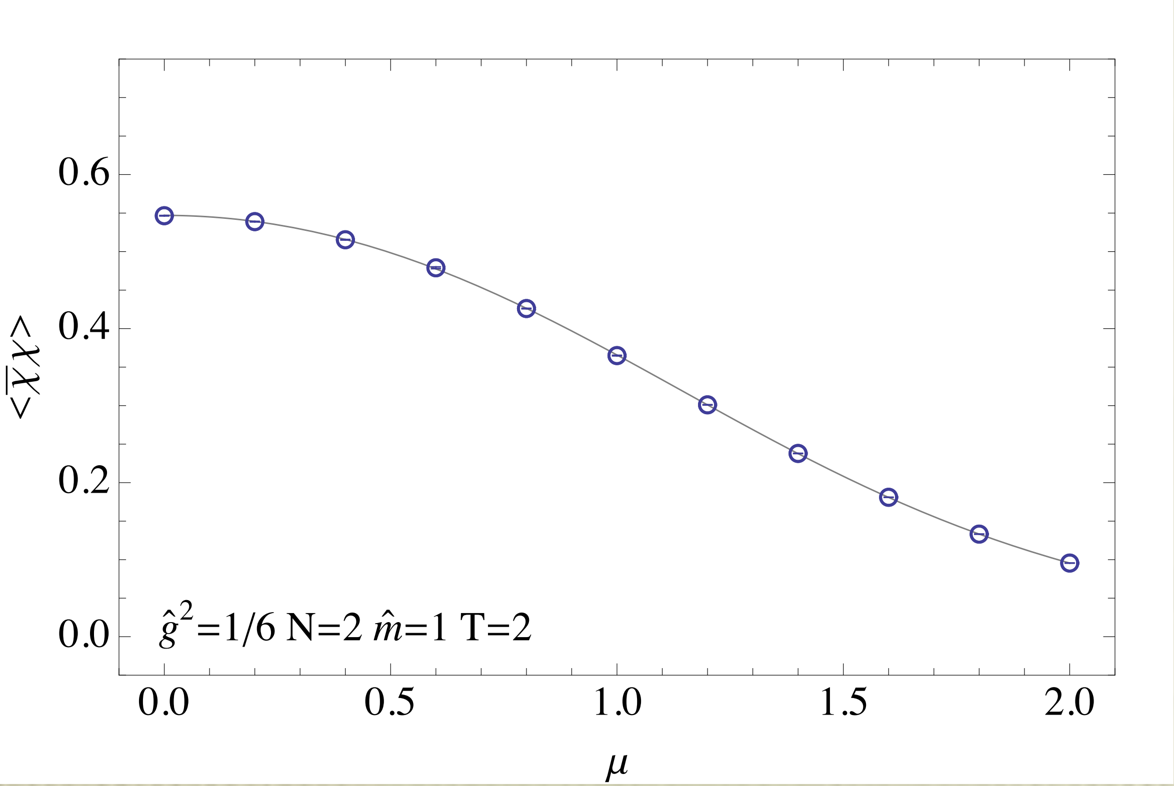
- This is *not* the same phase as in the phase quenched theory.

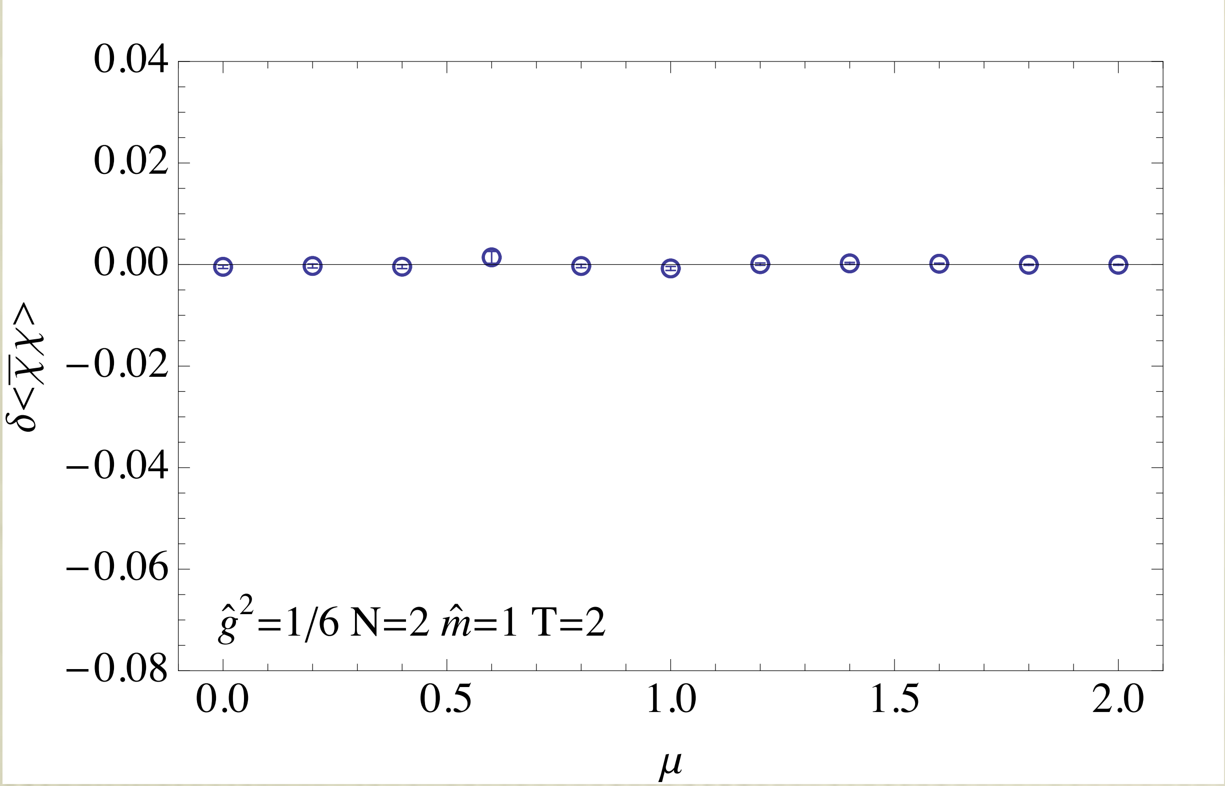
- The sign fluctuations of the residual phase are observable but mild in our model.



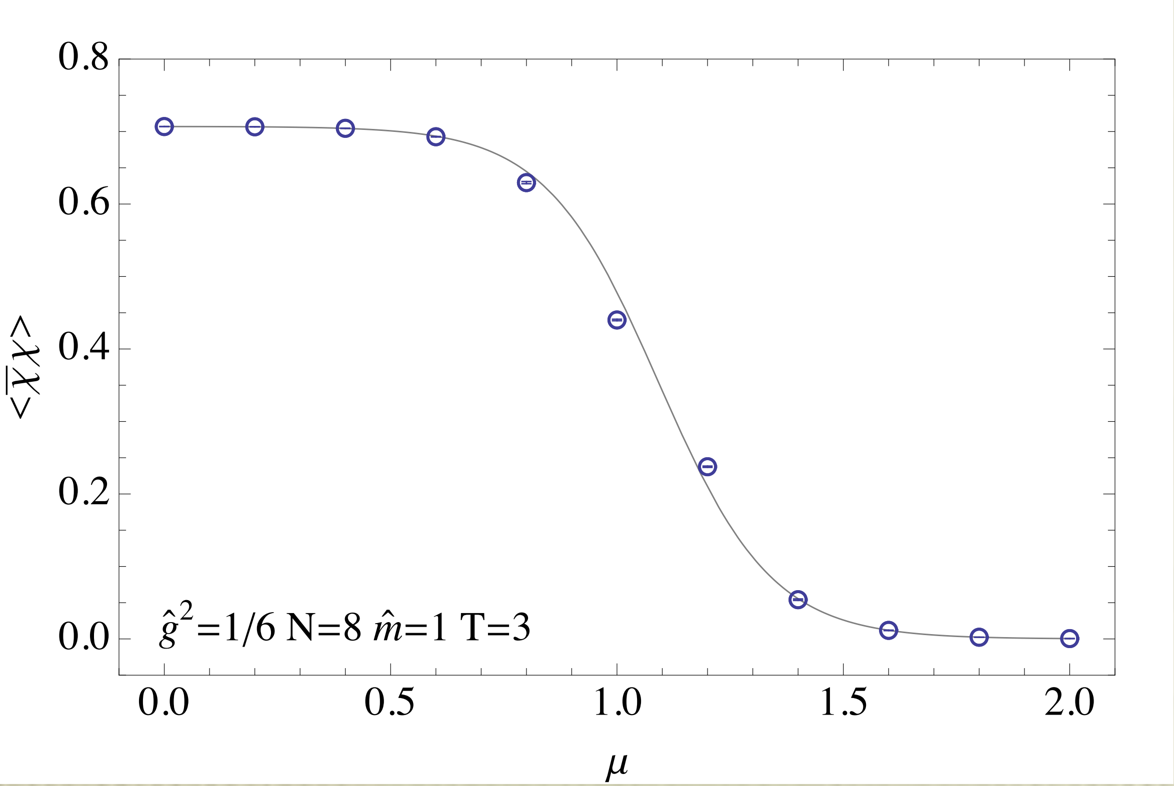


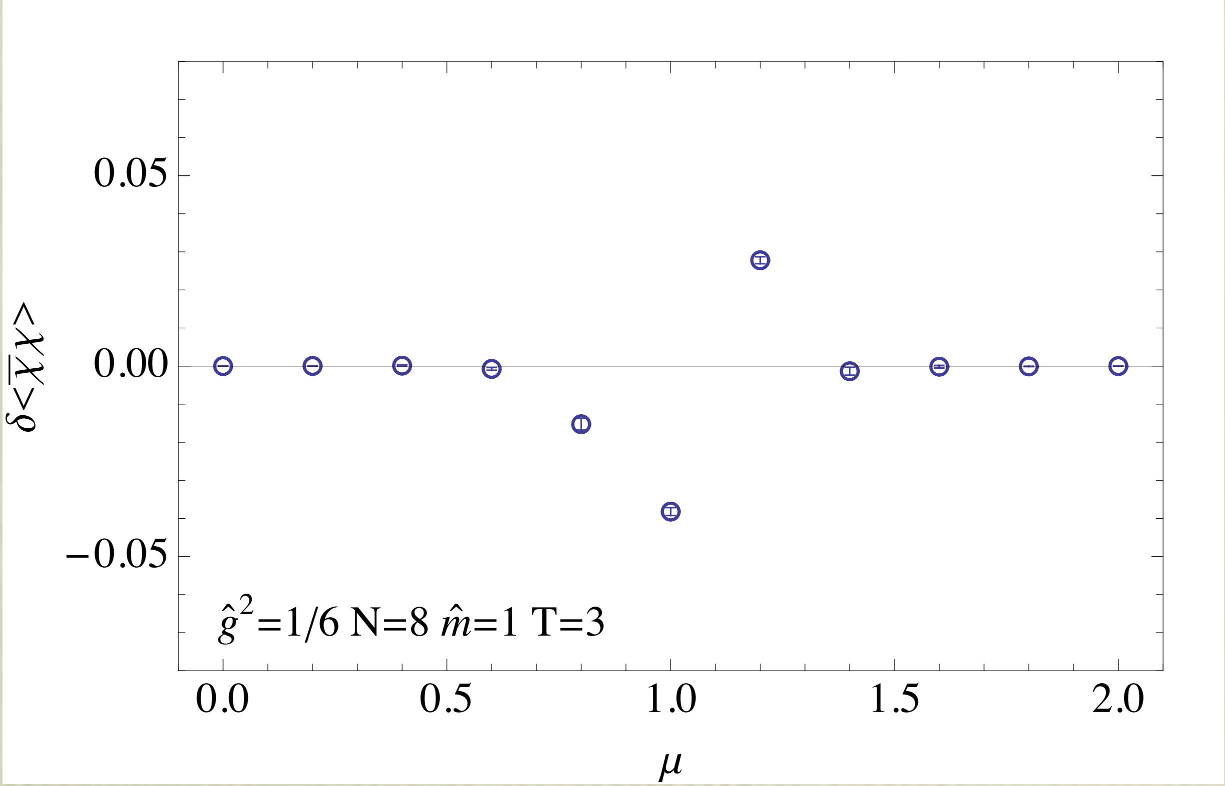
Weak coupling



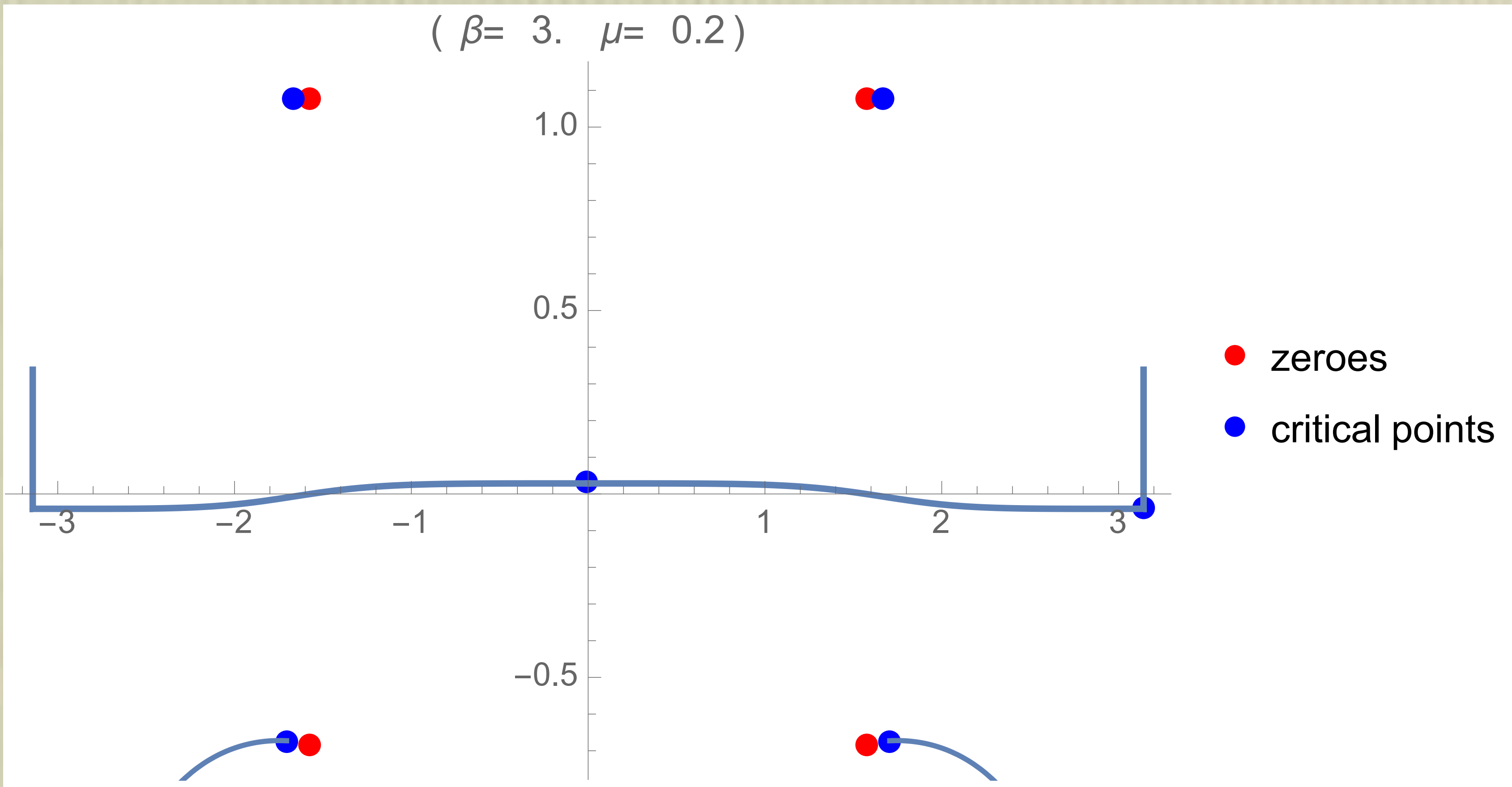


Weak coupling (low temp)

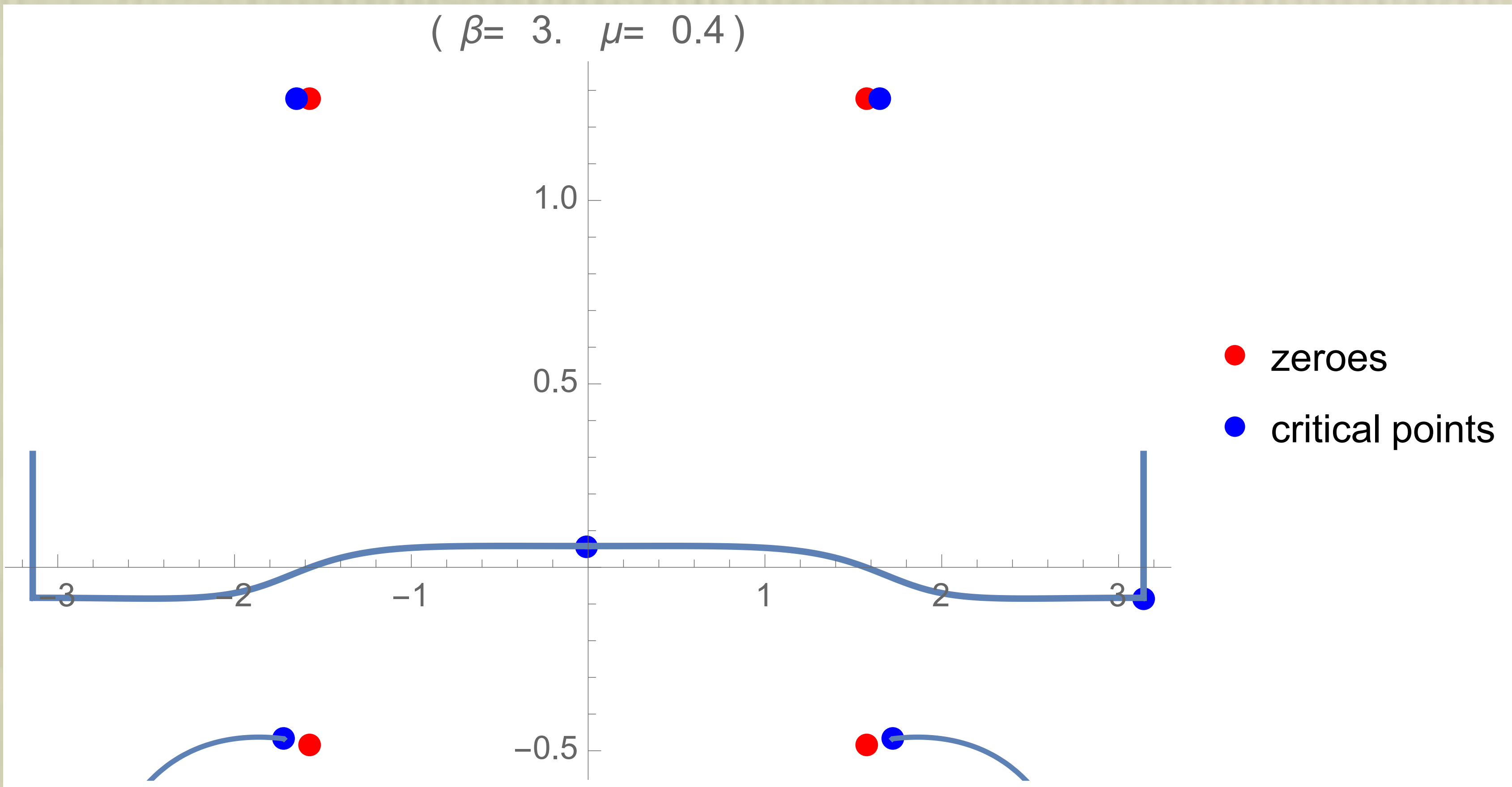




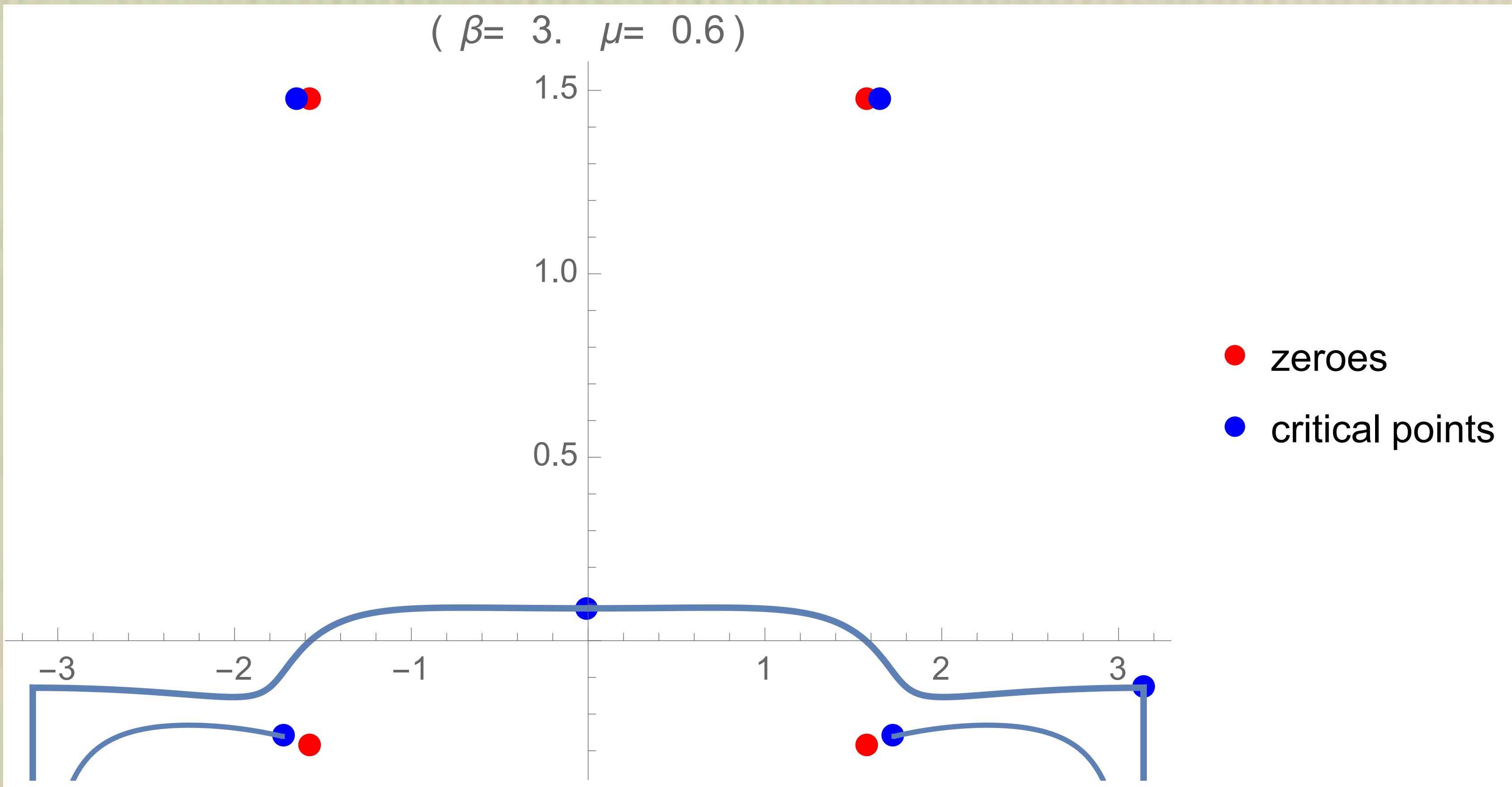
Thimble contributions



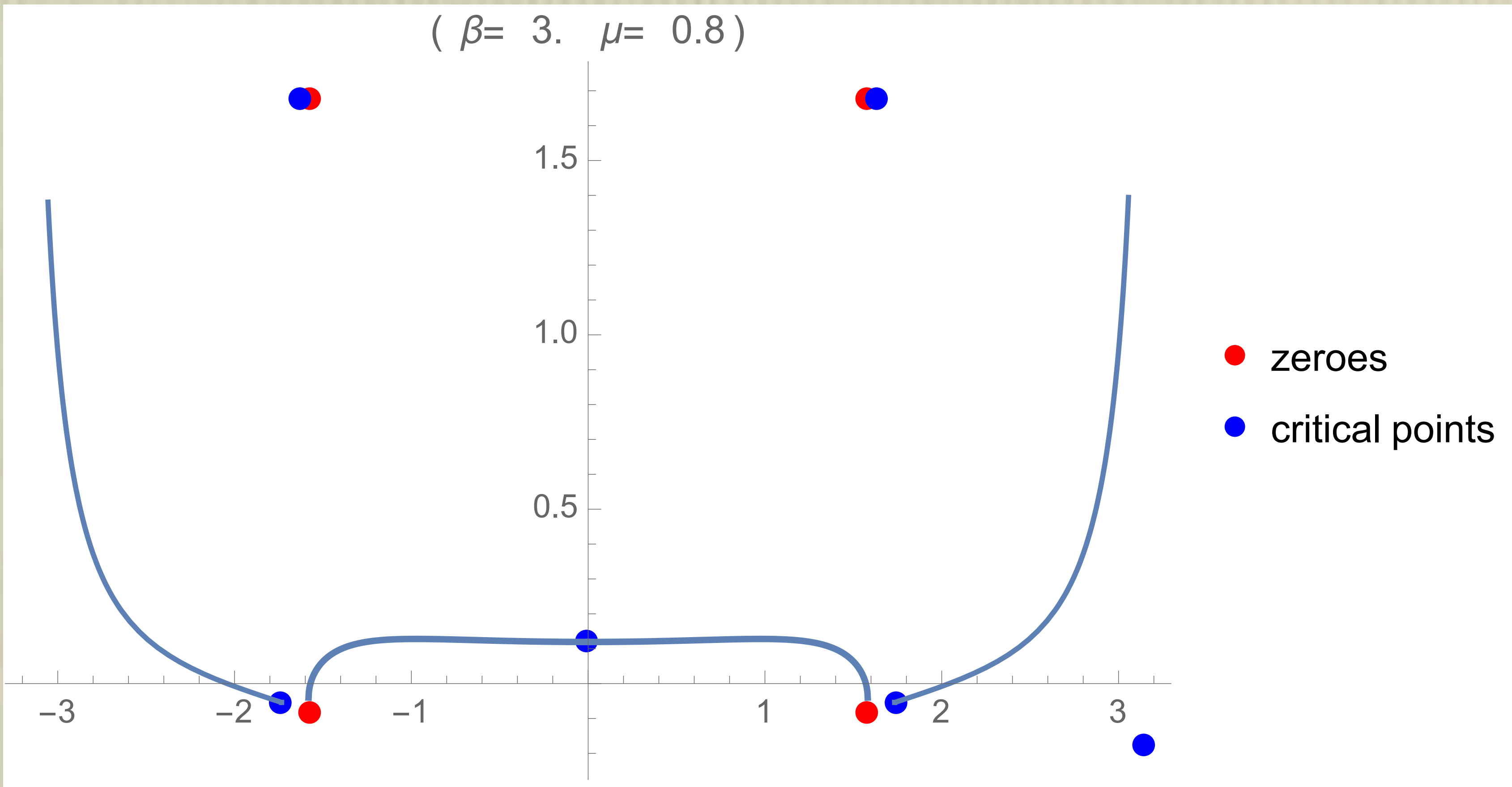
Thimble contributions



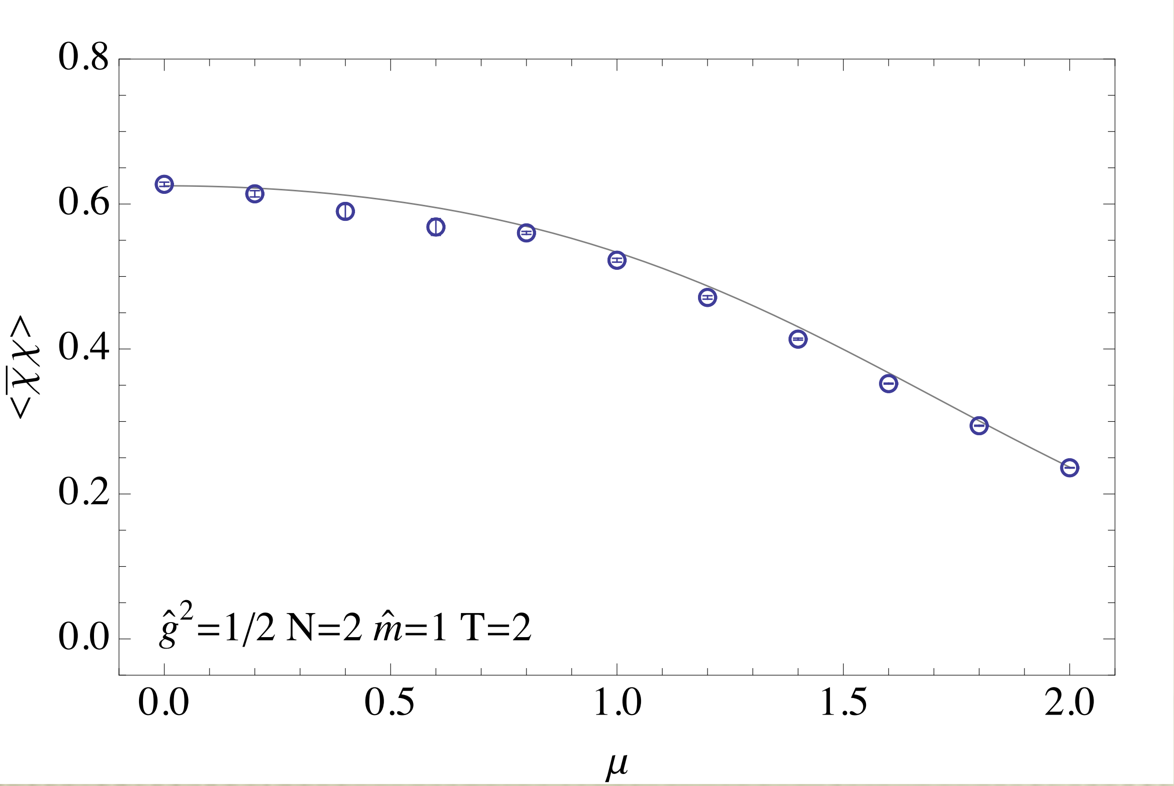
Thimble contributions

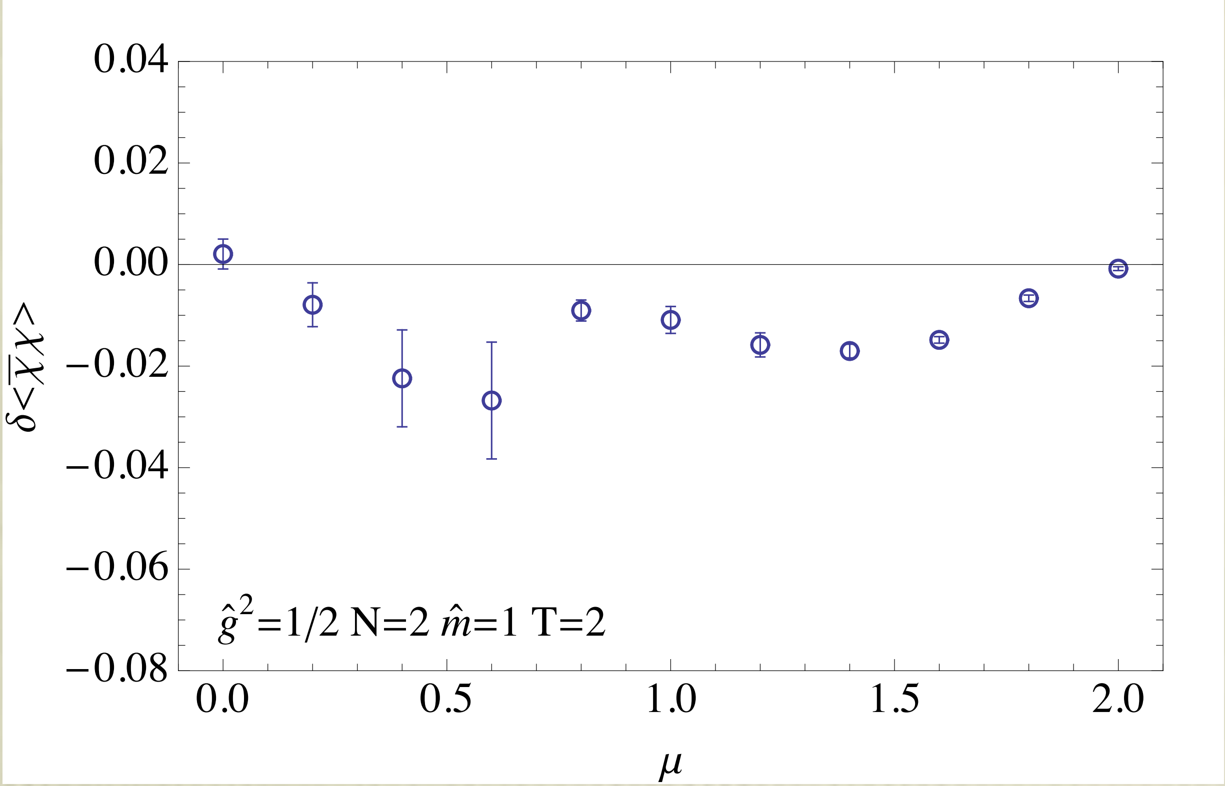


Thimble contributions

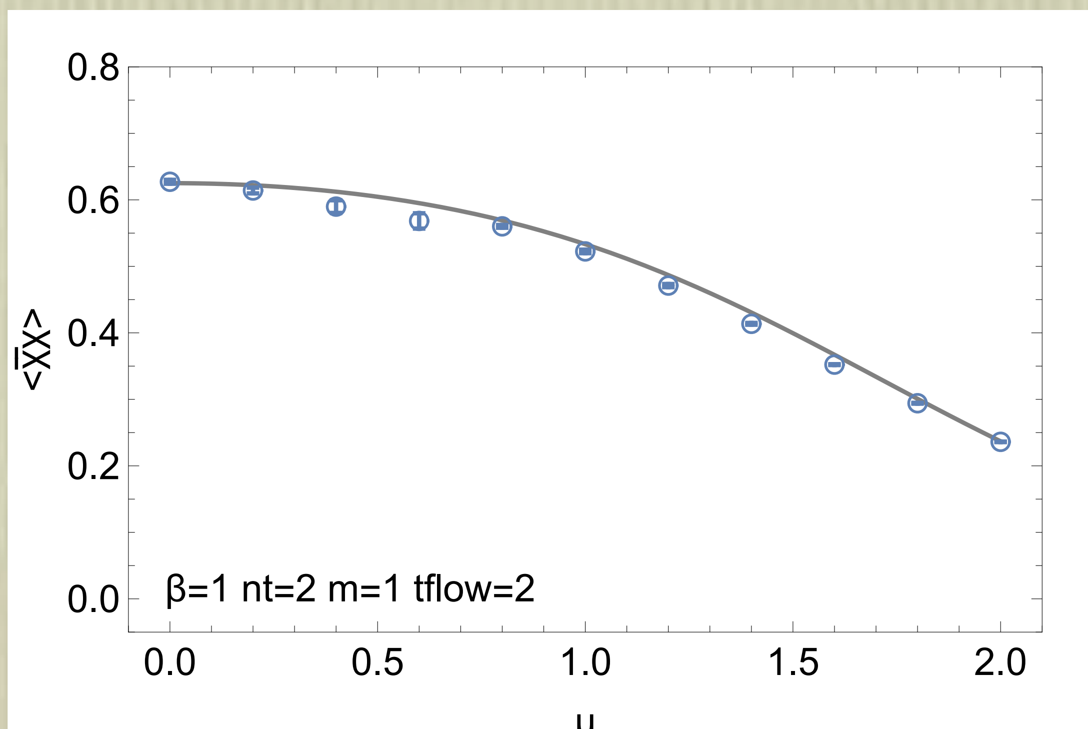


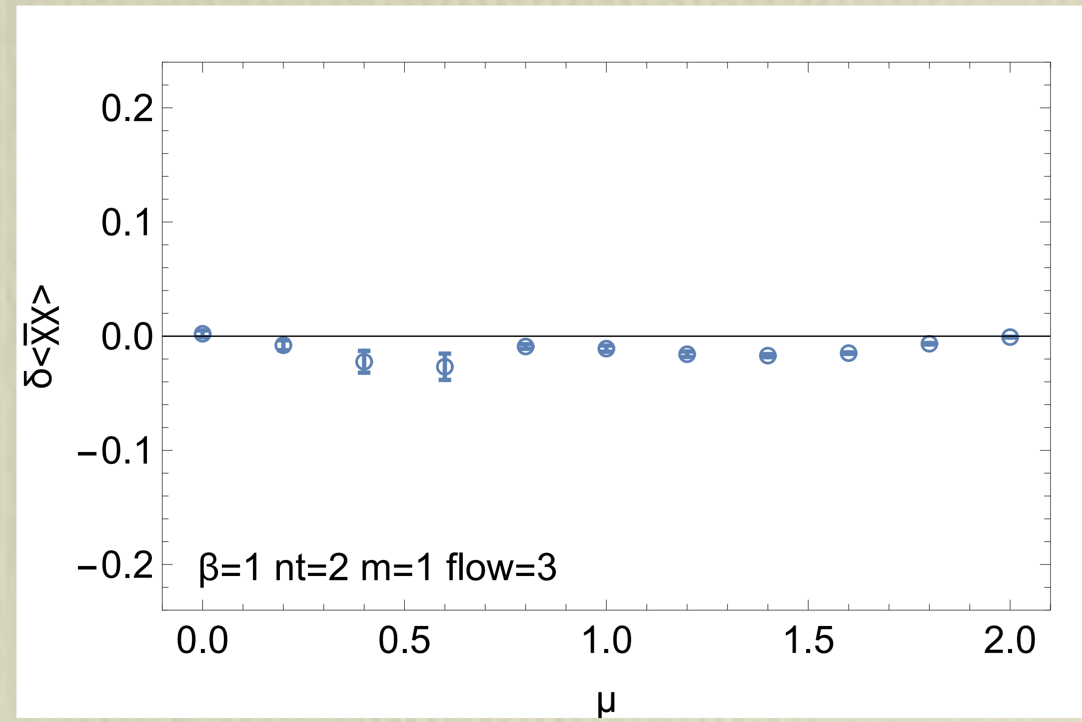
Strong coupling

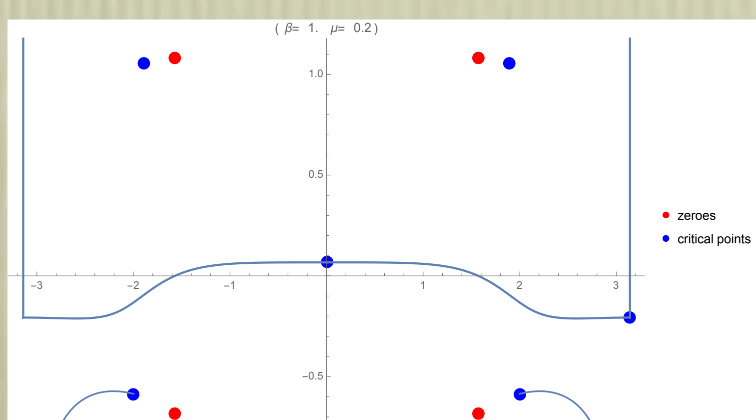


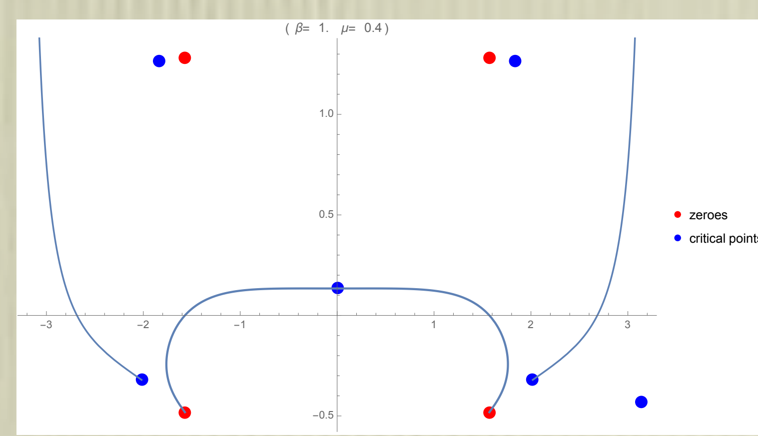


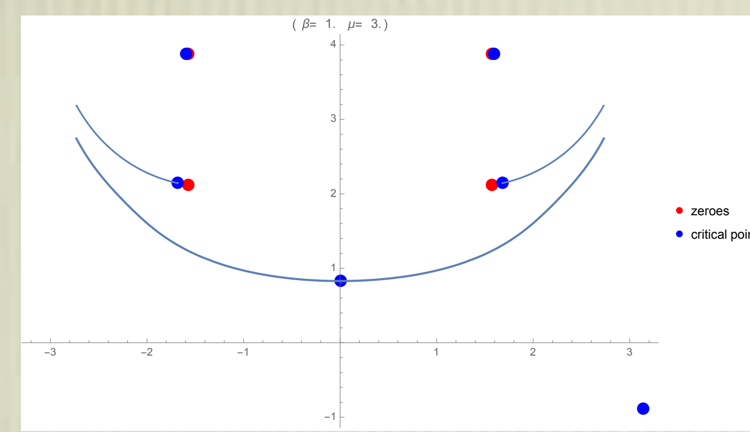
Contributing thimbles



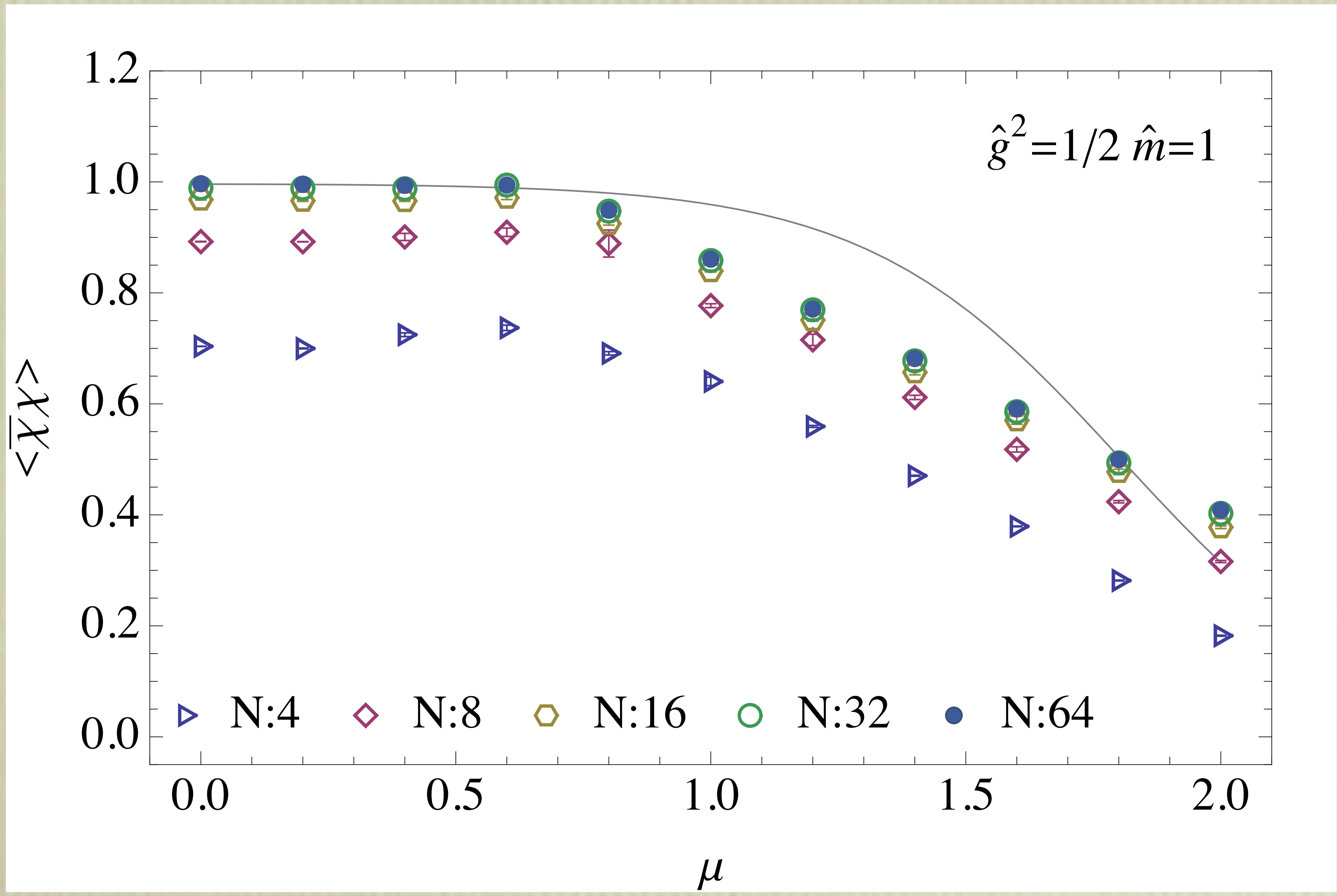






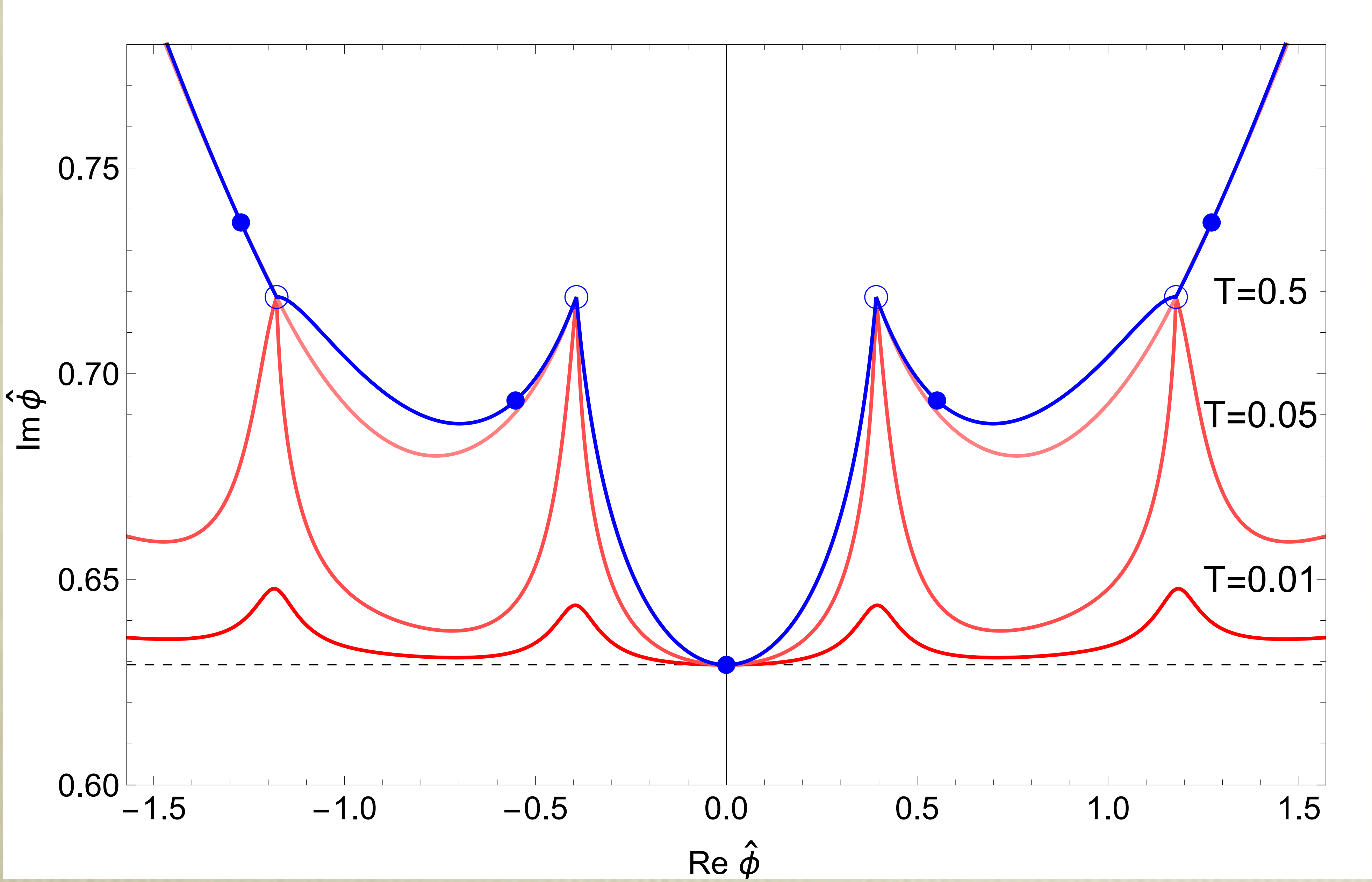


Strong coupling (cont limit)

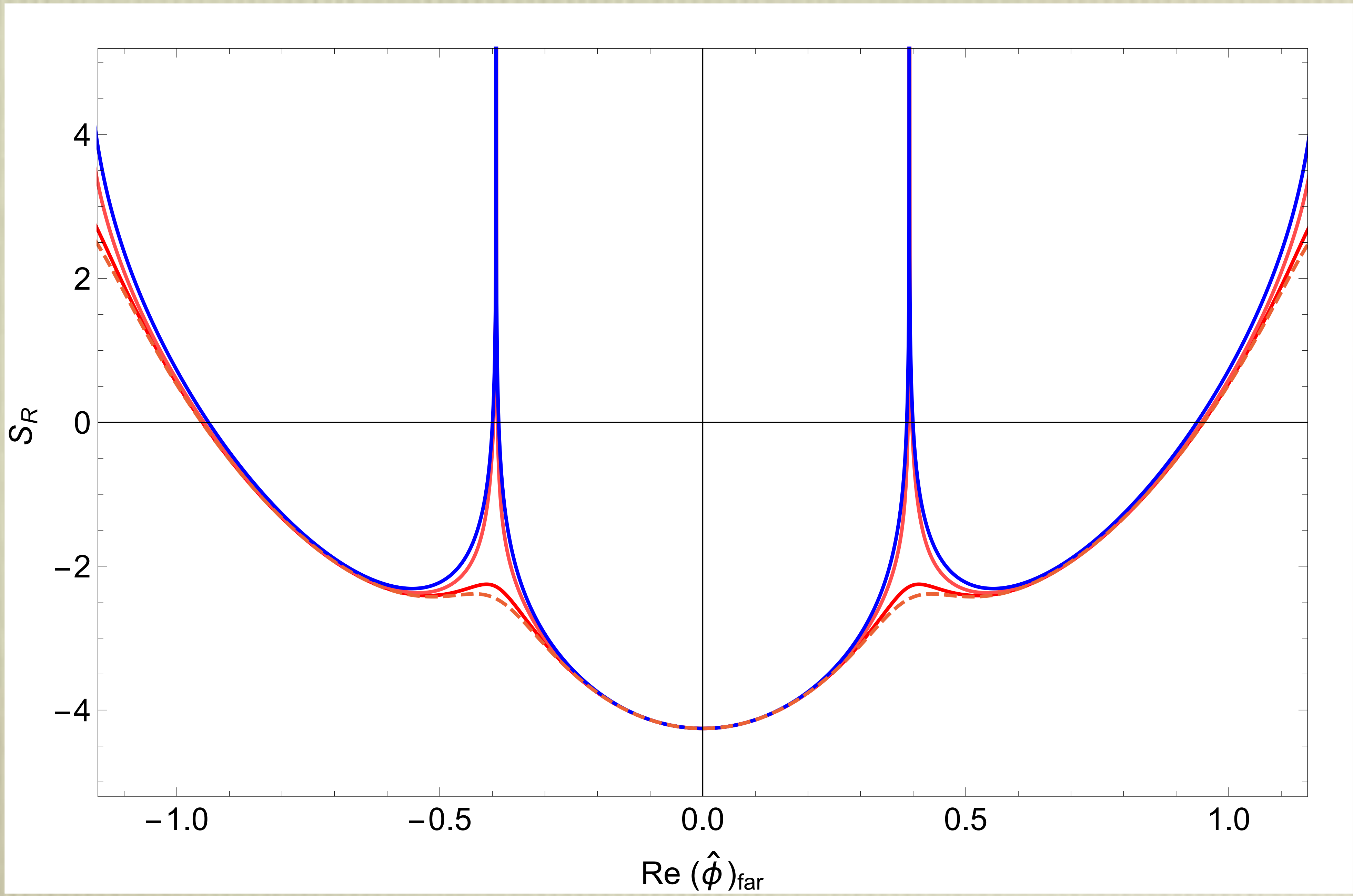


Beyond thimbles

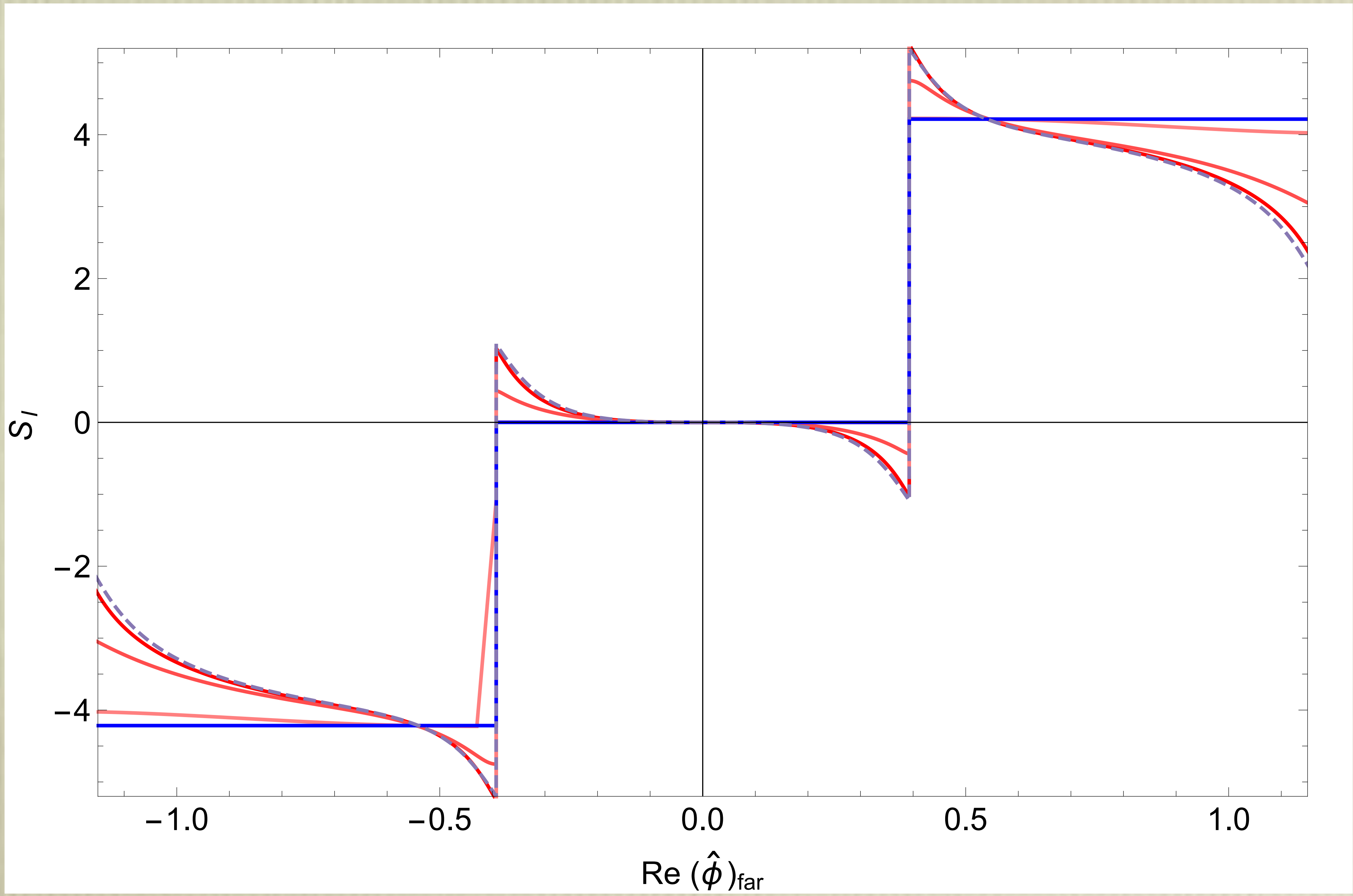
Thimble approximations



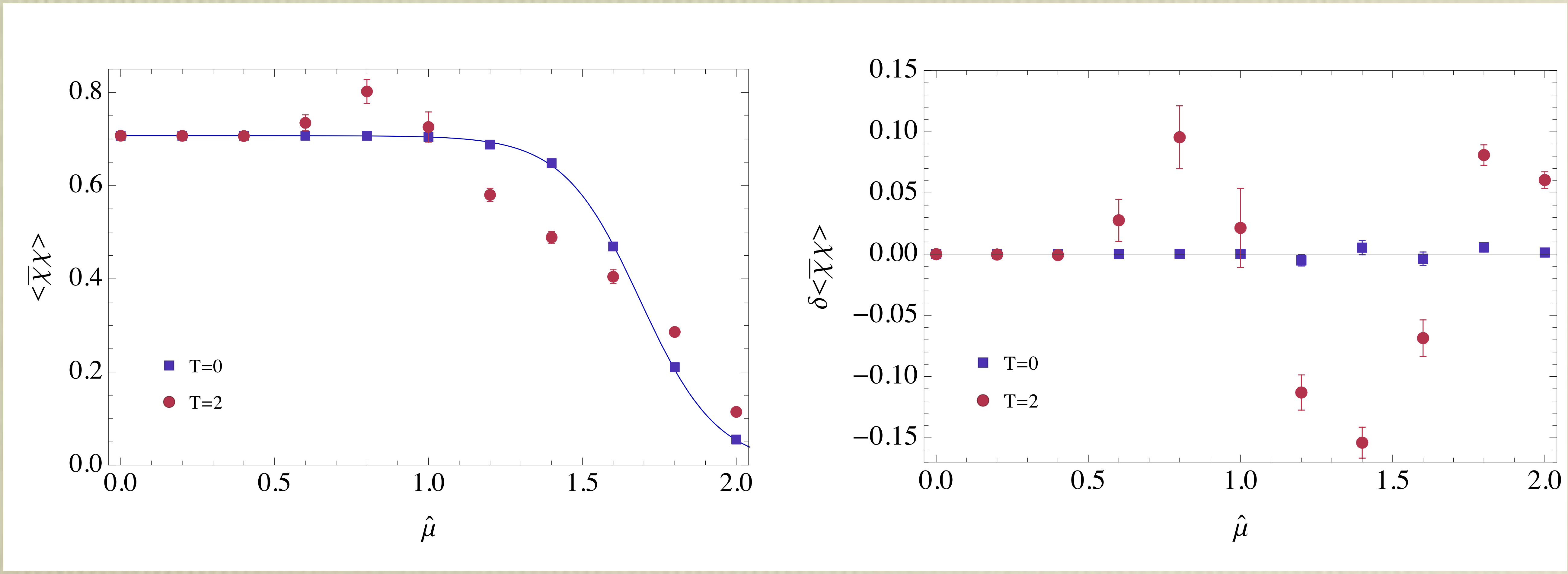
Action on thimbles



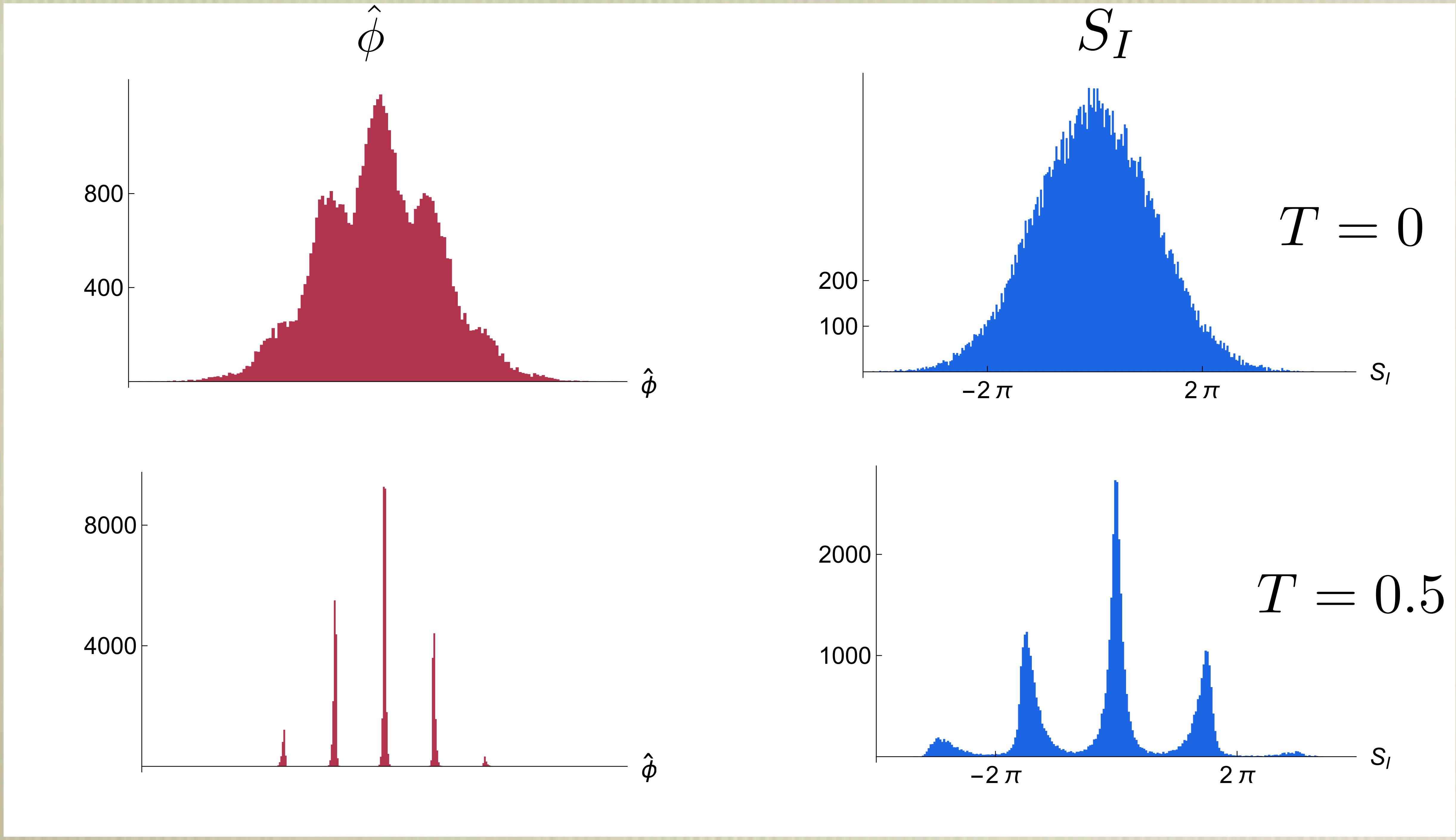
Action on thimbles



Strong coupling (revisited)



Taming the sign fluctuations



Conclusions and outlook

- Thimble integration is feasible for both bosonic and fermionic systems
- The residual phase fluctuations are mild
- In general multiple thimbles need to be considered, but it is still possible that in certain cases one thimble dominates
- Other manifolds might be more practical for numerical simulations, especially when thimble decomposition becomes cumbersome
- A number of challenges need to be overcome to attack large systems: hessian diagonalization, flow integration, etc.