DEFORMING PATH INTEGRALS: APPLICATIONS TO FERMIONS AT FINITE DENSITY

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Finite Density & The Sign Problem

$$\langle \mathcal{O} \rangle = \frac{1}{Z} \mathrm{tr}(\mathrm{e}^{-\beta(H-\mu N)} \mathcal{O}) = \frac{\int DA \; \mathrm{e}^{-S(A)} \mathcal{O}(A)}{\int DA \; \mathrm{e}^{-S(A)}}$$

where $DA = \prod_{\mu x} dA_{\mu,x}$

Problem: S is complex

Monte Carlo with complex actions:

1. Reweighting

$$\langle \mathcal{O} \rangle = \frac{\int DA \; \mathrm{e}^{-S(A)} \mathcal{O}(A)}{\int DA \; \mathrm{e}^{-S(A)}}$$

$$= \frac{\int DA \; \mathrm{e}^{-\mathrm{Re}S(A)} \mathrm{e}^{-i\mathrm{Im}S(A)} \mathcal{O}(A) / \int DA \; \mathrm{e}^{-\mathrm{Re}S(A)}}{\int DA \; \mathrm{e}^{-\mathrm{Re}S(A)} \mathrm{e}^{-i\mathrm{Im}S(A)} / \int DA \; \mathrm{e}^{-\mathrm{Re}S(A)}}$$

$$= \frac{\langle \mathrm{e}^{-i\mathrm{Im}S(A)} \mathcal{O}(A) \rangle_{\mathrm{Re}S}}{\langle \mathrm{e}^{-i\mathrm{Im}S(A)} \rangle_{\mathrm{Re}S}} \text{, with } \mathrm{Pr}(A) = \frac{\mathrm{e}^{-\mathrm{Re}S(A)}}{\int DA \; \mathrm{e}^{-\mathrm{Re}S(A)}}$$

Monte Carlo with complex actions:

2. Sample according to $\Pr(A) = \dfrac{\mathrm{e}^{-\mathrm{Re}S(A)}}{\int DA\ \mathrm{e}^{-\mathrm{Re}S(A)}}$

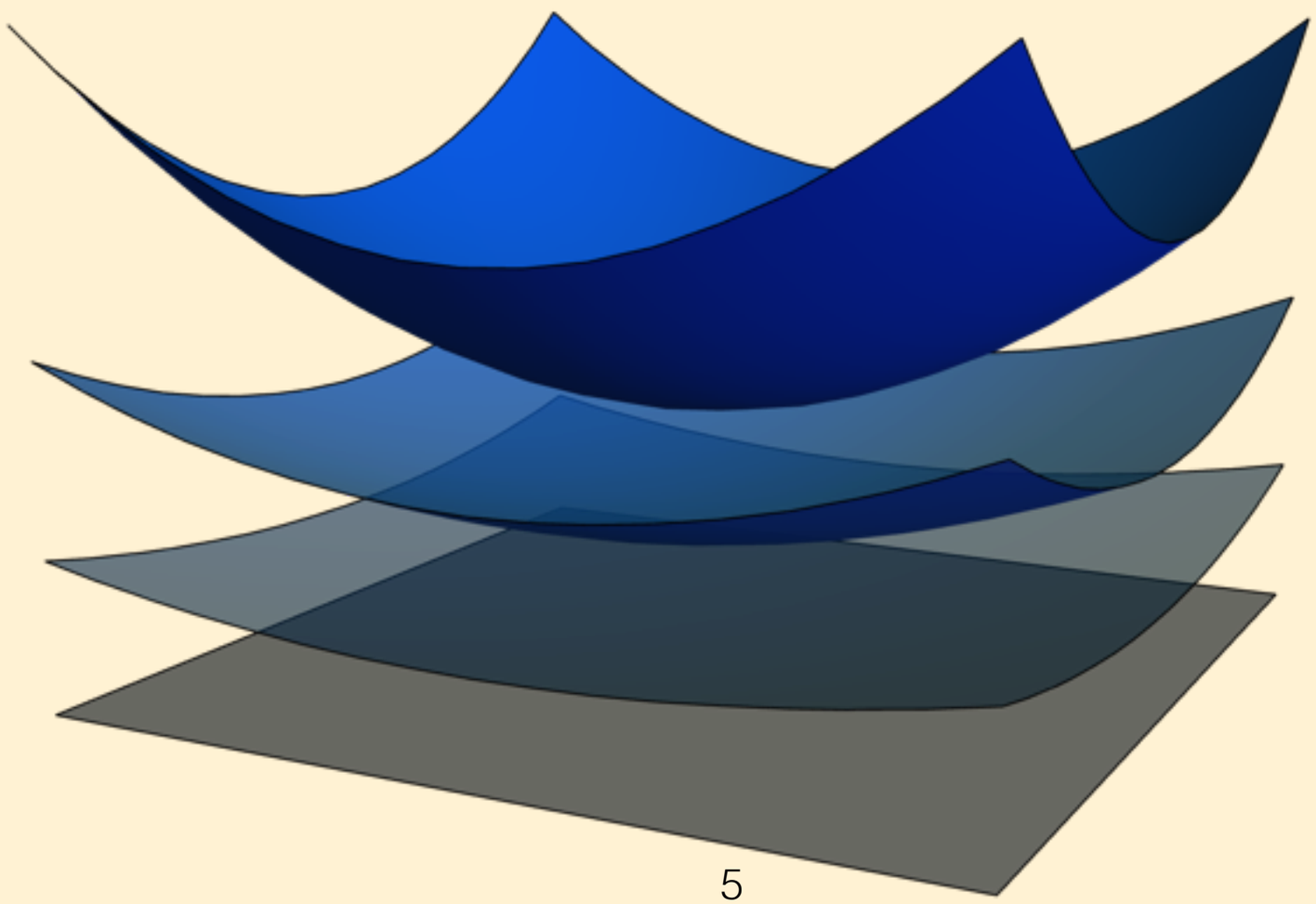
3. Estimate averages

$$\langle \mathcal{O} \rangle = \frac{\langle \mathrm{e}^{-i\mathrm{Im}S(A)} \mathcal{O}(A) \rangle_{\mathrm{Re}S}}{\langle \mathrm{e}^{-i\mathrm{Im}S(A)} \rangle_{\mathrm{Re}S}} \simeq \frac{\frac{1}{\mathcal{N}} \sum_{n=1}^{\mathcal{N}} \mathrm{e}^{-i\mathrm{Im}S(A_n)} \mathcal{O}(A_n)}{\frac{1}{\mathcal{N}} \sum_{n=1}^{\mathcal{N}} \mathrm{e}^{-i\mathrm{Im}S(A_n)}}$$

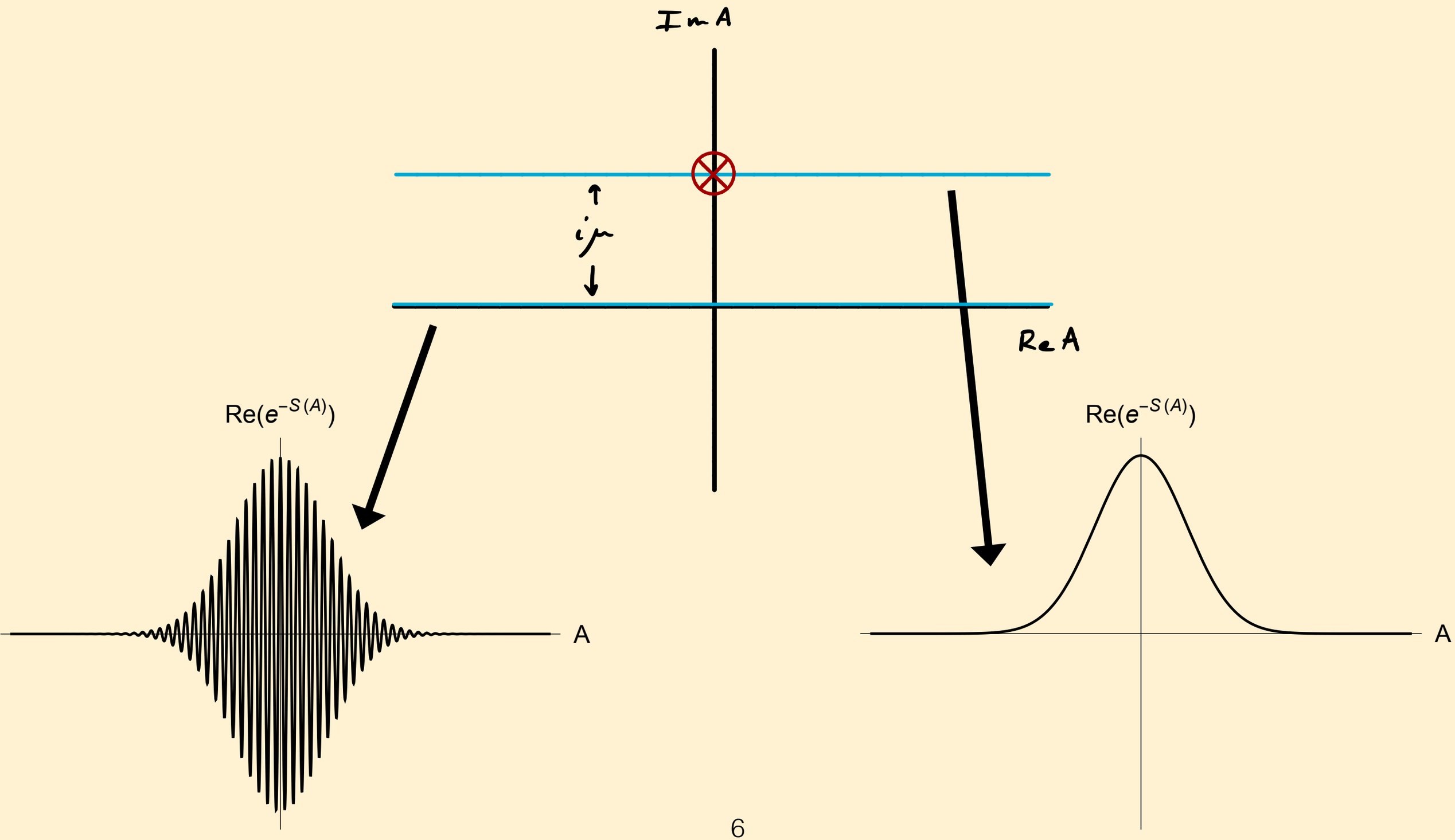
exponentially small in spacetime volume

Main Idea: Deform the Contour

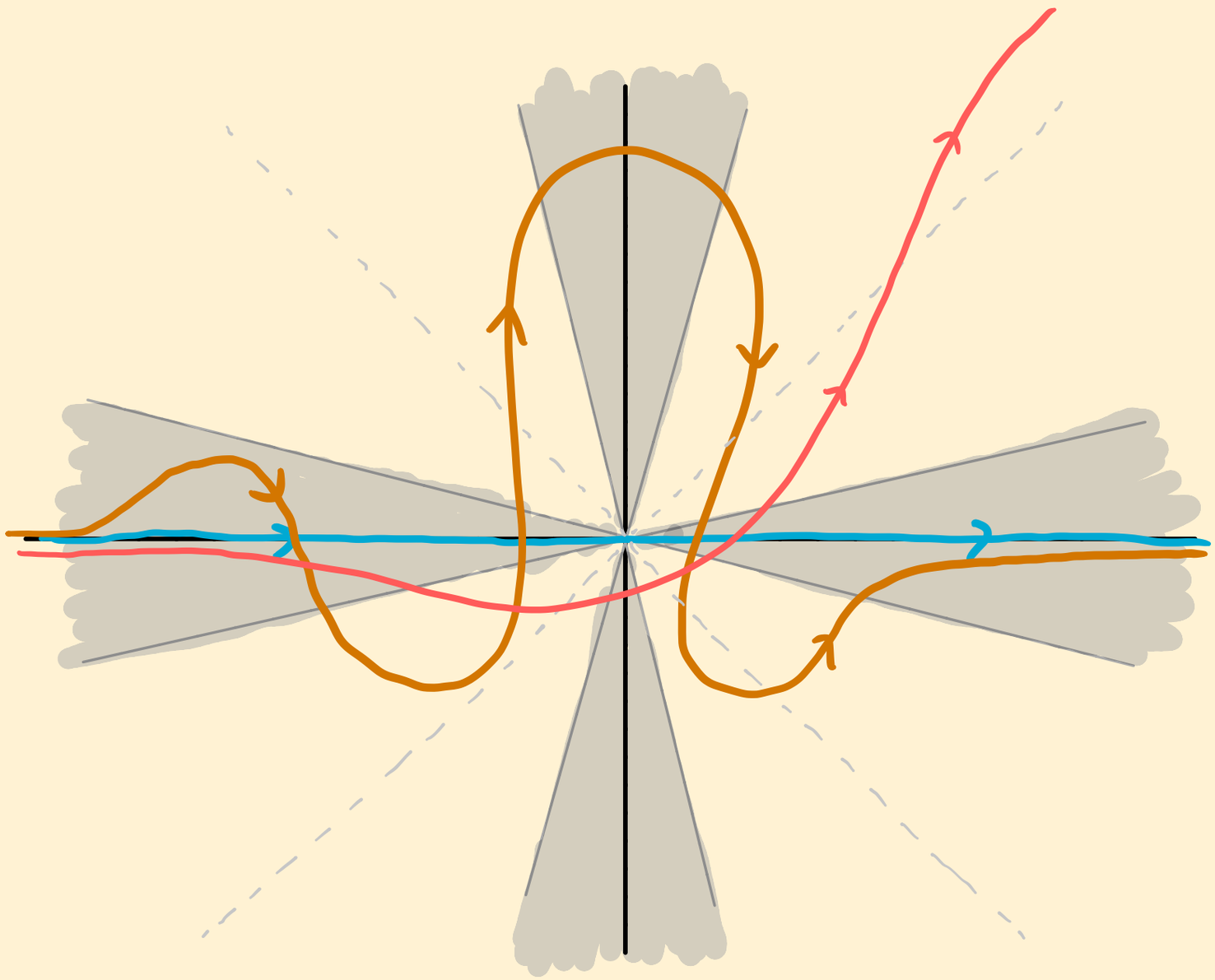
$$\int_{\mathbb{R}^N} DA\, \mathrm{e}^{-S(A)} = \int_{\mathcal{M}} D\tilde{A}\, \mathrm{e}^{-S(\tilde{A})}$$



$$Z = \int dA \; \mathrm{e}^{-(A-i\mu)^2} = \sqrt{\pi}$$



$$Z = \int dA \; \mathrm{e}^{-S(A)} \quad , \quad S(A) = A^4 + mA^2 + i\mu A$$



all contours yield the same integral

=

same homology class

Integrating in Principle

$$\langle \mathcal{O} \rangle = \frac{\int_{\mathbb{R}^n} DA \; \mathrm{e}^{-S} \mathcal{O}(A)}{\int_{\mathbb{R}^n} DA \; \mathrm{e}^{-S}}$$

Cauchy's theorem

$$= \frac{\int_{\mathcal{M}} D\tilde{A} \; \mathrm{e}^{-S} \mathcal{O}(\tilde{A})}{\int_{\mathcal{M}} D\tilde{A} \; \mathrm{e}^{-S}}$$

Choose coordinates

$$= \frac{\int_{\mathbb{R}^n} DA \; \det J(A) \mathrm{e}^{-S} \mathcal{O}(\tilde{A}(A))}{\int_{\mathbb{R}^n} DA \; \det J(A) \mathrm{e}^{-S}}$$

Integrating in Practice

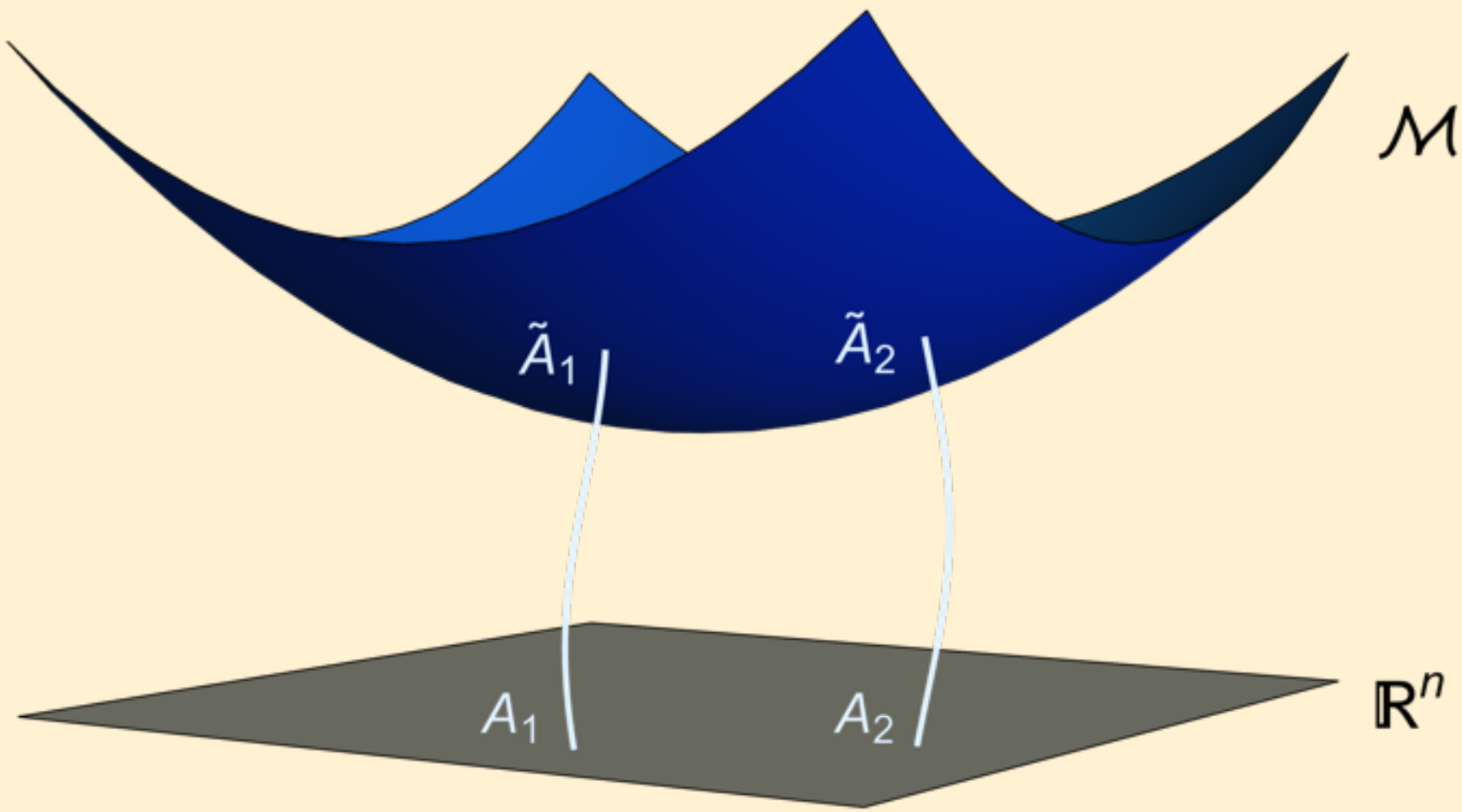
1. Define $S_{\text{eff}}(A) = S(\tilde{A}(A)) - \ln J(A)$

2. Sample according to $\Pr(A) = \dfrac{\mathrm{e}^{-\mathrm{Re}S_{\text{eff}}(A)}}{\int DA\ \mathrm{e}^{-\mathrm{Re}S_{\text{eff}}(A)}}$

3. Reweigh $\langle \mathcal{O} \rangle = \dfrac{\langle \mathrm{e}^{-i\mathrm{Im}S_{\text{eff}}(A)} \mathcal{O}(A) \rangle_{\mathrm{Re}S_{\text{eff}}}}{\langle \mathrm{e}^{-i\mathrm{Im}S_{\text{eff}}(A)} \rangle_{\mathrm{Re}S_{\text{eff}}}}$

Holomorphic Gradient Flow

Evolve points as $\frac{dA}{ds} = \overline{\frac{\partial S}{\partial A}}$

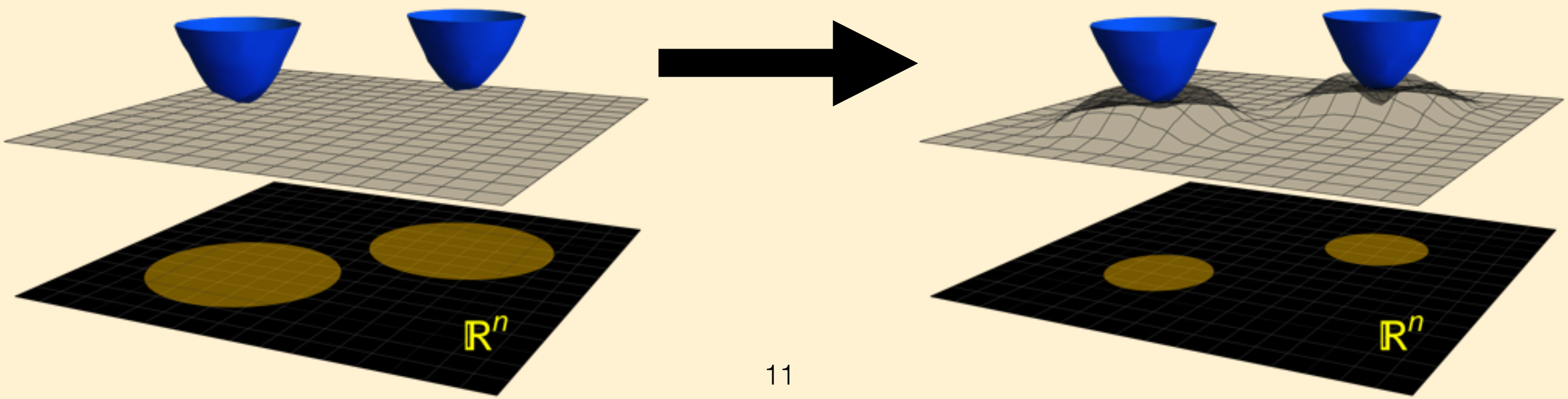


Jacobian evolves as $\frac{dJ}{ds} = \overline{(HJ)}$ with $H_{ij} = \frac{\partial^2 S}{\partial A_i \partial A_j}$

How is the sign problem tamed?

$\mathrm{Re}(S)$ strictly increases while $\mathrm{Im}(S)$ is stationary:

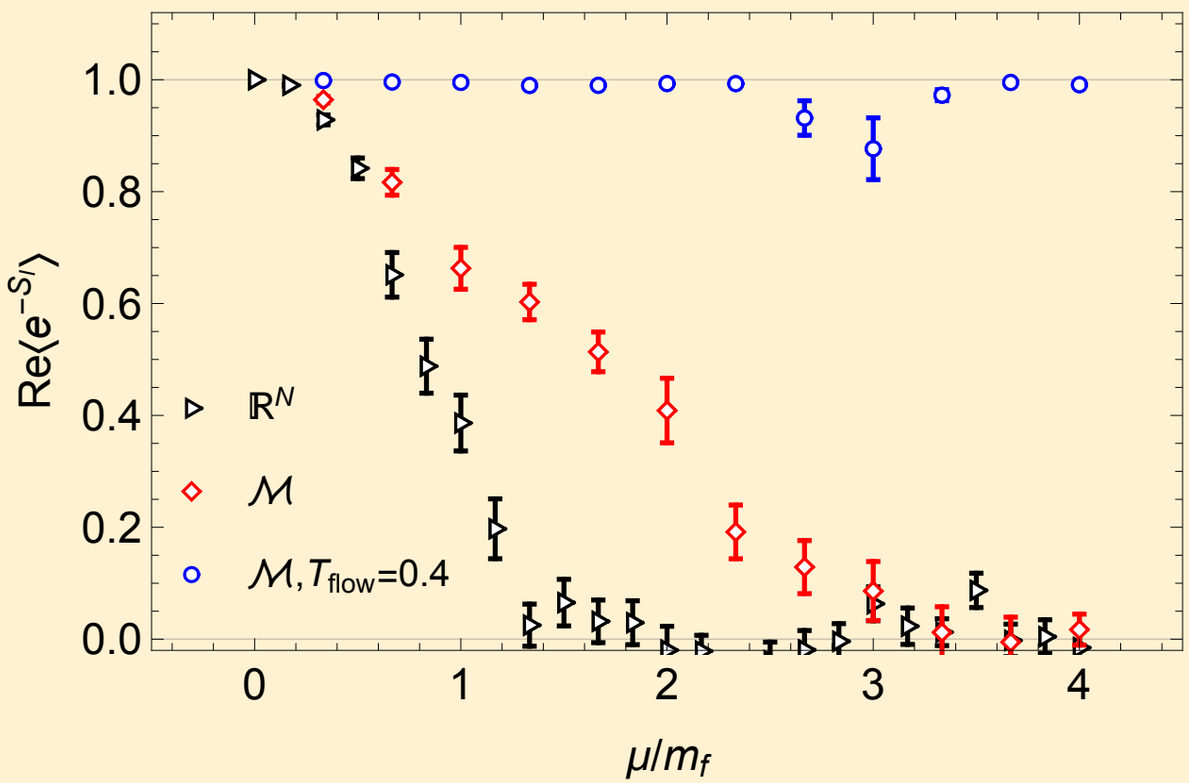
$$\frac{d}{ds}S(A) = \frac{\partial S}{\partial A_i}\frac{dA_i}{ds} = \frac{\partial S}{\partial A_i}\overline{\frac{\partial S}{\partial A_i}} > 0$$

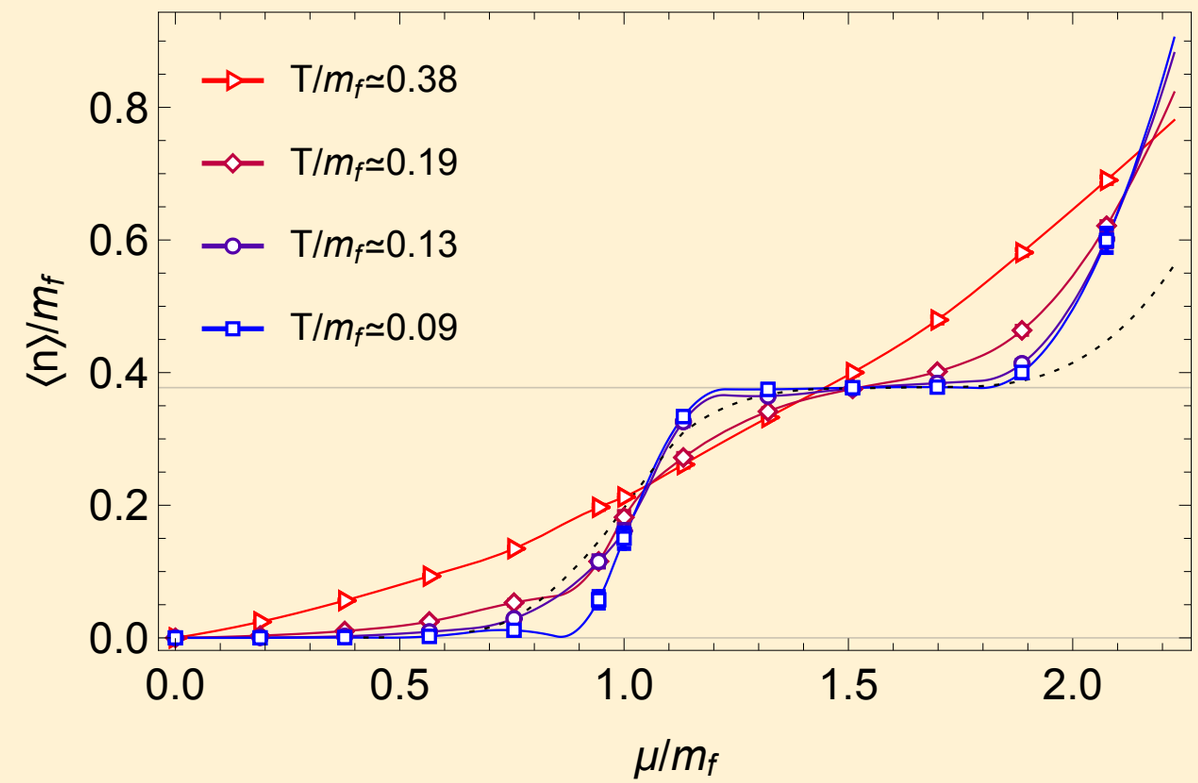


Application to (1+1) Thirring model

$$S = \int d^2x \Big[\overline{\psi}\Big(\gamma^\mu \partial_\mu + m + \mu\gamma^0\Big)\psi + \frac{g^2}{2}(\overline{\psi}\gamma^\mu\psi)^2\Big]$$

$$\longrightarrow \int d^2x \Big[\frac{1}{2g^2}A_\mu A^\mu + \overline{\psi}(\partial\!\!\!/ + iA\!\!\!/ + m + \mu\gamma^0)\psi\Big]$$





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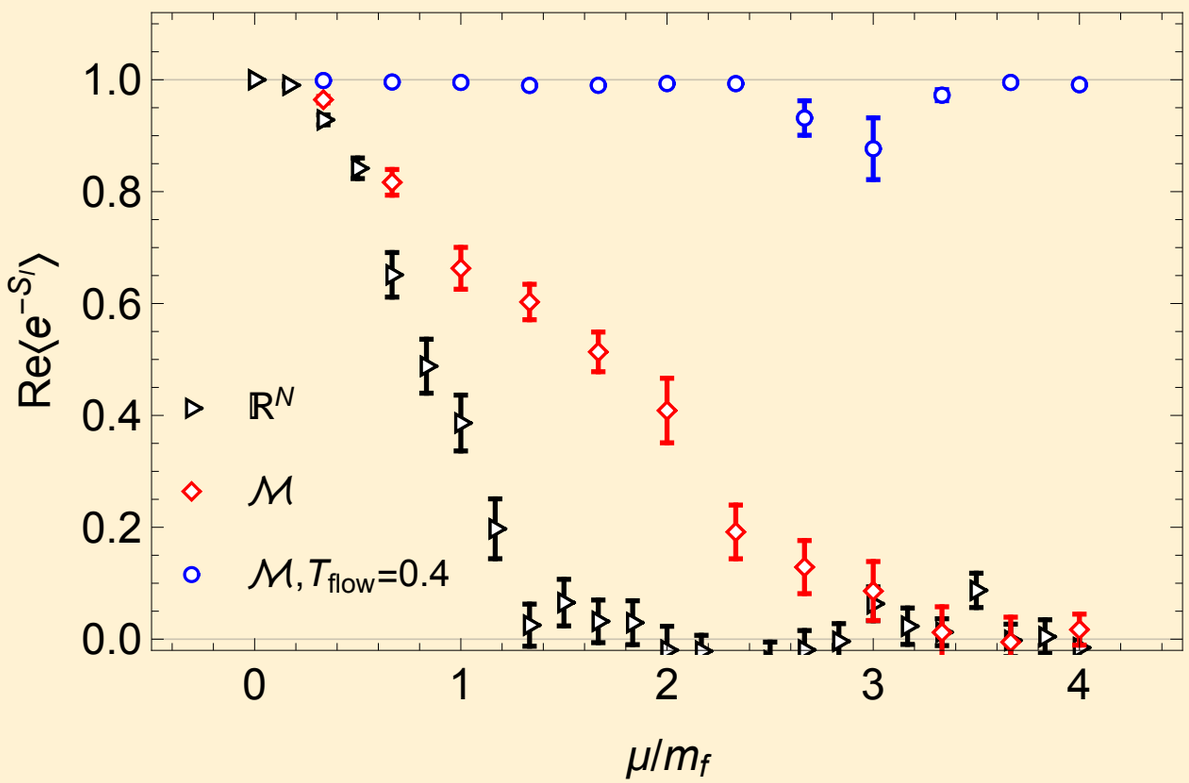
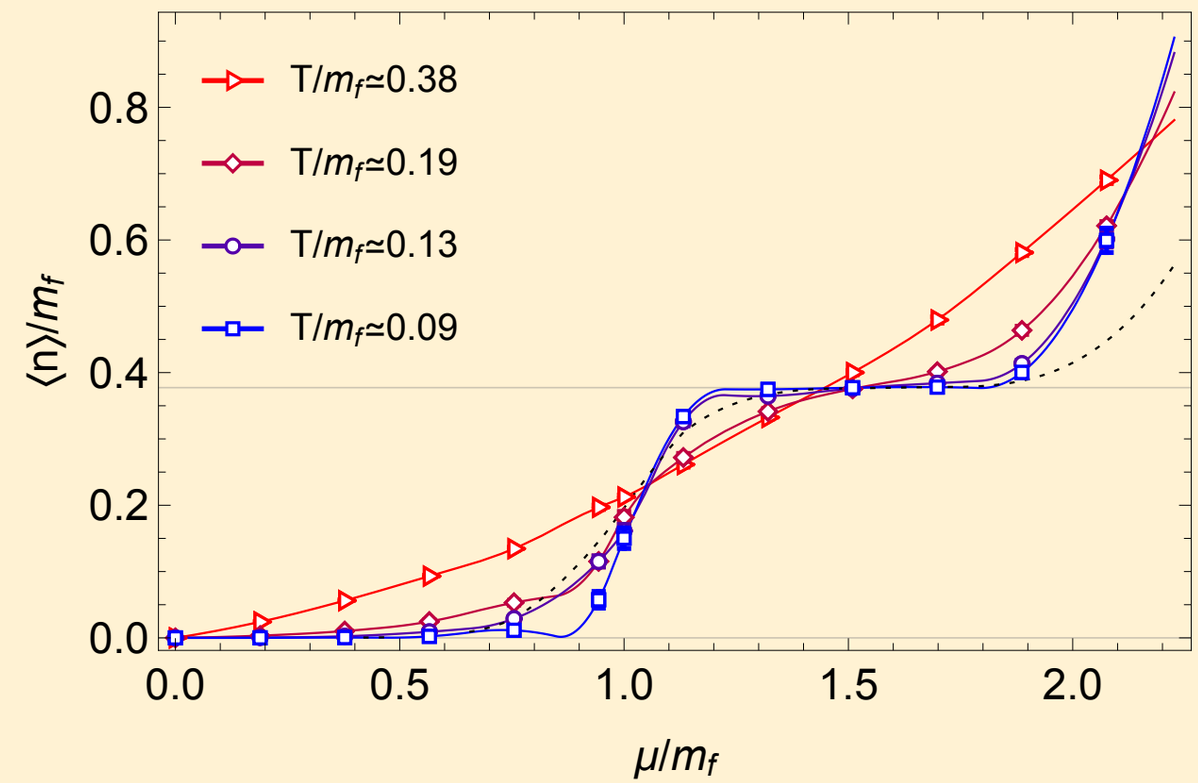




Issue: Jacobian is expensive

Solution: Sign Optimized Manifolds

Uncertainty in observables $\langle \mathcal{O} \rangle = \dfrac{\left\langle \mathcal{O}\ \mathrm{e}^{-i\mathrm{Im}(S)} \right\rangle_R}{\left\langle \mathrm{e}^{-i\mathrm{Im}(S)} \right\rangle_R}$

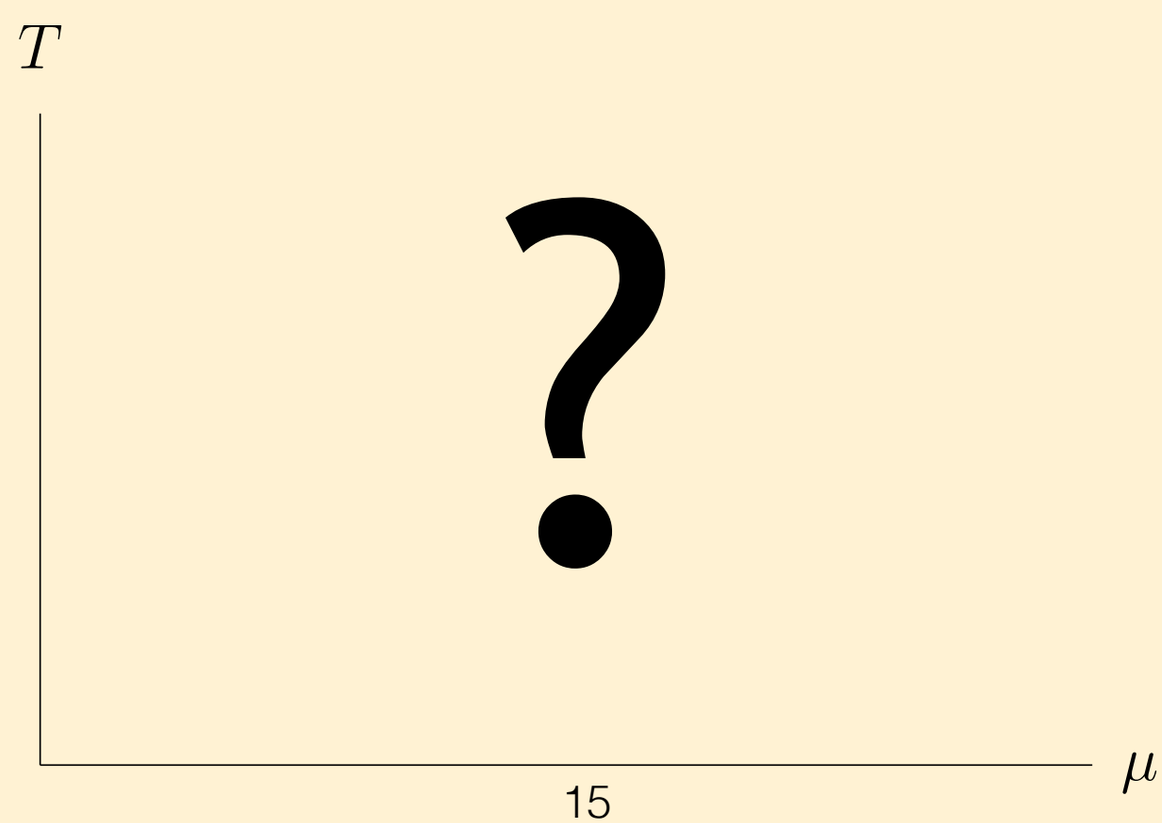
come from small "average sign" $\langle \sigma \rangle \equiv \left\langle \mathrm{e}^{-i\mathrm{Im}S} \right\rangle_R$

Maximize average sign over
family of manifolds with cheap Jacobians

Application to (2+1) Thirring model

$$S = \int d^3x \left[\overline{\psi}(\partial\!\!\!/ + m + \mu\gamma^0)\psi + \frac{g^2}{2}(\overline{\psi}\gamma^\mu\psi)^2 \right]$$

$$\longrightarrow \int d^3x \left[\frac{1}{2g^2} A_\mu A^\mu + \overline{\psi}(\partial\!\!\!/ + iA\!\!\!/ + m + \mu\gamma^0)\psi \right]$$



Sign Optimized Manifolds

1. Propose family of manifolds

$$\tilde{A}_{0x}(A) = A_{0x} + i(\lambda_1 + \lambda_2 \cos(A_{0x}) + \lambda_3 \cos(2A_{0x}))$$

three parameter family

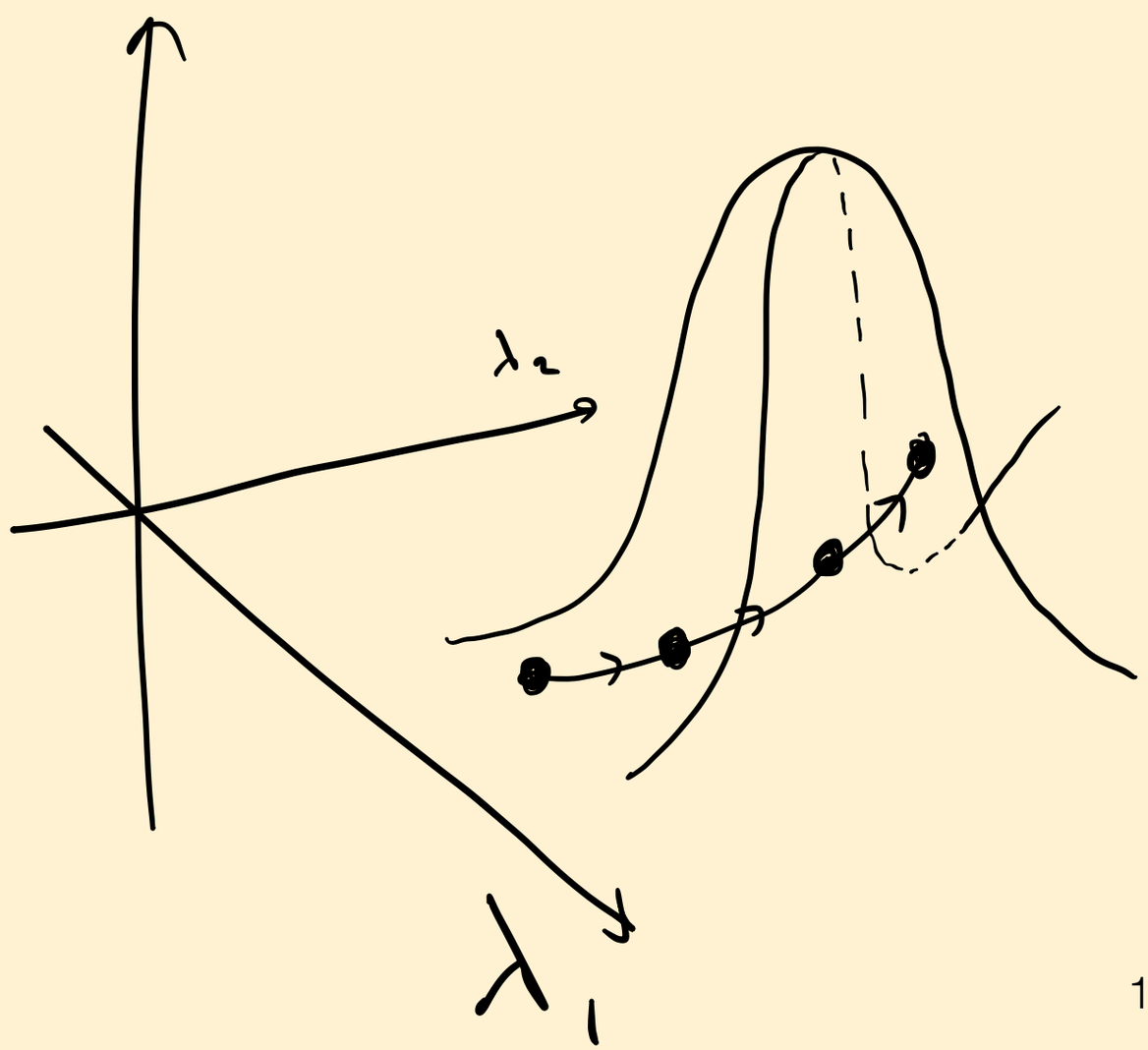
Feature: Manifold is factorizable

$$J_{xy} = \frac{\partial \tilde{A}_{0x}}{\partial A_{0y}} = \delta_{xy} \times g(A_{0x})$$

Sign Optimized Manifolds

2. Maximize average sign over family

$\langle e^{-i\,\mathrm{Im}\,S} \rangle_R$



$$\langle \mathcal{O} \rangle = \frac{\left\langle \mathcal{O}\ \mathrm{e}^{-i\mathrm{Im}(S)} \right\rangle_R}{\left\langle \mathrm{e}^{-i\mathrm{Im}(S)} \right\rangle_R}$$

need precision
if small

Sign Optimized Manifolds

2. Maximize average sign over family

$$\langle \sigma \rangle \equiv \langle \mathrm{e}^{-i\mathrm{Im}S} \rangle_R$$

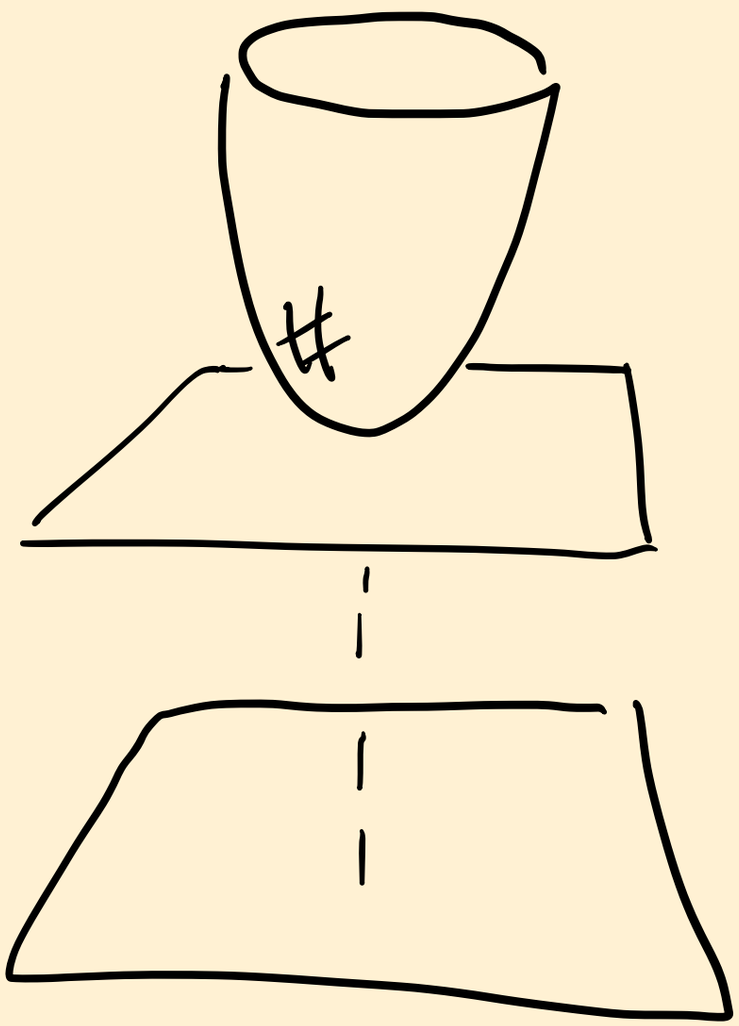
$$\nabla_\lambda \langle \sigma \rangle = |\langle \sigma \rangle| \frac{\int DA\ \mathrm{e}^{-\mathrm{Re}(S)} \left[\nabla_\lambda \mathrm{Re}(S) - \mathrm{tr}(J^{-1} \nabla_\lambda J) \right]}{\int DA\ \mathrm{e}^{-\mathrm{Re}(S)}}$$

sign problem free = cheap

Sign Optimized Manifolds

3. Integrate over optimal manifold

Tangent Shift



Saturation Limit

$$Z = \left(\int dA \, \mathrm{e}^{-S(A)} \right)^{\beta V}$$

$$\tilde{A}_{0x}(A) = A_{0x} + i(\lambda_1 + \lambda_2 \cos(A_{0x}) + \lambda_3 \cos(2A_{0x}))$$

Strategy

- Use sign opt. manifold
- HMC on manifold

HMC on Manifolds

$$Z = \int_{\mathbb{R}^N} DA \; \mathrm{e}^{-S(A)}$$

$$= \int_{\mathcal{M}} D\tilde{A} \; \mathrm{e}^{-S(\tilde{A})}$$

Cauchy's Theorem

$$= \int_{\mathbb{R}^N} DA \; \mathrm{det} J(A) \mathrm{e}^{-S(A)}$$

Choose coordinates

Want to sample as $\mathrm{Pr}(A) \propto |\mathrm{det} J(A)| \; \mathrm{e}^{-\mathrm{Re} S(A)}$

HMC on Manifolds

Standard HMC: $H(\pi, A) = \frac{1}{2}\sum_x \pi_x^2 + S(A)$

$$P(\pi, A) \propto \mathrm{e}^{-H(\pi,A)} \xrightarrow{\text{marginalize}} \sum_\pi P(\pi, A) \propto \mathrm{e}^{-S(A)}$$

HMC on Manifolds

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$$P(\pi, A) \propto \mathrm{e}^{-H(\pi,A)} \xrightarrow{\text{marginalize}} \sum_\pi P(\pi, A) \propto \mathrm{e}^{-S(A)}$$

Kinetic: $\frac{1}{2}\sum_x \pi_x^2 \longrightarrow \frac{1}{2}\sum_x \pi_x \left[J(A)J^\dagger(A)\right]^{-1}_{xy} \pi_y$

HMC on Manifolds

Standard HMC: $H(\pi, A) = \frac{1}{2}\sum_x \pi_x^2 + S(A)$

$$P(\pi, A) \propto \mathrm{e}^{-H(\pi,A)} \xrightarrow{\text{marginalize}} \sum_\pi P(\pi, A) \propto \mathrm{e}^{-S(A)}$$

Kinetic: $\frac{1}{2}\sum_x \pi_x^2 \longrightarrow \frac{1}{2}\sum_x \pi_x \left[J(A)J^\dagger(A)\right]^{-1}_{xy} \pi_y$

Manifold HMC: $H(\pi, A) = \frac{1}{2}\sum_x \pi_x \left[J(A)J^\dagger(A)\right]^{-1}_{xy} \pi_y + S(A)$

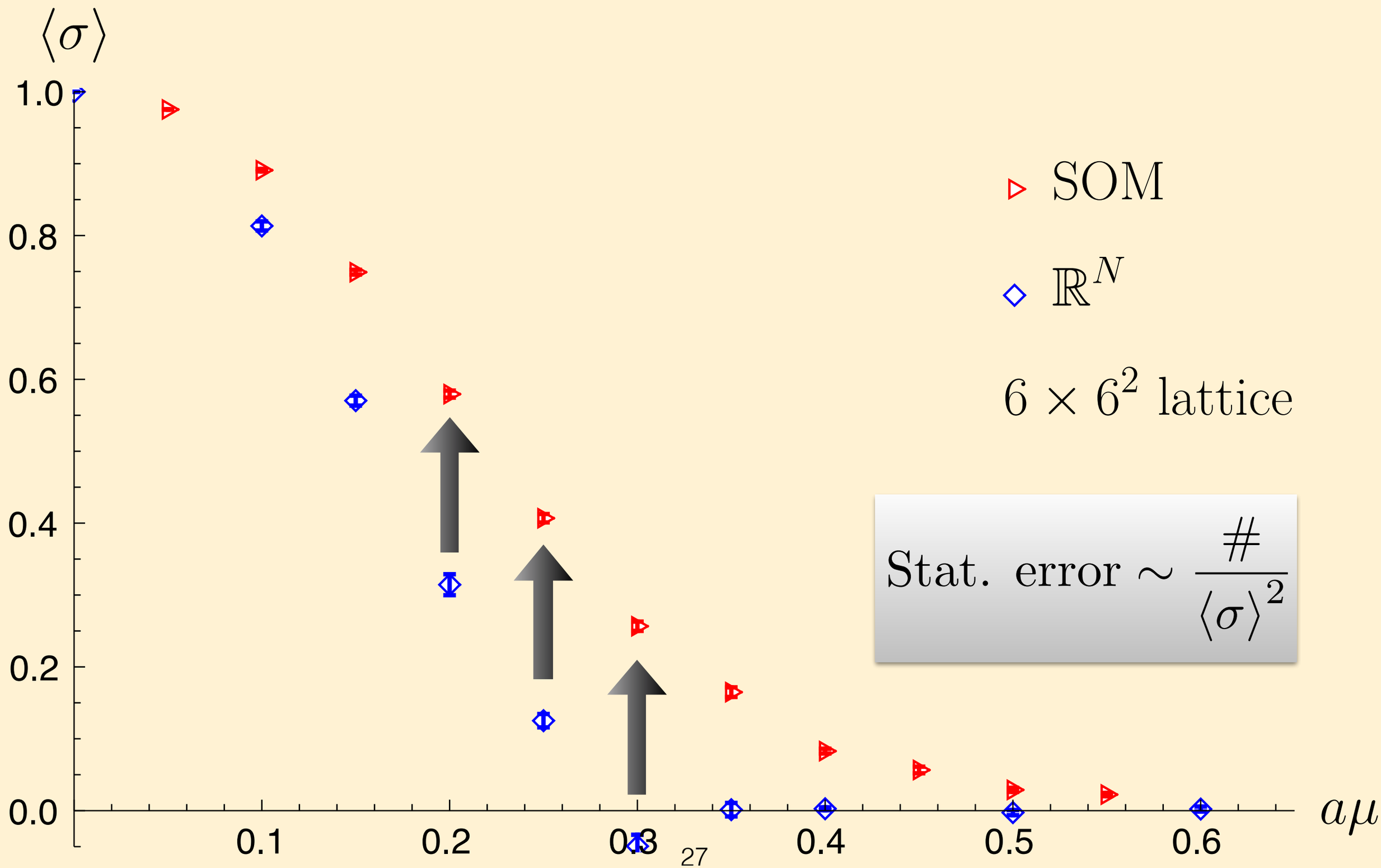
$$P(\pi, \phi) \propto e^{-H(\pi,\phi)} \xrightarrow{\text{marginalize}} \sum_\pi P(\pi, A) \propto \mathrm{e}^{-S(A)} |\det J(A)|$$

$$H(\pi, A) = \frac{1}{2} \sum_x \pi_x \left[J(A) J^\dagger(A) \right]^{-1}_{xy} \pi_y + S(A)$$

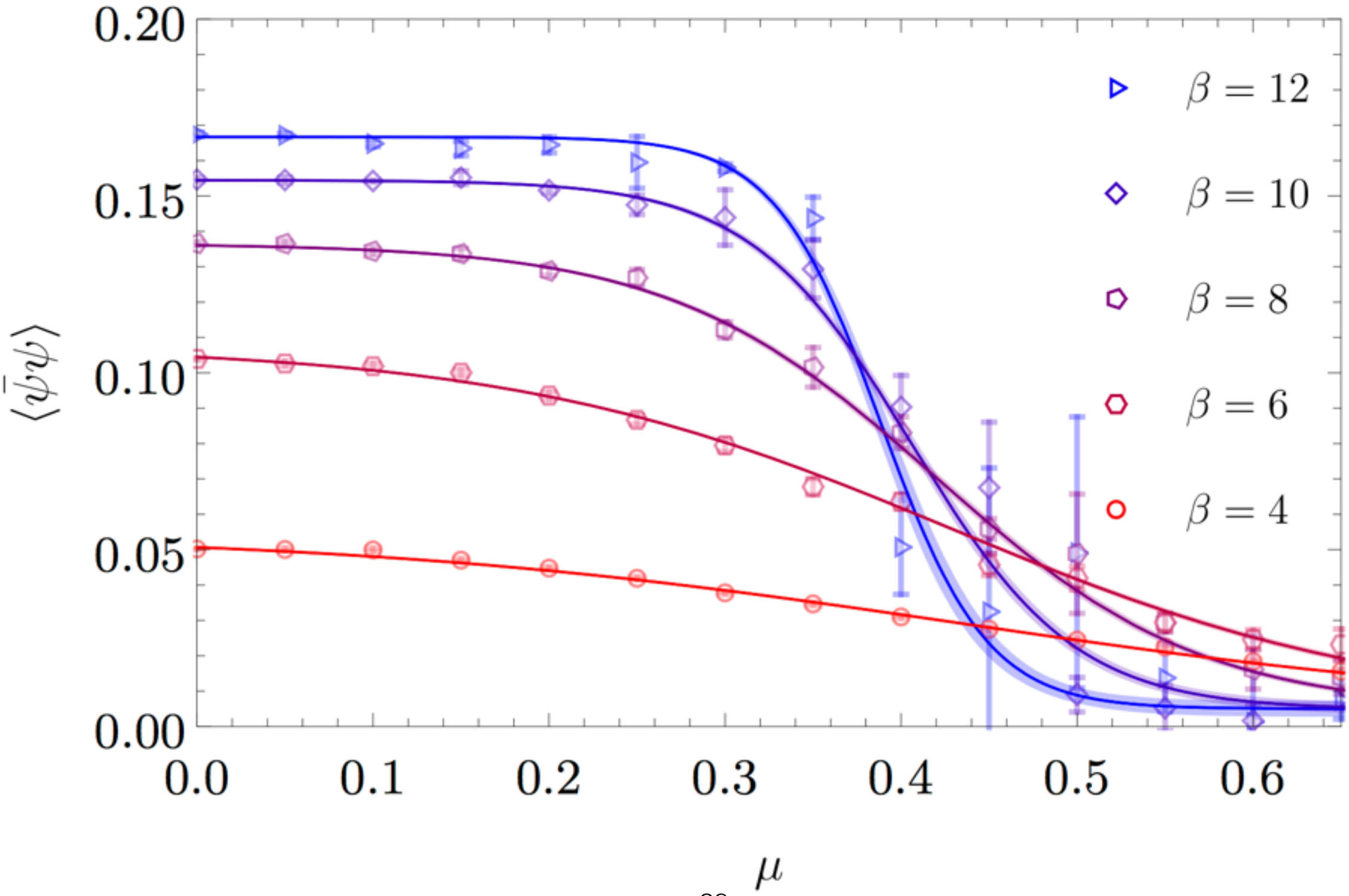
difficult if non-separable

SOM is key to HMC on manifolds

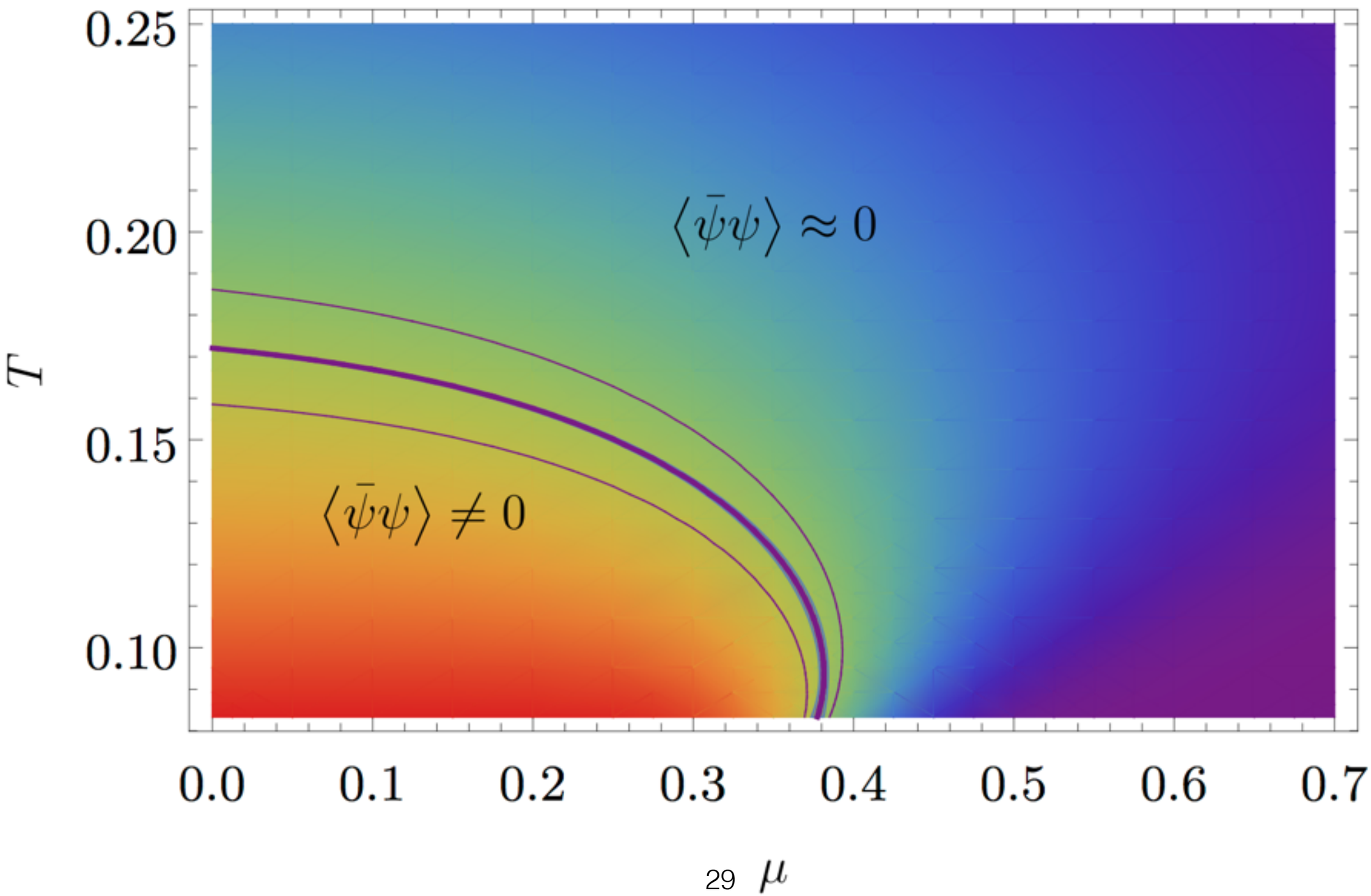
Sign Increases



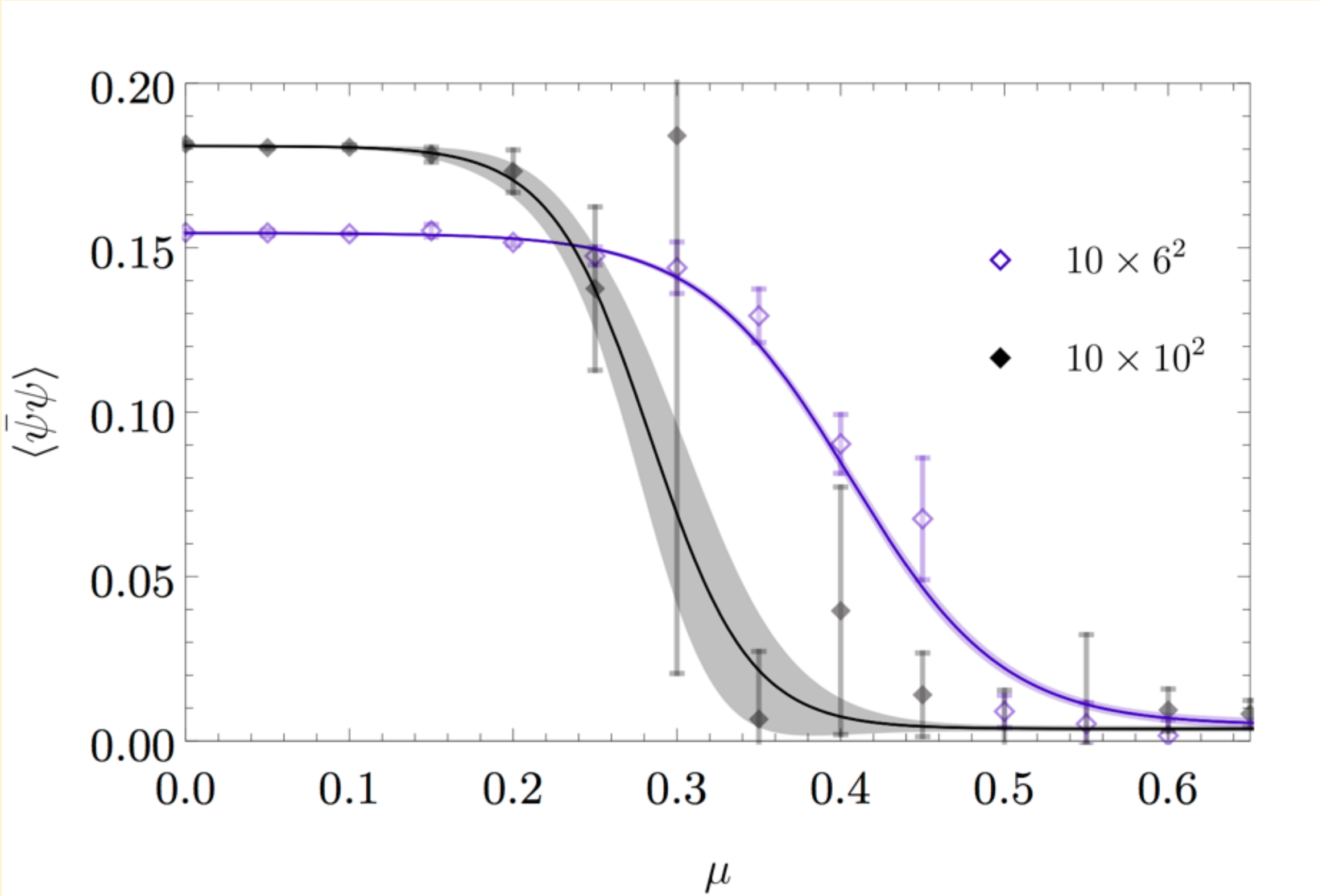
Chiral Condensate

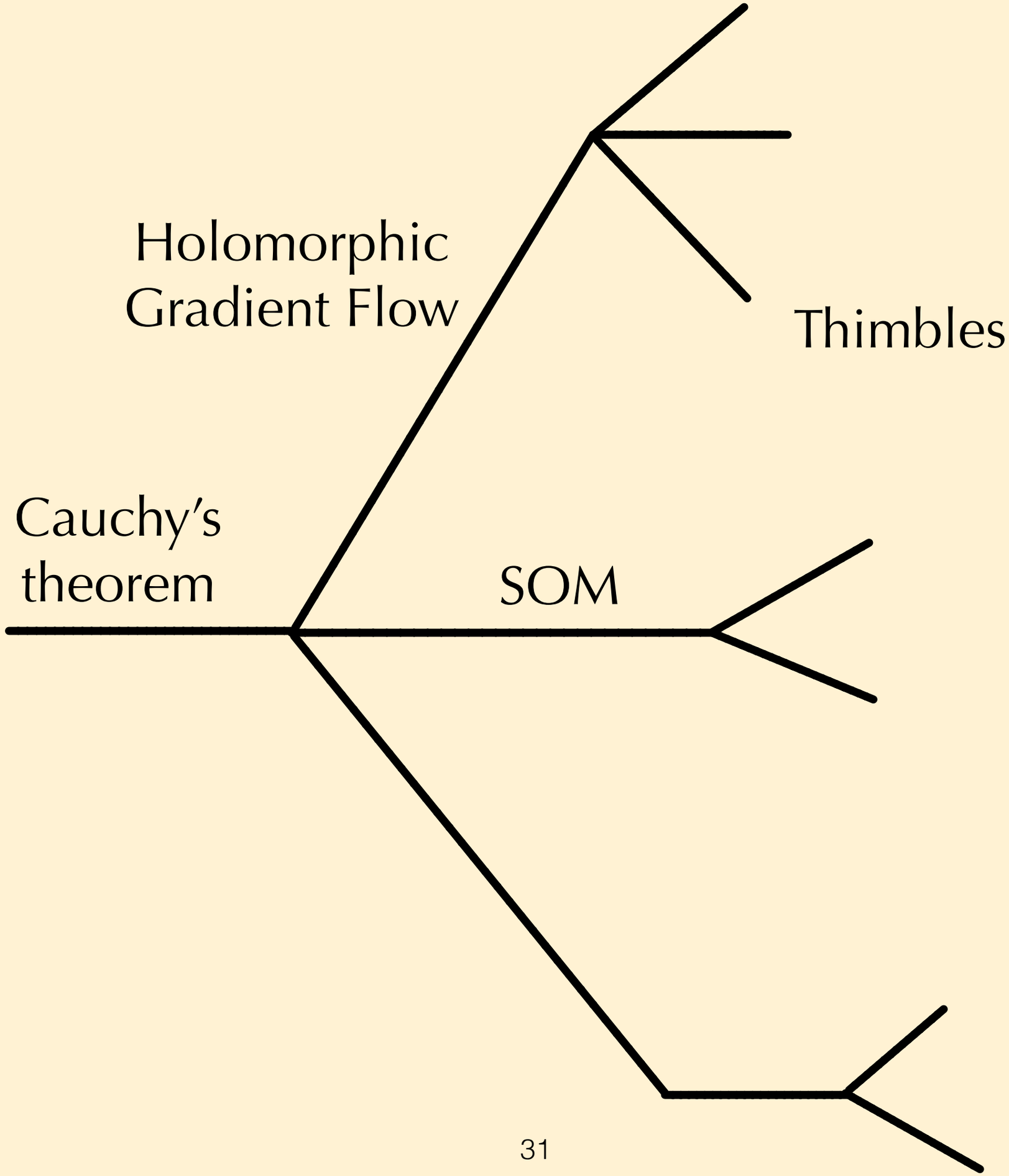


(T, μ) Phase Diagram



Current Limit




Holomorphic
Gradient Flow
Thimbles
Cauchy's
theorem
SOM

Next step

Nearest Neighbor Manifold

$$\tilde{A}_{0x}(A) = A_{0x} + if(A_{0x}, A_{0,x+\hat{0}})$$

$$\tilde{A}_{1x}(A) = A_{1x}$$

$$\tilde{A}_{2x}(A) = A_{2x}$$

Polyakov Loop Manifold

$$\tilde{A}_{0x}(A) = A_{0x} + if(\sum_{x_0} A_{0x})$$

$$\tilde{A}_{1x}(A) = A_{1x}$$

$$\tilde{A}_{2x}(A) = A_{2x}$$

More Applications

Thermodynamics:

Phys. Rev. D. 94, 045017
Phys. Rev. D. 95, 014502

Real time dynamics:

Phys. Rev. Lett. 117, 081602
Phys. Rev. D 95, 114501

Gauge Theories:

Phys. Rev. D 034506

Thank you!