Thimbles: A Geometric Solution to the Sign Problem

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Roadmap:

- The Sign Problem
- Motivational 1D example
- Thimbles in path integrals
- The Beltway Algorithm
- Application to Relativistic Bose Gas at Finite Density

The Sign Problem

Observables in QFT

$$\langle \mathcal{O} \rangle = \frac{1}{Z} \int \mathcal{O}[\phi] \mathrm{e}^{-S[\phi]} D[\phi]$$

$$Z = \int \mathrm{e}^{-S[\phi]} D[\phi]$$

The Sign Problem

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In practice, generate fields $\{\phi_i\}$ distributed as $\mathrm{Pr}[\phi] = \dfrac{\mathrm{e}^{-S[\phi]}}{Z}$

The Sign Problem

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Then, $\langle \mathcal{O} \rangle = \dfrac{1}{N} \displaystyle\sum_{i=1}^{N} \mathcal{O}[\phi_i]$ with statistical errors.

The Sign Problem

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Then, $\langle \mathcal{O} \rangle = \dfrac{1}{N} \displaystyle\sum_{i=1}^{N} \mathcal{O}[\phi_i]$ with statistical errors.

But if $S = S_R + iS_I$ ….then what? You've got a "sign problem".

The Sign Problem

A complex action occurs in a variety of situations

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So, is there a way around?

Reweighting

$$\langle \mathcal{O} \rangle = \frac{\int \mathrm{e}^{-S_R(\phi)} \mathrm{e}^{-iS_I(\phi)} \mathcal{O}(\phi) d^n\phi}{\int \mathrm{e}^{-S_R(\phi)} \mathrm{e}^{-iS_I(\phi)} d^n\phi}$$

$$= \frac{\int \mathrm{e}^{-S_R(\phi)} \mathrm{e}^{-iS_I(\phi)} \mathcal{O}(\phi) d^n\phi}{\int \mathrm{e}^{-S_R(\phi)} d^n\phi} \frac{\int \mathrm{e}^{-S_R(\phi)} d^n\phi}{\int \mathrm{e}^{-S_R(\phi)} \mathrm{e}^{-iS_I(\phi)} d^n\phi}$$

$$= \frac{\langle \mathrm{e}^{-iS_I} \mathcal{O} \rangle_{S_R}}{\langle \mathrm{e}^{-iS_I} \rangle_{S_R}}$$

average phase $\sim \mathrm{e}^{-\#\beta V}$

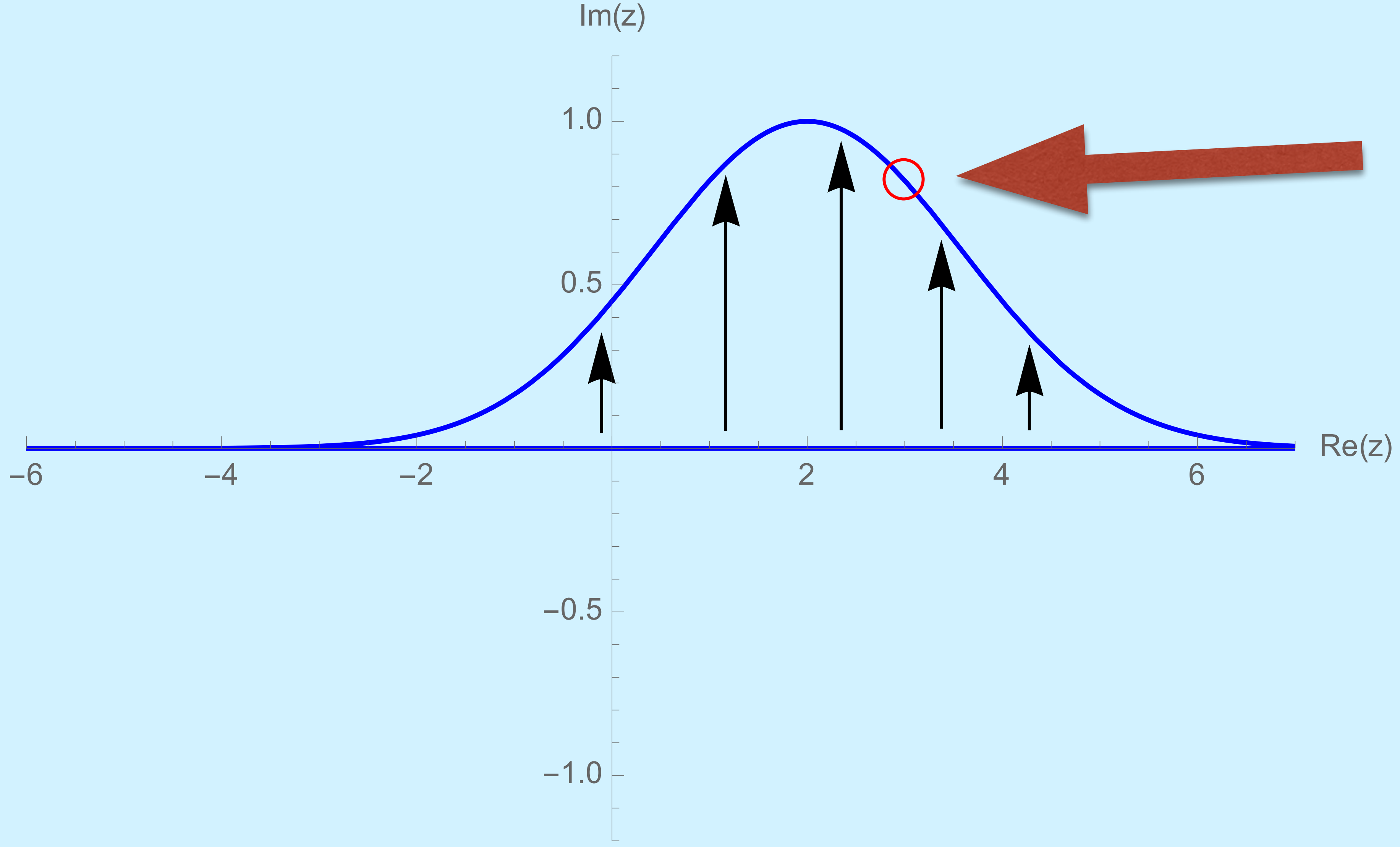
Geometric Solution

$$\phi \in \mathbb{R}^N \longrightarrow \phi \in \mathbb{C}^N$$

What's a thimble?

Thimble = a surface of steepest descent/stationary phase

$$\int_{-\infty}^{\infty} \mathrm{e}^{-S(x)} f(x) dx = \mathrm{e}^{-iS_I} \int_{\mathcal{C}} \mathrm{e}^{-S_R(z)} f(z) dz$$



$$\frac{dS}{dz} = 0$$

What's a thimble?

To find thimbles, solve flow equations

$$\frac{dz}{d\tau} = -\overline{\left(\frac{\partial S}{\partial z}\right)}$$

$$z(\tau) \xrightarrow{\tau\to\infty} z_c$$

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Rewriting $z(\tau) = x(\tau) + iy(\tau)$:

$$\frac{dx}{d\tau} = -\frac{\partial S_R}{\partial x} = -\frac{\partial S_I}{\partial y}$$

$$\frac{dy}{d\tau} = -\frac{\partial S_R}{\partial y} = \frac{\partial S_I}{\partial x}$$

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Gradient Flow of S_R

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Gradient Flow of S_R

Hamiltonian Flow of S_I

1D Example

1D Example: $S(z) = -z^2 + z^4 + (h_R + ih_I)z$

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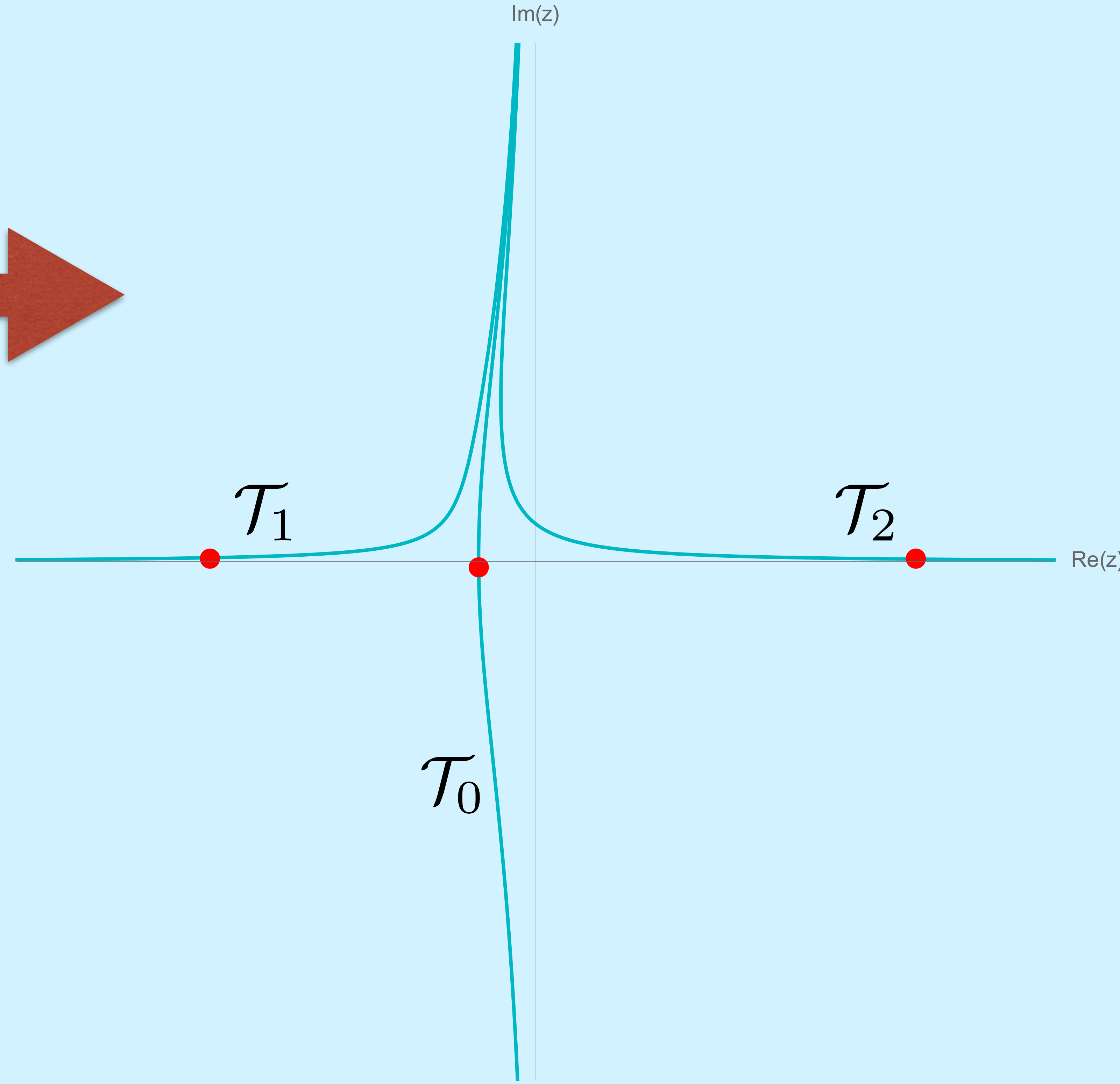

1D Example

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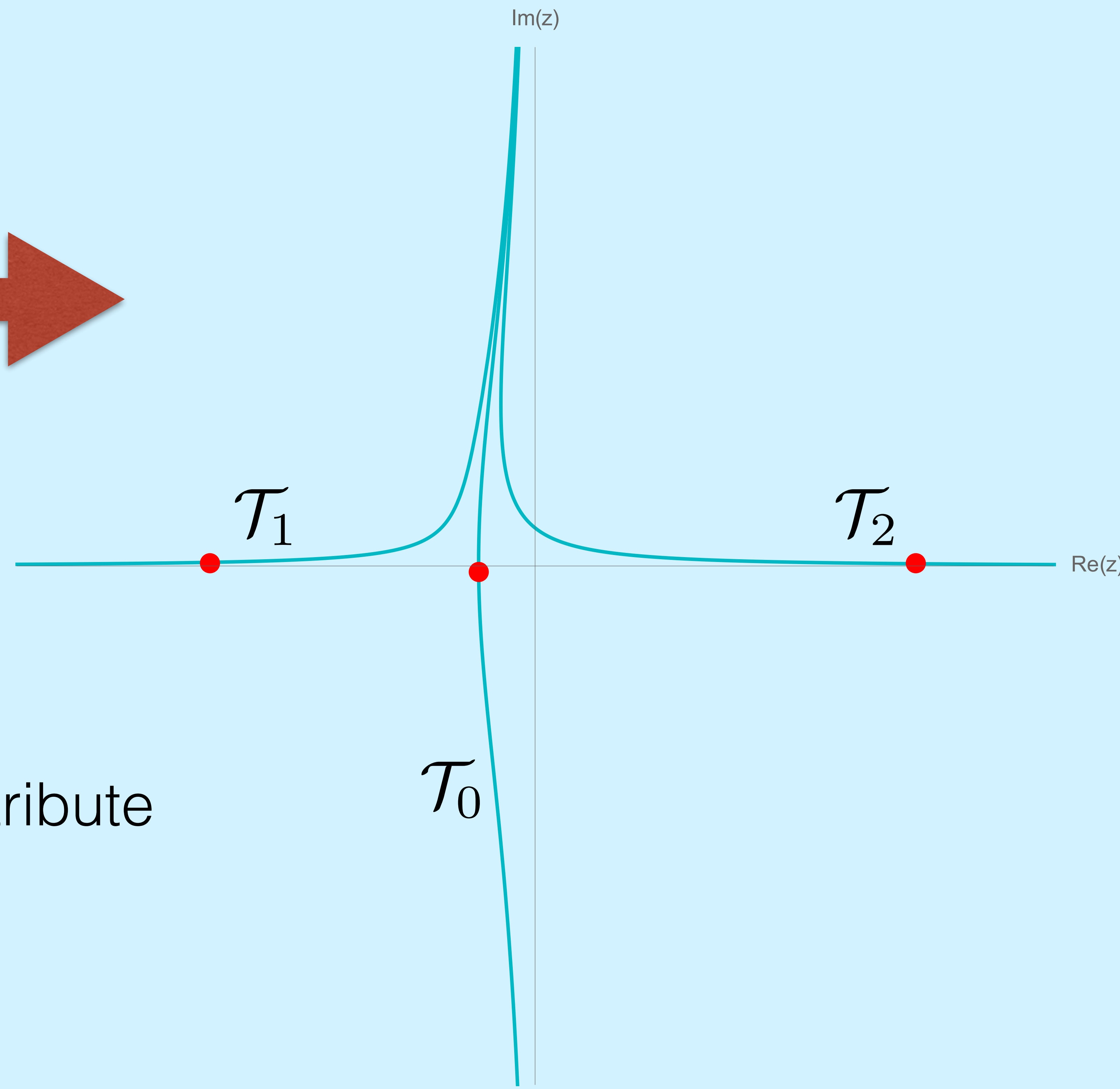
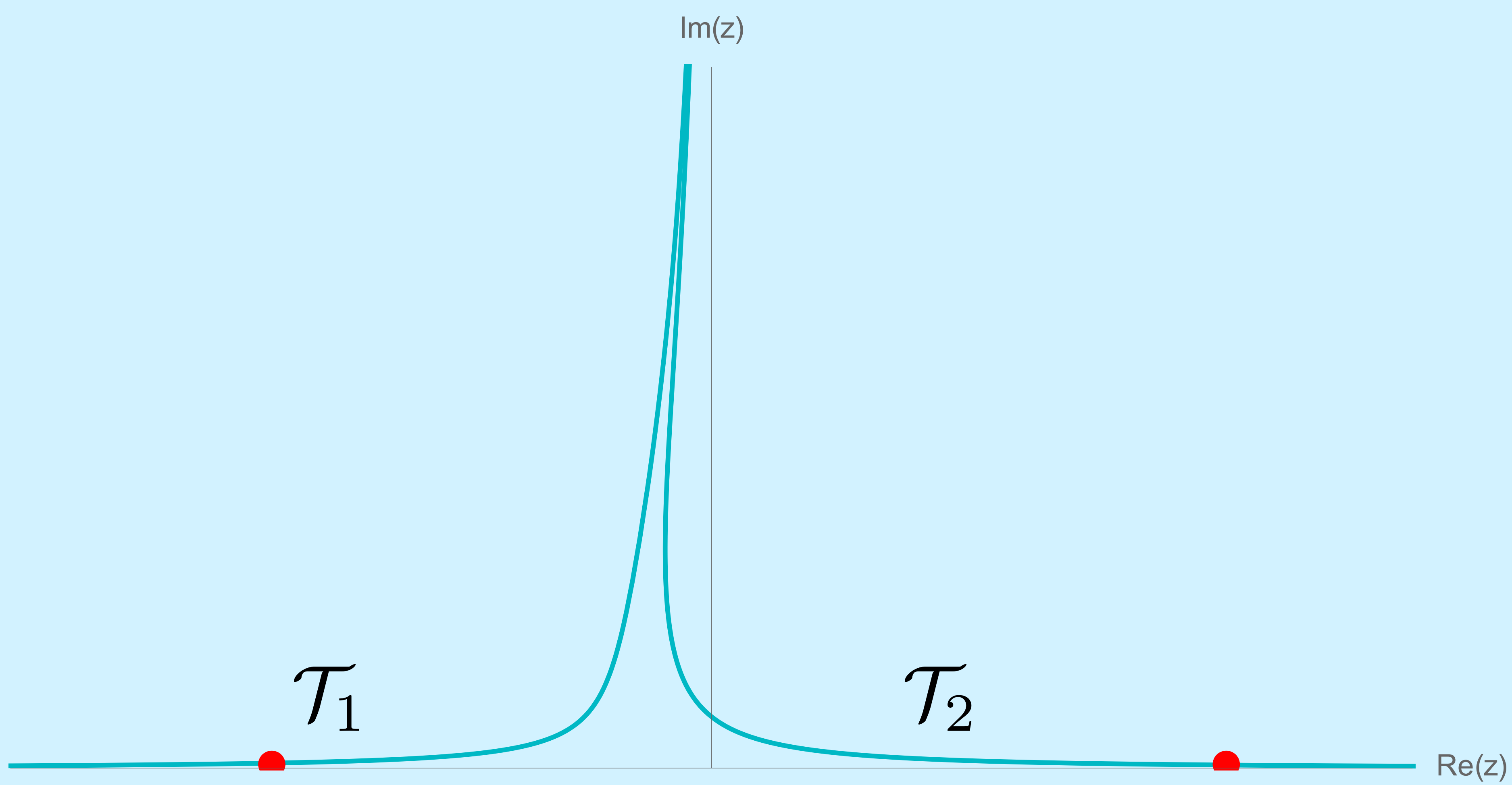


Notice: Not all thimbles contribute to integral

1D Example

In general:

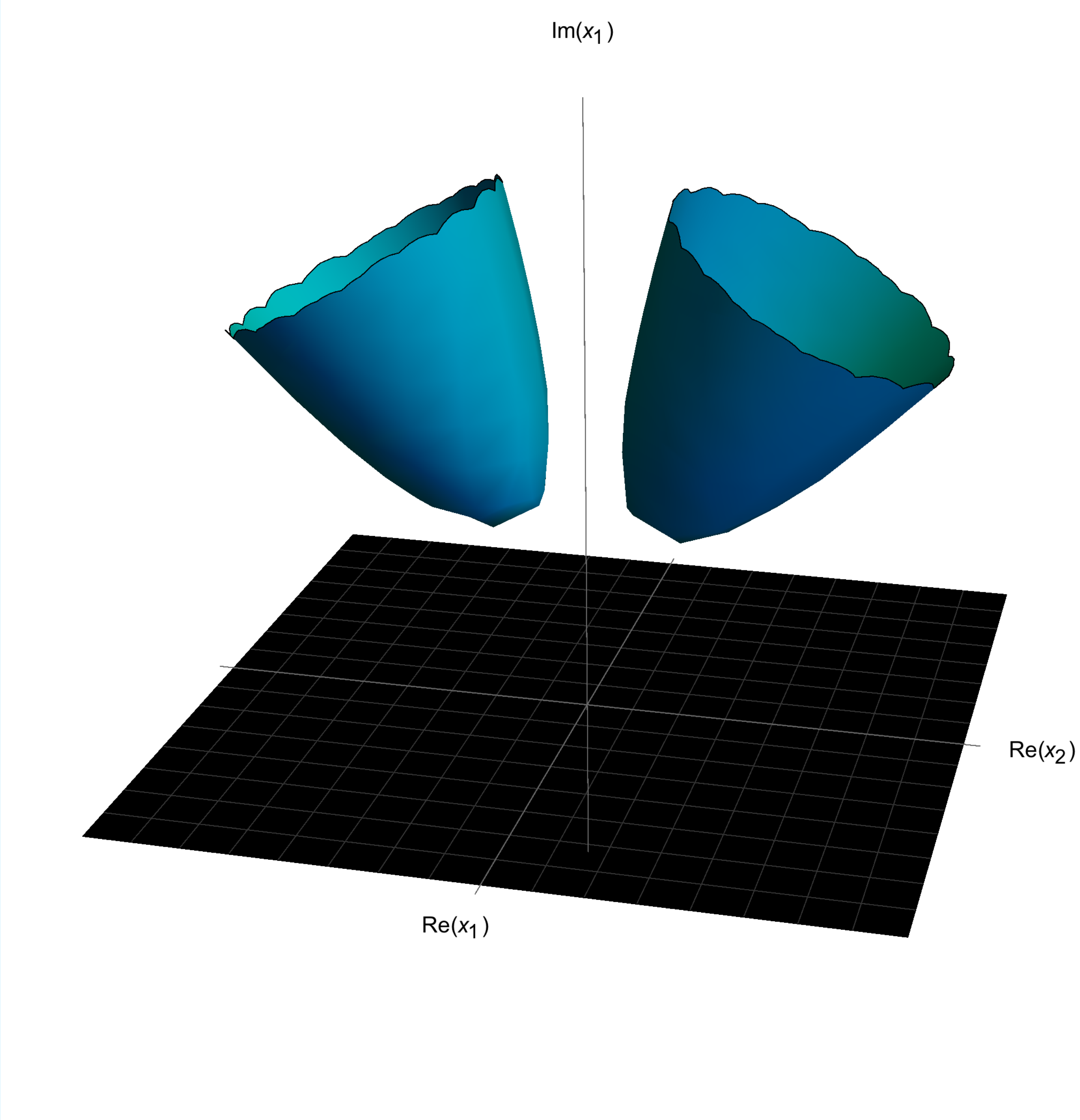
$$\int_{-\infty}^{\infty} \mathrm{e}^{-S(x)} f(x)dx = \sum_{\sigma=0}^{N} n_\sigma \mathrm{e}^{-iS_I(\sigma)} \int_{\mathcal{T}_\sigma} \mathrm{e}^{-S_R(z)} f(z)dz$$



Many Variables

$$S = S(z_1, \ldots, z_n) \longrightarrow \frac{dz_i}{d\tau} = -\overline{\left(\frac{\partial S}{\partial z_i}\right)}$$

$$z(\tau) \xrightarrow{\tau \to \infty} z_c$$



Many Variables

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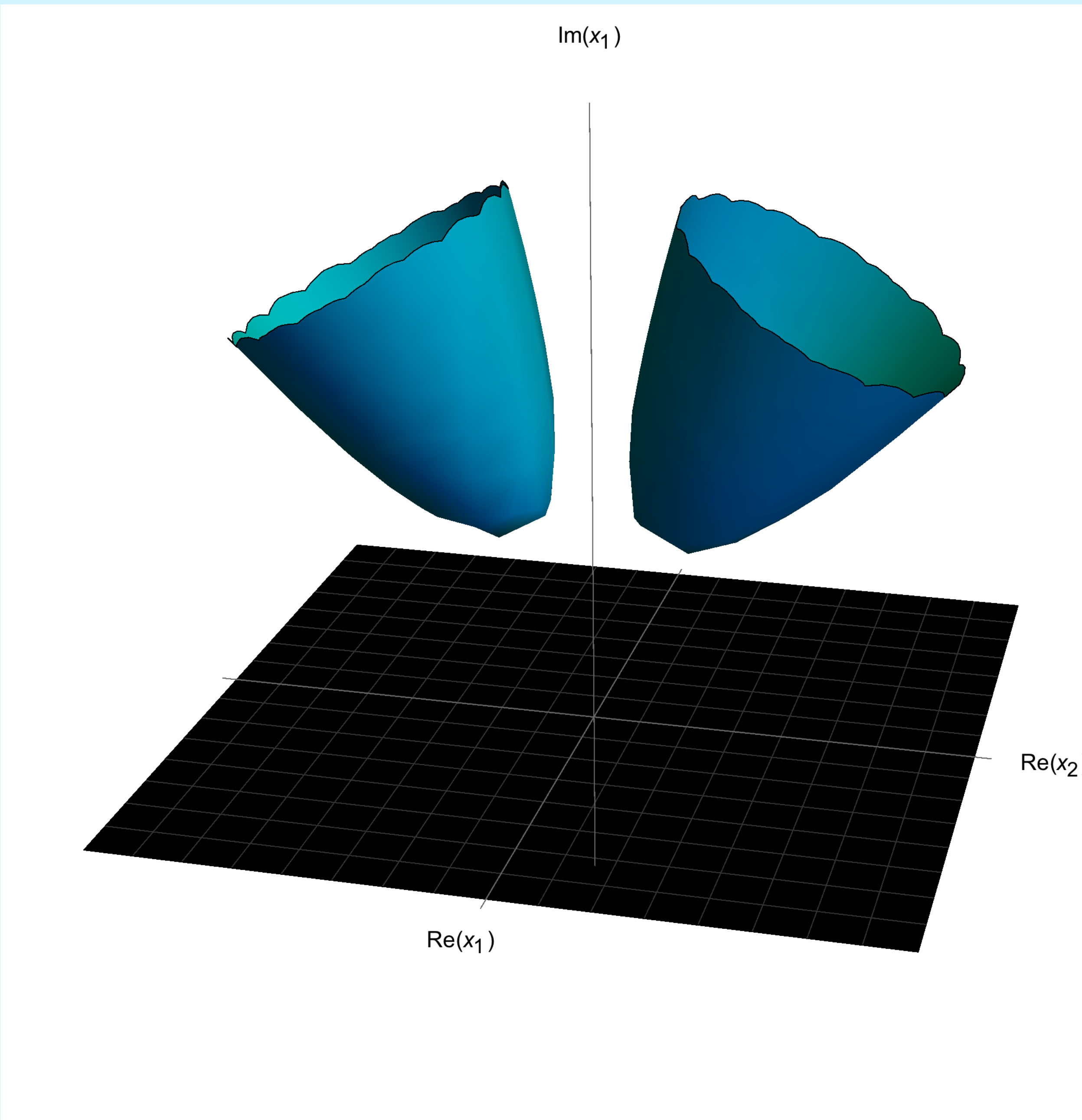
$$\frac{dz_i}{d\tau} = -\left(\overline{\frac{\partial S}{\partial z_i}}\right)$$

$$z(\tau) \xrightarrow{\tau \to \infty} z_c$$

$$\Downarrow$$

$$\frac{dx_i}{dt} = -\frac{\partial S_R}{\partial x_i} = -\frac{\partial S_I}{\partial y_i}$$

$$\frac{dy_i}{dt} = -\frac{\partial S_R}{\partial y_i} = \frac{\partial S_I}{\partial x_i}$$



Gradient Flow of S_R

Hamiltonian Flow of S_I

Many Variables

Harder to see (no pictures):

$$\int_{\mathbb{R}^n} \mathrm{e}^{-S(x)} f(x) dx = \sum_{\sigma=0}^{N} n_\sigma \mathrm{e}^{-iS_I(\sigma)} \int_{\mathcal{T}_\sigma} \mathrm{e}^{-S(z)} f(z) dz$$

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Recall: $\langle \mathcal{O} \rangle = \dfrac{\int \mathrm{e}^{-S(\phi)} \mathcal{O}(\phi) d^n\phi}{\int \mathrm{e}^{-S(\phi)} d^n\phi}$

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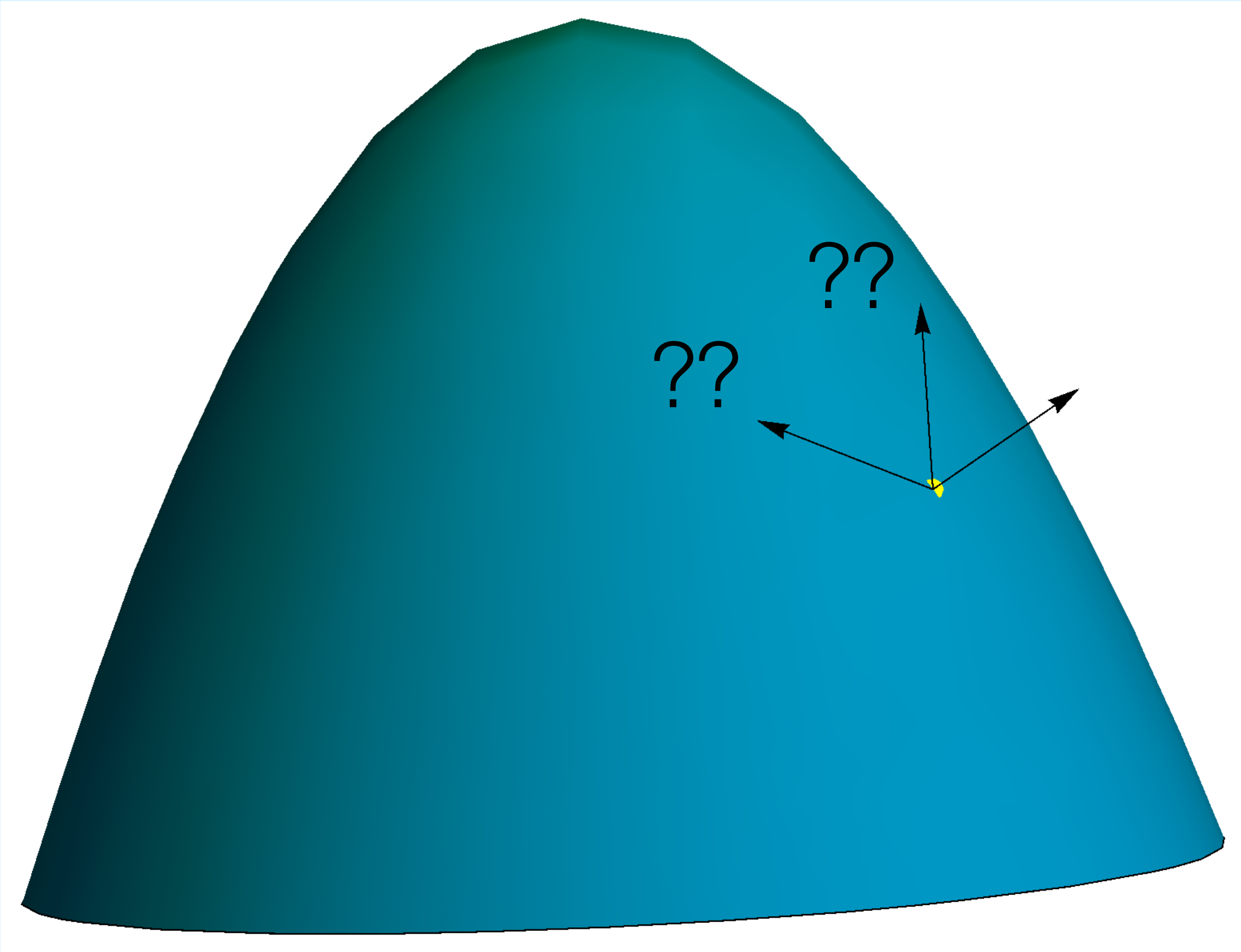
Recall: $\langle \mathcal{O} \rangle = \dfrac{\int \mathrm{e}^{-S(\phi)} \mathcal{O}(\phi) d^n\phi}{\int \mathrm{e}^{-S(\phi)} d^n\phi}$

$$\implies \langle \mathcal{O} \rangle = \frac{\sum\limits_{\sigma=0}^{N} n_\sigma \mathrm{e}^{-iS_I(\sigma)} \int\limits_{\mathcal{T}_\sigma} \mathrm{e}^{-S_R(\phi)} \mathcal{O}(\phi) d^n\phi}{\sum\limits_{\sigma=0}^{N} n_\sigma \mathrm{e}^{-iS_I(\sigma)} \int\limits_{\mathcal{T}_\sigma} \mathrm{e}^{-S_R(\phi)} d^n\phi}$$

Beltway Algorithm

Start with one thimble integration: $\langle \mathcal{O} \rangle_0 = \dfrac{\int_{\mathcal{T}_0} \mathrm{e}^{-S_R(\phi)} \mathcal{O}(\phi) d^n \phi}{\int_{\mathcal{T}_0} \mathrm{e}^{-S_R(\phi)} d^n \phi}$



Generate points **on the thimble** according to:

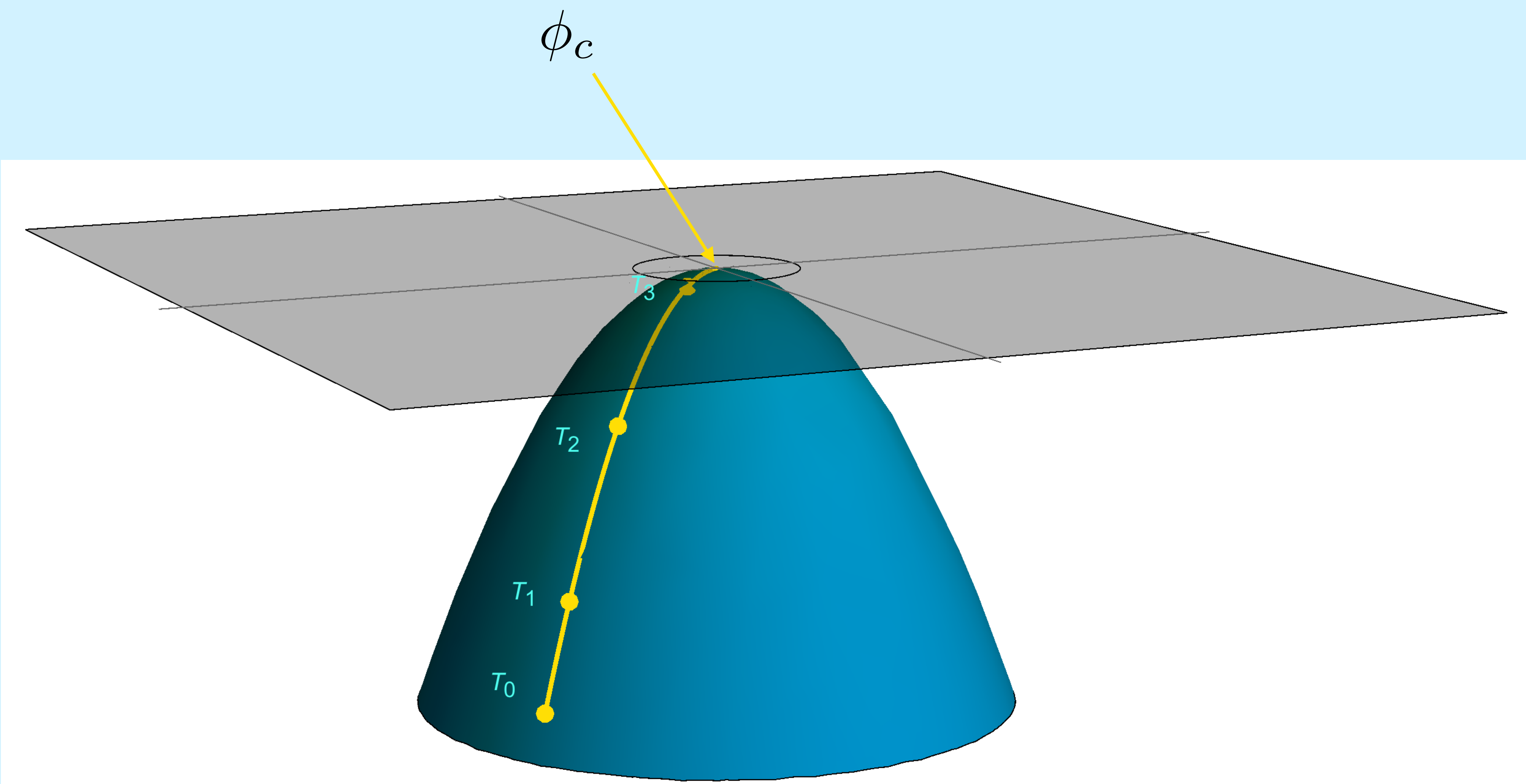
$$\mathrm{Pr}[\phi] = \frac{\mathrm{e}^{-S_R(\phi)}}{\int_{\mathcal{T}_0} \mathrm{e}^{-S_R(\phi)}}$$

Non-trivial task!

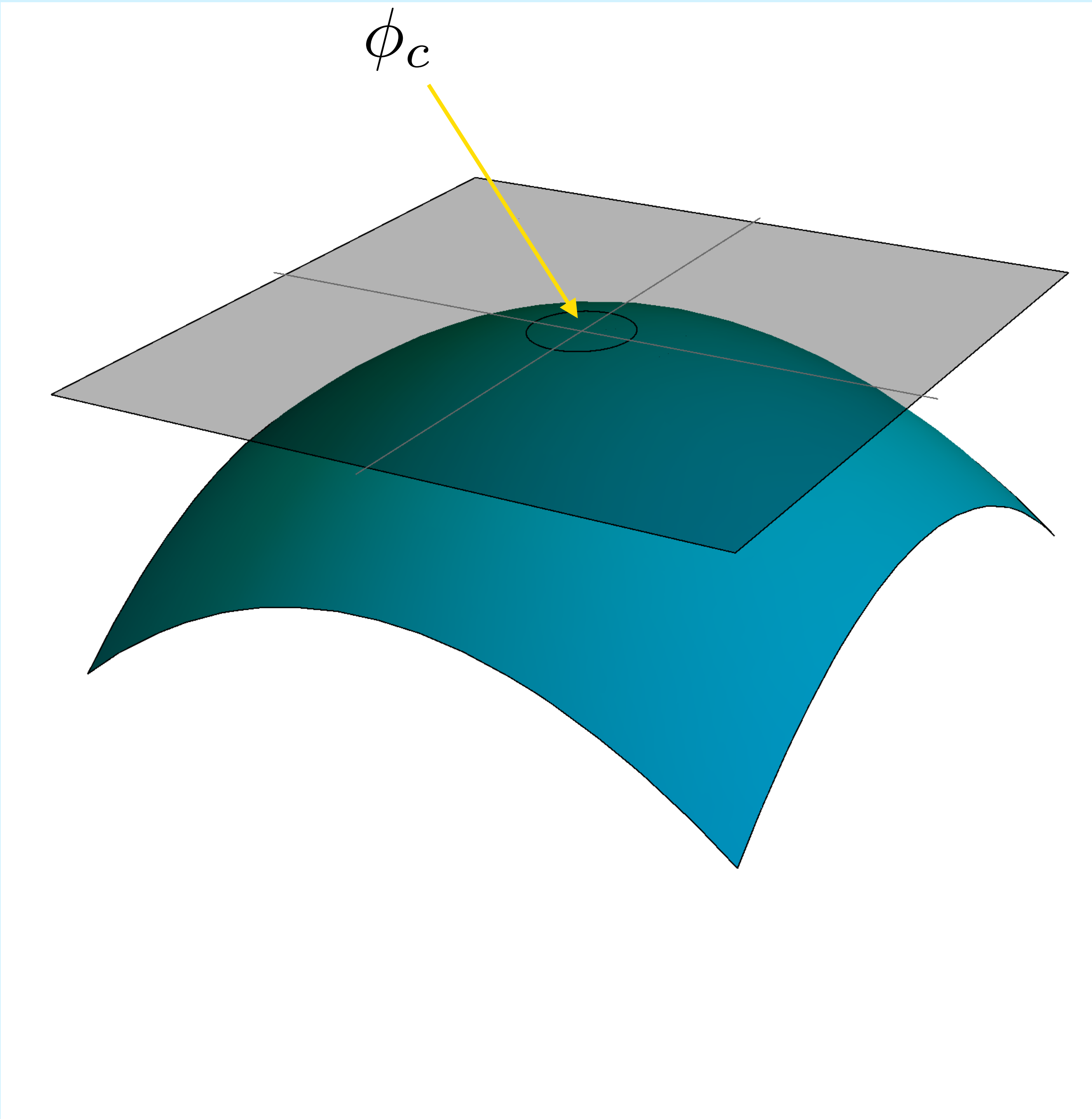
Beltway Algorithm

$$\tilde{\phi} = \mathrm{Flow}(\phi, T)$$

Tangent space parameterization



Beltway Algorithm



Near critical point,

$$\frac{d\phi_i}{d\tau} = -\left(\overline{\frac{\partial S}{\partial \phi_i}}\right) \simeq -\overline{H_{ij}\phi_j}$$

$\Longrightarrow$ spanned by $\{\hat{\rho}_i\}$

such that $\overline{H\hat{\rho}_i} = \lambda_i \hat{\rho}_i$

Beltway Algorithm

$$\langle \mathcal{O} \rangle = \frac{\int \mathrm{e}^{-S_R(\phi)} \mathcal{O}(\phi) d\phi}{\int \mathrm{e}^{-S_R(\phi)} d\phi} = \frac{\int \mathrm{e}^{-S_R(\tilde{\phi})} \mathcal{O}(\tilde{\phi}) \det\left(\frac{d\phi}{d\tilde{\phi}}\right) d\tilde{\phi}}{\int \mathrm{e}^{-S_R(\tilde{\phi})} \det\left(\frac{d\phi}{d\tilde{\phi}}\right) d\tilde{\phi}}$$

$$\equiv J = \mathrm{e}^{\mathrm{Re}(lnJ) + i\mathrm{Im}(lnJ)}$$

Beltway Algorithm

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$$\equiv J = \mathrm{e}^{\mathrm{Re}(lnJ) + i\mathrm{Im}(lnJ)}$$

$$\equiv S_{eff}$$

$$= \frac{\int \mathrm{e}^{-(S_R(\tilde{\phi}) - \mathrm{Re}(lnJ))} \mathrm{e}^{i\mathrm{Im}(lnJ)} \mathcal{O}(\tilde{\phi}) d\tilde{\phi}}{\int \mathrm{e}^{-(S_R(\tilde{\phi}) - \mathrm{Re}(lnJ))} \mathrm{e}^{i\mathrm{Im}(lnJ)} d\tilde{\phi}}$$

$$\equiv \text{“residual phase”}$$

Beltway Algorithm

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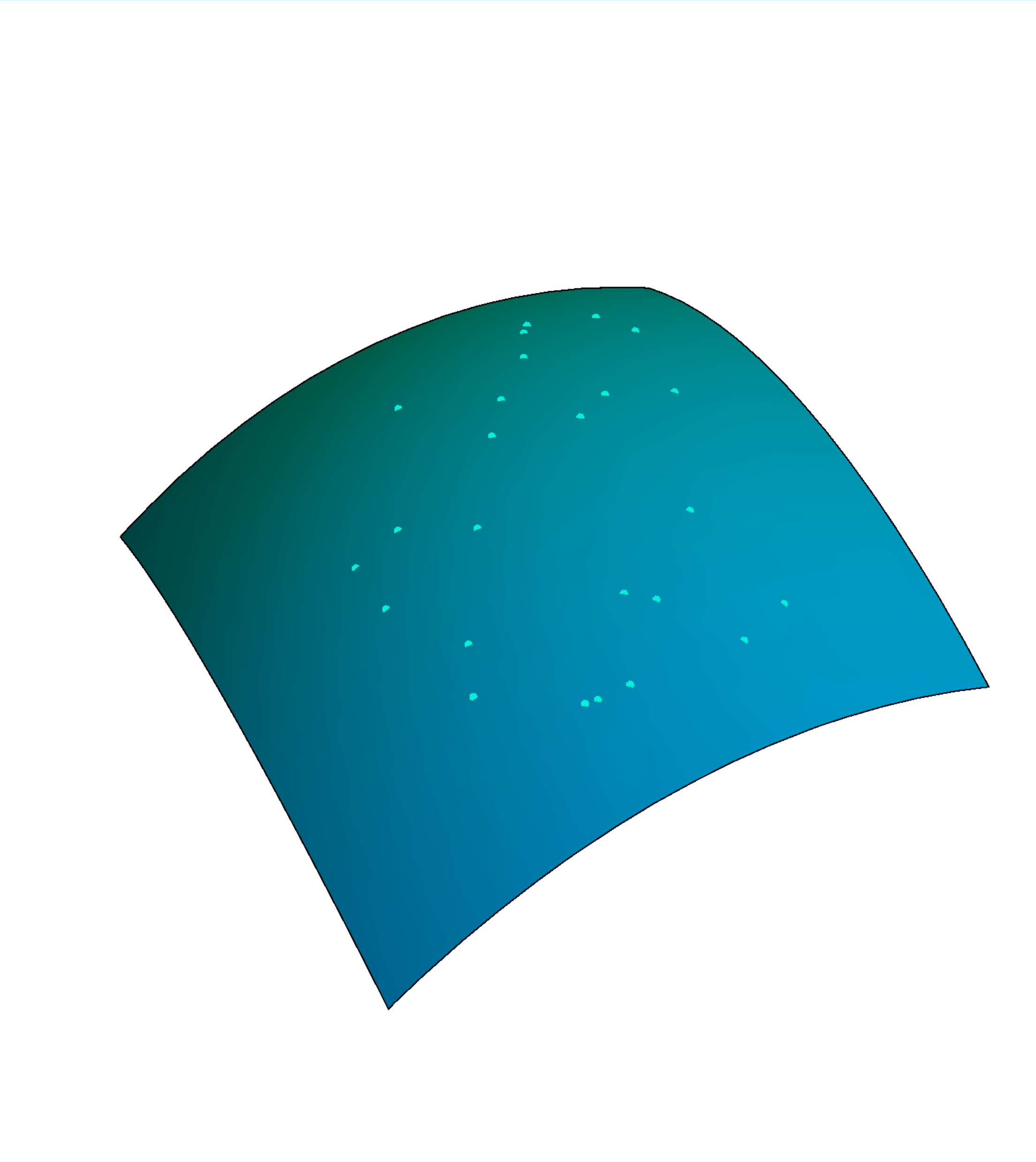
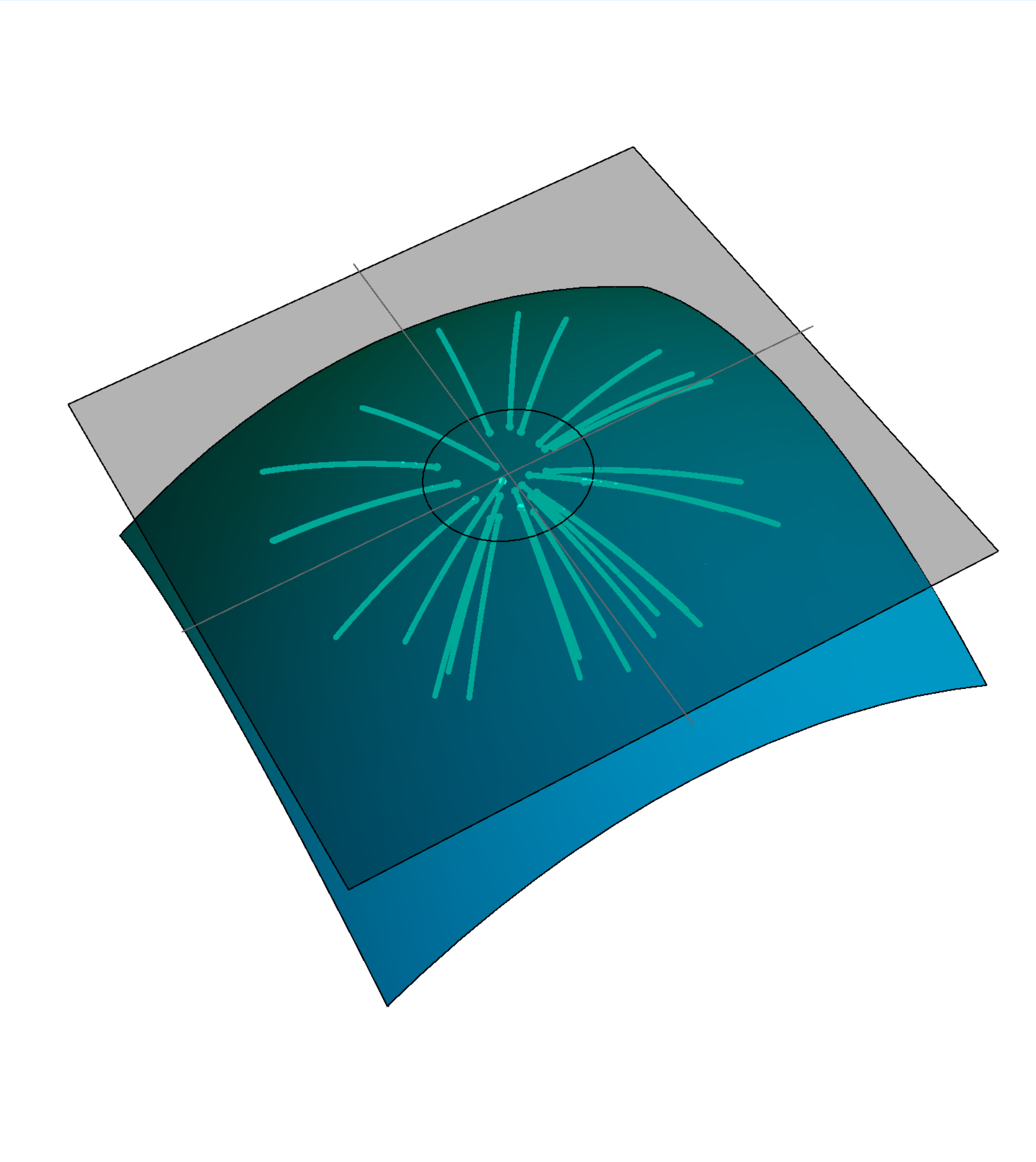
$$= \frac{\langle \mathcal{O} \mathrm{e}^{i\mathrm{Im}(lnJ)} \rangle_{S_{eff}}}{\langle \mathrm{e}^{i\mathrm{Im}(lnJ)} \rangle_{S_{eff}}}$$

Beltway Algorithm

$$(\phi, S_R) \quad = \quad (\tilde{\phi}, S_{eff})$$





Relativistic Bose Gas

$$S[\phi] = \int \Big(|\partial\phi|^2 + (m^2 - \mu^2)|\phi|^2 + \mu j_0 + \lambda|\phi|^4 + h(\phi_1 + \phi_2)\Big) d^4x$$

Where: $\phi = \phi_1 + i\phi_2$

$$j_0 = 2i\mathrm{Im}\big(\phi\partial_0\phi^* - \phi^*\partial_0\phi\big)$$

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Here's the sign problem!

$$S = \left(4 + \frac{m^2}{2}\right)\sum_{x,a}\phi_{a,x}{}^2 - \sum_{x,a}\sum_{\nu=1}^{3}\Big(\phi_{a,x}\phi_{a,x+\hat{\nu}}\Big)$$
$$+ \sum_{x,a,b}\Big(\cosh\mu\ \phi_{a,x}\phi_{b,x+\hat{0}}\delta_{a,b} - i\sinh\mu\ \epsilon_{ab}\phi_{a,x}\phi_{b,x+\hat{0}}\Big)$$
$$+\frac{\lambda}{4}\sum_x\Big(\phi_{1,x}^2 + \phi_{2,x}^2\Big)^2 + h\sum_x \phi_{1,x} + \phi_{2,x}$$

Relativistic Bose Gas

Global min of $S[\phi]$ $\Longrightarrow$ constant field solution

Relativistic Bose Gas

Global min of $S[\phi]$ $\Longrightarrow$ constant field solution

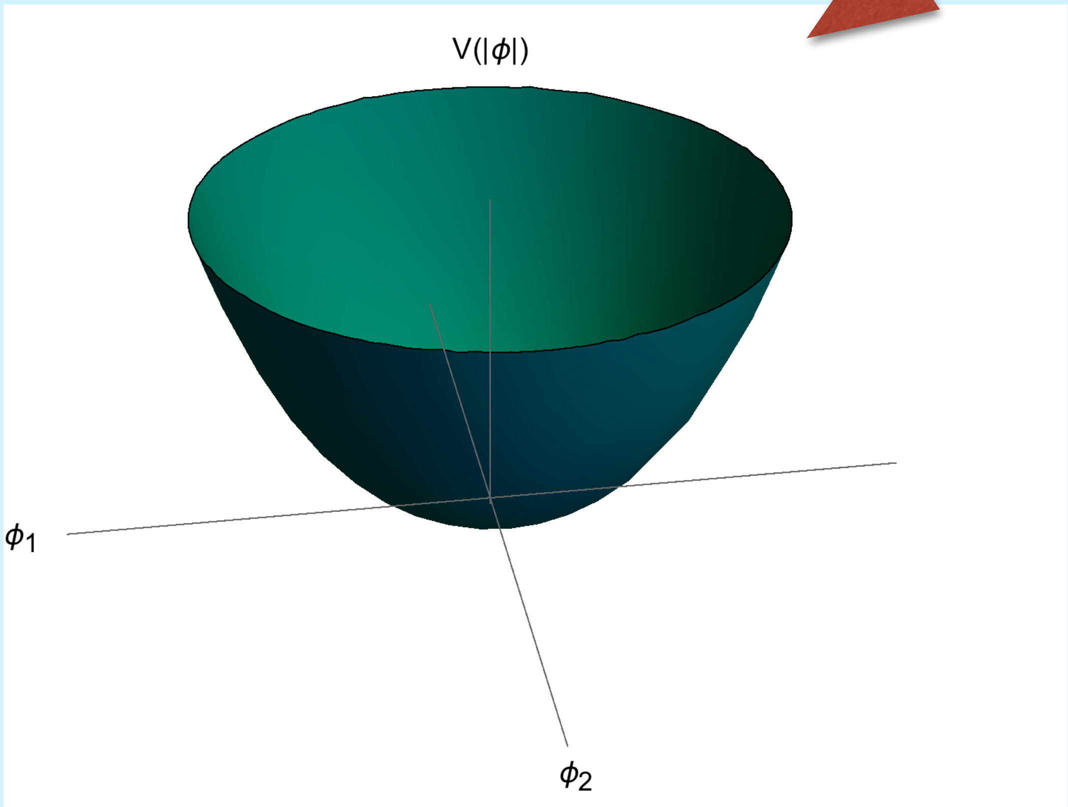
$$\longrightarrow \quad V(\phi) = (m^2 - \mu^2)|\phi|^2 + \lambda|\phi|^4 + h(\phi_1 + \phi_2)$$

Relativistic Bose Gas

Global min of $S[\phi]$ $\Longrightarrow$ constant field solution

$$V(\phi) = (m^2 - \mu^2)|\phi|^2 + \lambda|\phi|^4 + h(\phi_1 + \phi_2)$$

$\mu < \mu_{crit}$



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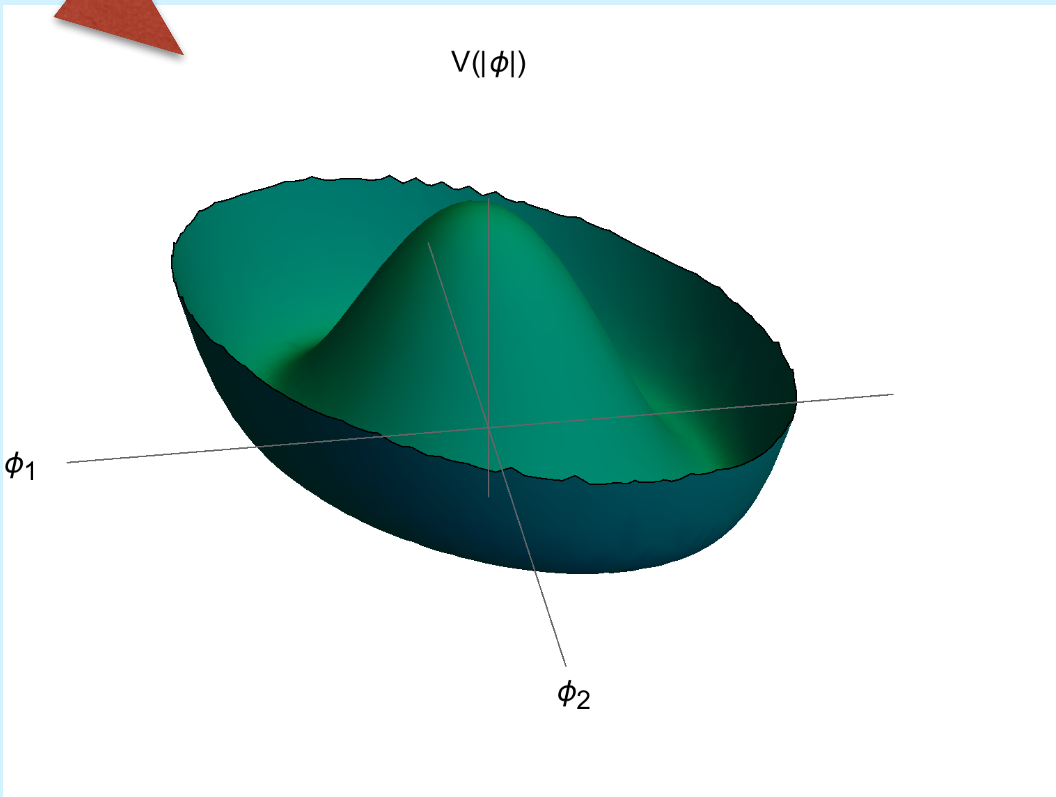
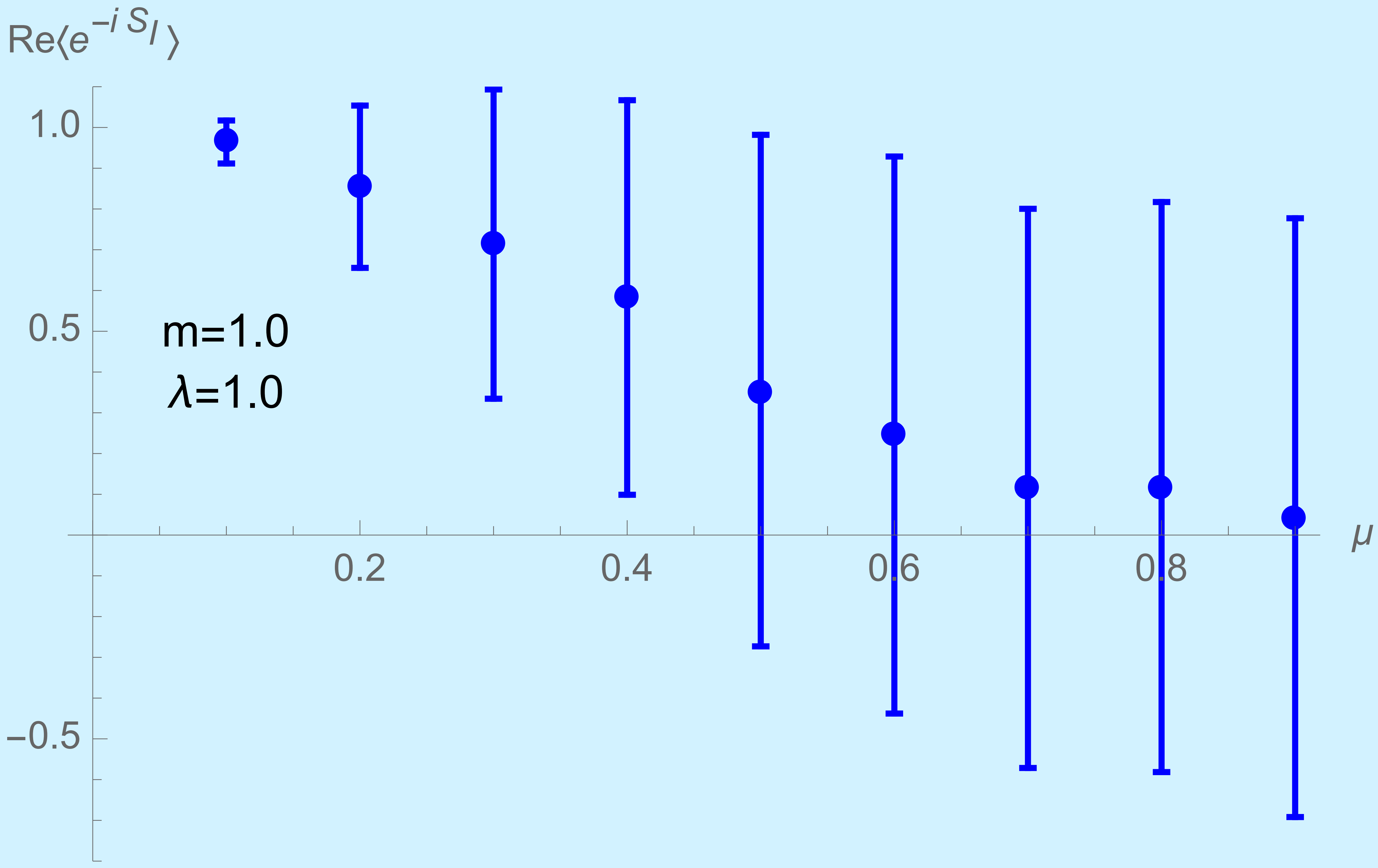


$$\mu < \mu_{crit}$$

Is there a sign problem?



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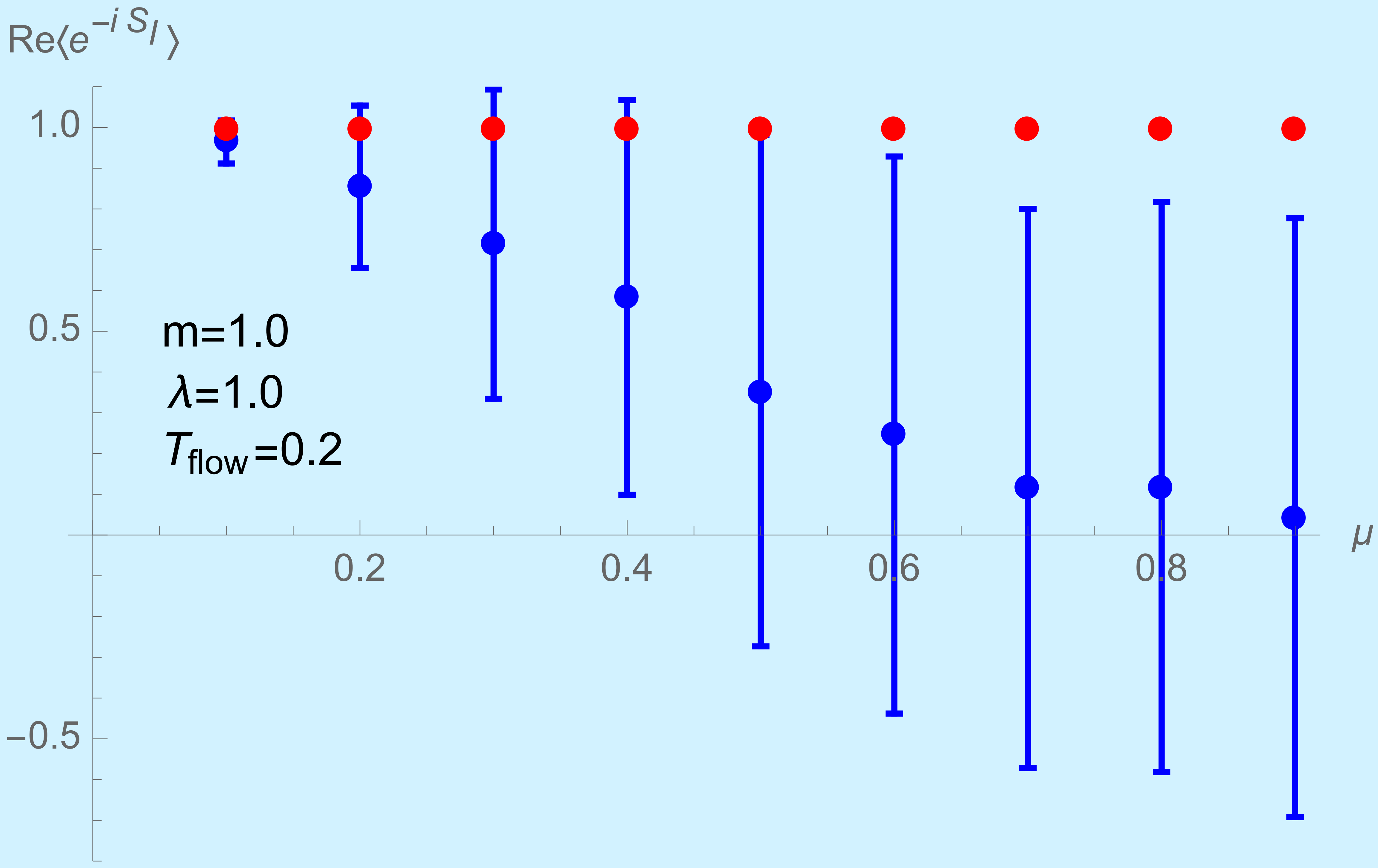
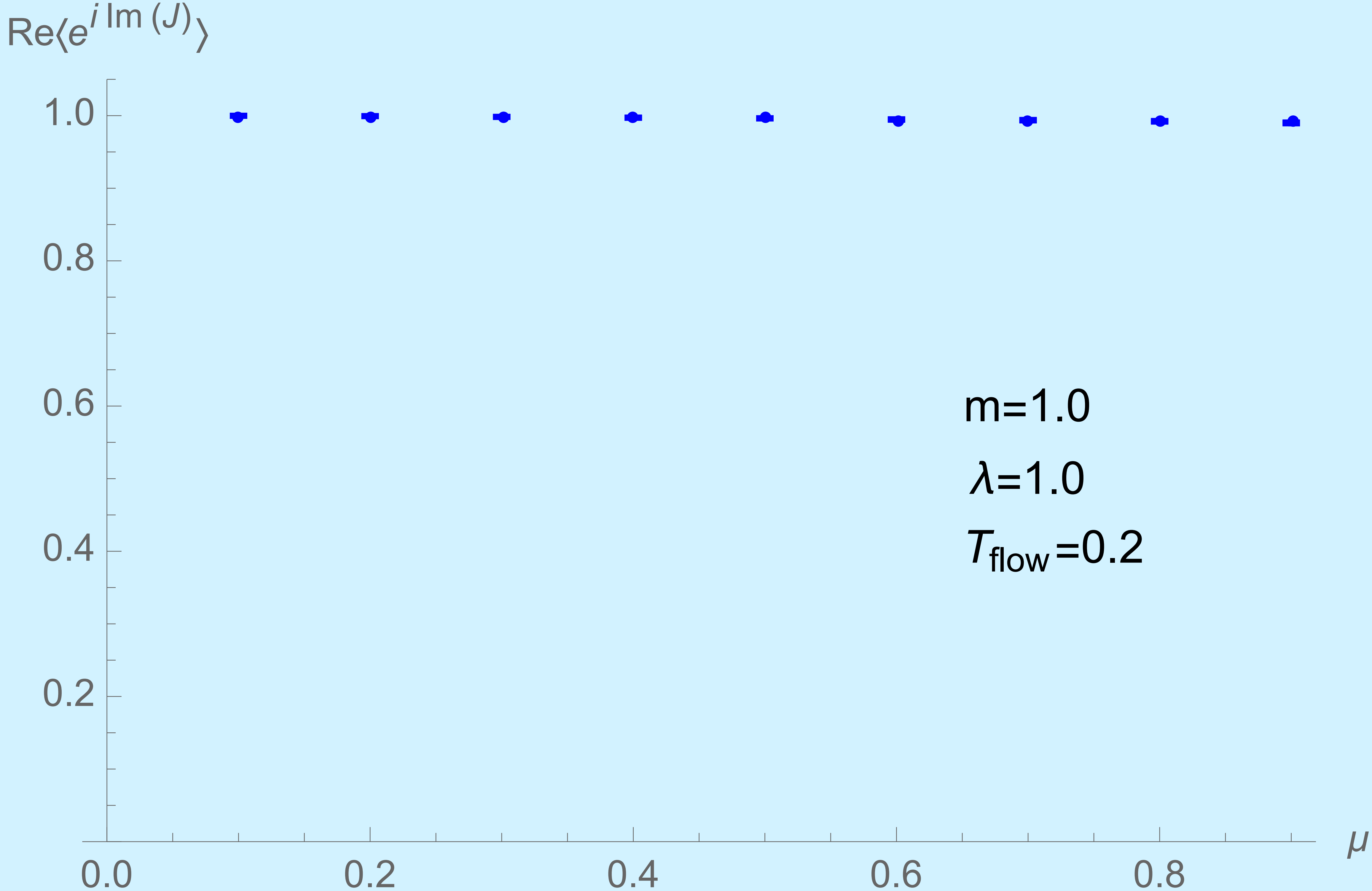
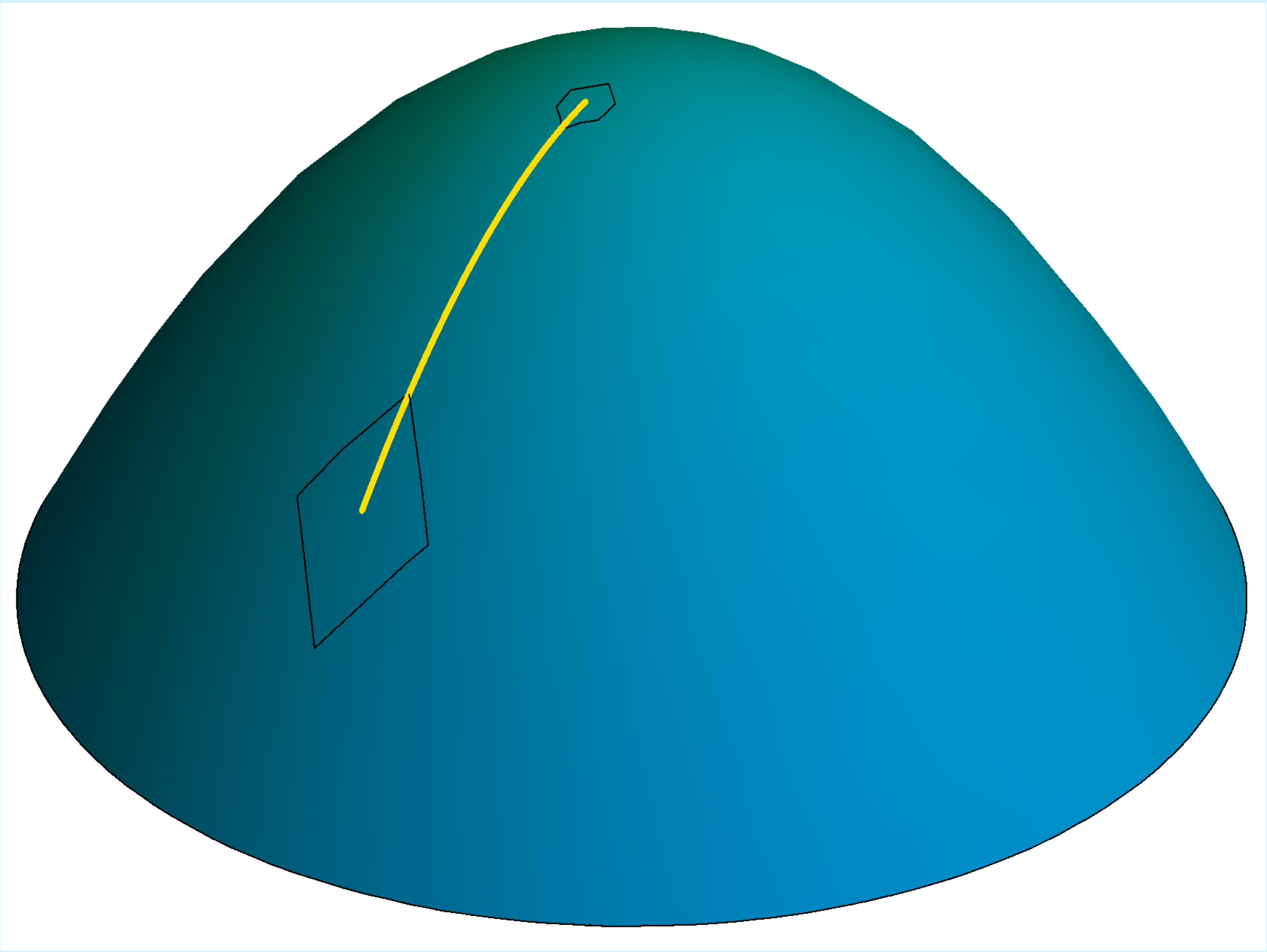


Phase due to curvature?



The Jacobian

$$S_{eff}(\tilde{\phi}) = S_R(\phi(\tilde{\phi})) - \mathrm{Re}(\ln J(\tilde{\phi}))$$



$$\frac{\mathrm{Flow}(\mathrm{V}(\tilde{\phi}), T_{flow})}{\mathrm{V}(\tilde{\phi})}$$

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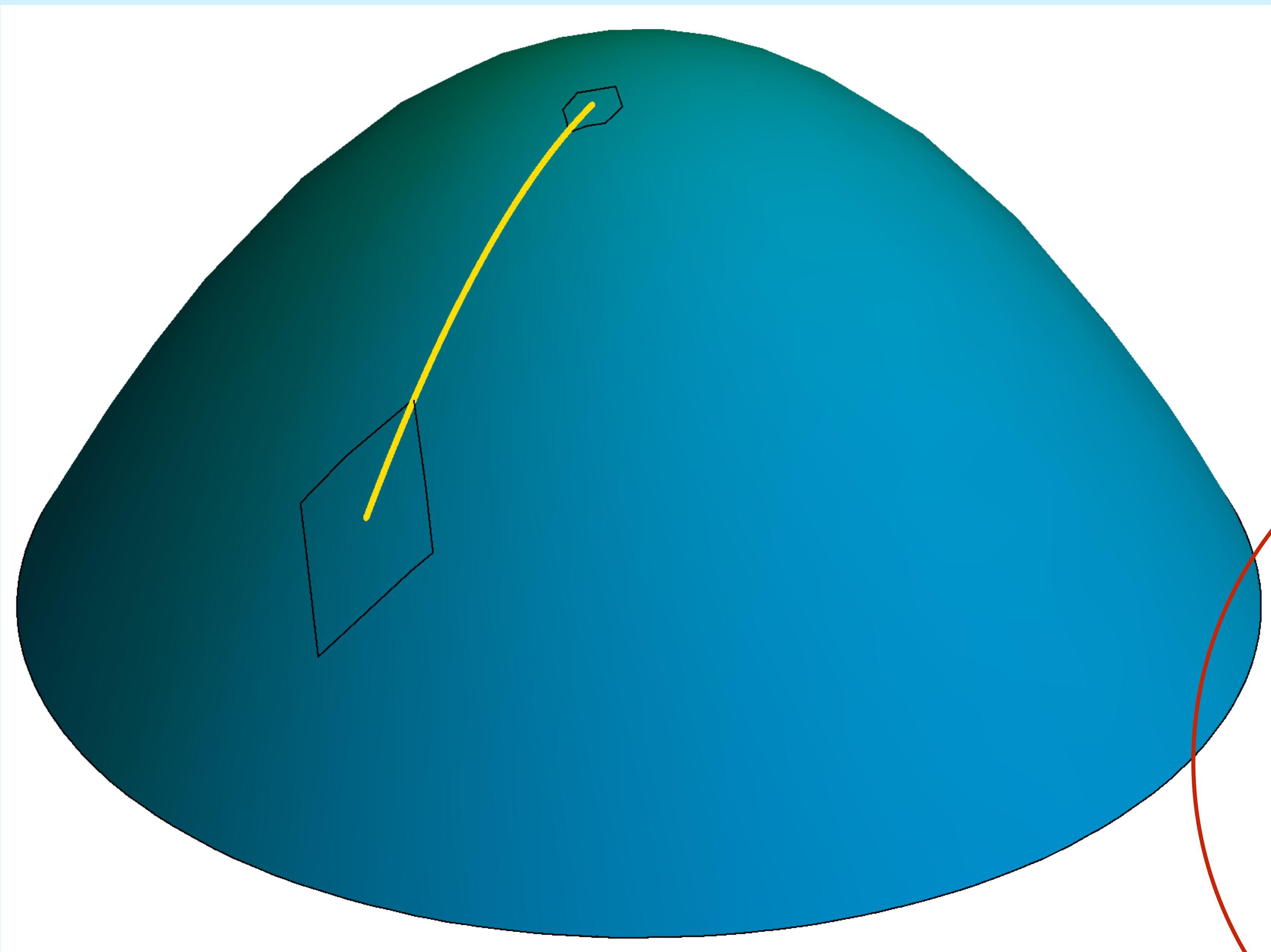

$$\frac{\mathrm{Flow}(\mathrm{V}(\tilde{\phi}), T_{flow})}{\mathrm{V}(\tilde{\phi})}$$

Evolves as:

$$J = \det(M)$$

$$\frac{dM}{d\tau} = \overline{HM}$$

$$M(0) = \left(\hat{\rho}_1, \hat{\rho}_2, \ldots, \hat{\rho}_V\right)$$

This is really hard to do!

Compromise: Reweighting

$$\langle \mathcal{O} \rangle = \frac{\int \mathrm{e}^{-\left[S_R(\tilde{\phi}) - \mathrm{Re}[\log(J)]\right]} \mathrm{e}^{\mathrm{Im}(\log(J))} \mathcal{O}(\tilde{\phi}) d\tilde{\phi}}{\int \mathrm{e}^{-\left[S_R(\tilde{\phi}) - \mathrm{Re}[\log(J)]\right]} \mathrm{e}^{\mathrm{Im}(\log(J))} d\tilde{\phi}}$$

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$$= \frac{\int \mathrm{e}^{-\left[S_R(\tilde{\phi}) - \mathrm{Re}[\log(W_1)]\right]} \mathrm{e}^{\mathrm{Re}\left[\log(J) - \log(W_1)\right]} \mathrm{e}^{\mathrm{Im}(\log(J))} \mathcal{O}(\tilde{\phi}) d\tilde{\phi}}{\int \mathrm{e}^{-\left[S_R(\tilde{\phi}) - \mathrm{Re}[\log(J)]\right]} \mathrm{e}^{\mathrm{Re}\left[\log(J) - \log(W_1)\right]} \mathrm{e}^{\mathrm{Im}(\log(J))} d\tilde{\phi}}$$

Modified distribution

“reweighting factor”

Compromise: Reweighting

$$\langle \mathcal{O} \rangle = \frac{\int \mathrm{e}^{-\left[S_R(\tilde{\phi}) - \mathrm{Re}[\log(J)]\right]} \mathrm{e}^{\mathrm{Im}(\log(J))} \mathcal{O}(\tilde{\phi}) d\tilde{\phi}}{\int \mathrm{e}^{-\left[S_R(\tilde{\phi}) - \mathrm{Re}[\log(J)]\right]} \mathrm{e}^{\mathrm{Im}(\log(J))} d\tilde{\phi}}$$

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Modified distribution

"reweighting factor"

$$= \frac{\left\langle \mathrm{e}^{\mathrm{Re}\left[\log(J) - \log(W_1)\right]} \mathrm{e}^{\mathrm{Im}(\log(J))} \mathcal{O} \right\rangle_{S_R(\tilde{\phi}) - \mathrm{Re}[\log(W_1)]}}{\left\langle \mathrm{e}^{\mathrm{Re}\left[\log(J) - \log(W_1)\right]} \mathrm{e}^{\mathrm{Im}(\log(J))} \right\rangle_{S_R(\tilde{\phi}) - \mathrm{Re}[\log(W_1)]}}$$

The Estimators

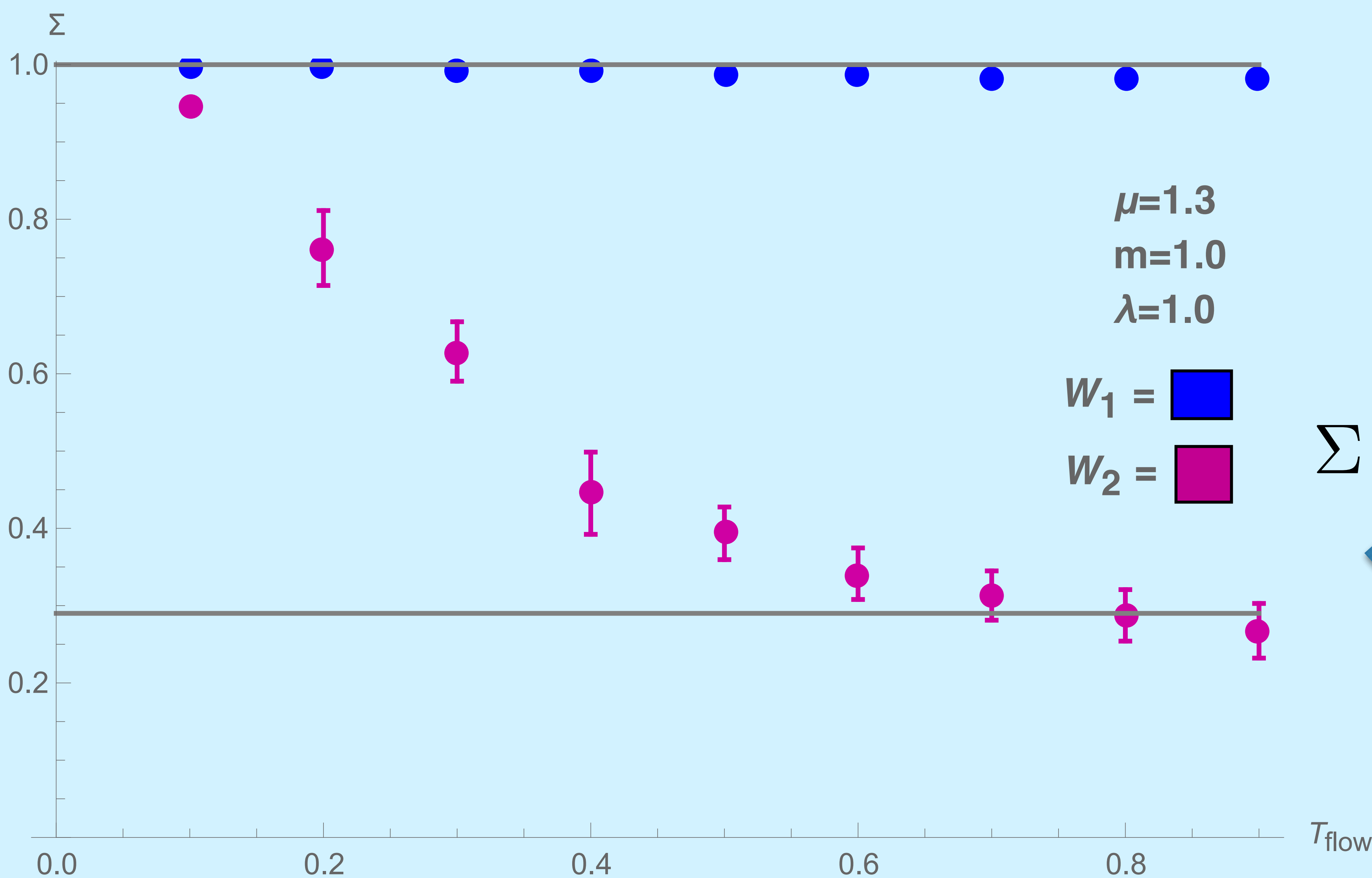
The problem: $\log(J) = \log(\det(M)) \sim \mathcal{O}(N^3)$

Solution 1: $\log(W_1) = \int\limits_0^{T_{flow}} dt' \sum_a \rho_a^\dagger \overline{H}(t')\overline{\rho_a} \sim \mathcal{O}(N)$

Solution 2: $\log(W_2) = \int\limits_0^{T_{flow}} dt' \mathrm{Tr}(\overline{H(t')}) \sim \mathcal{O}(N)$

Just reweigh after the fact!

Do they work?



$$= 1$$

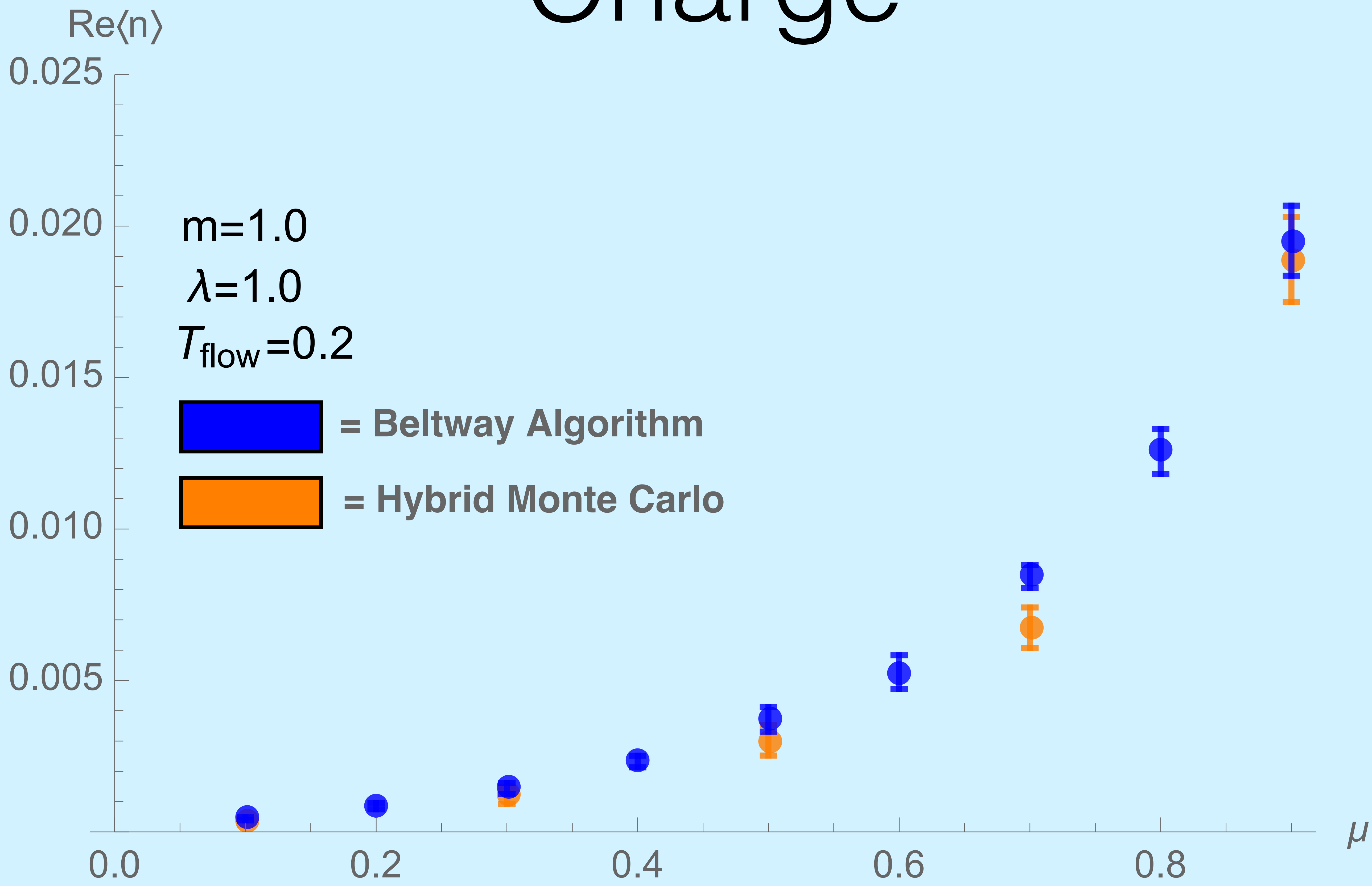
$$\{r_i\} = \{\frac{1}{N}, \dots, \frac{1}{N}\}$$

$$\Sigma = \frac{1}{N}\frac{\langle r \rangle^2}{\langle r^2 \rangle}$$

$$\{r_i\} = \{1, 0, \dots, 0\}$$

$$= \frac{1}{N}$$

Charge



[1] H. Fujii, D. Honda, M. Kato, Y. Kikukawa, S. Komatsu, and T. Sano. Hybrid Monte Carlo on Lefschetz thimbles- A study of the residual sign problem. JHEP, 10:147, 2013.

Conclusions

- One thimble computations below μ_c
- Fast jacobian estimator makes algorithm possible
- Analysis of Bose gas above μ_c possible with alternate surfaces

Marching on

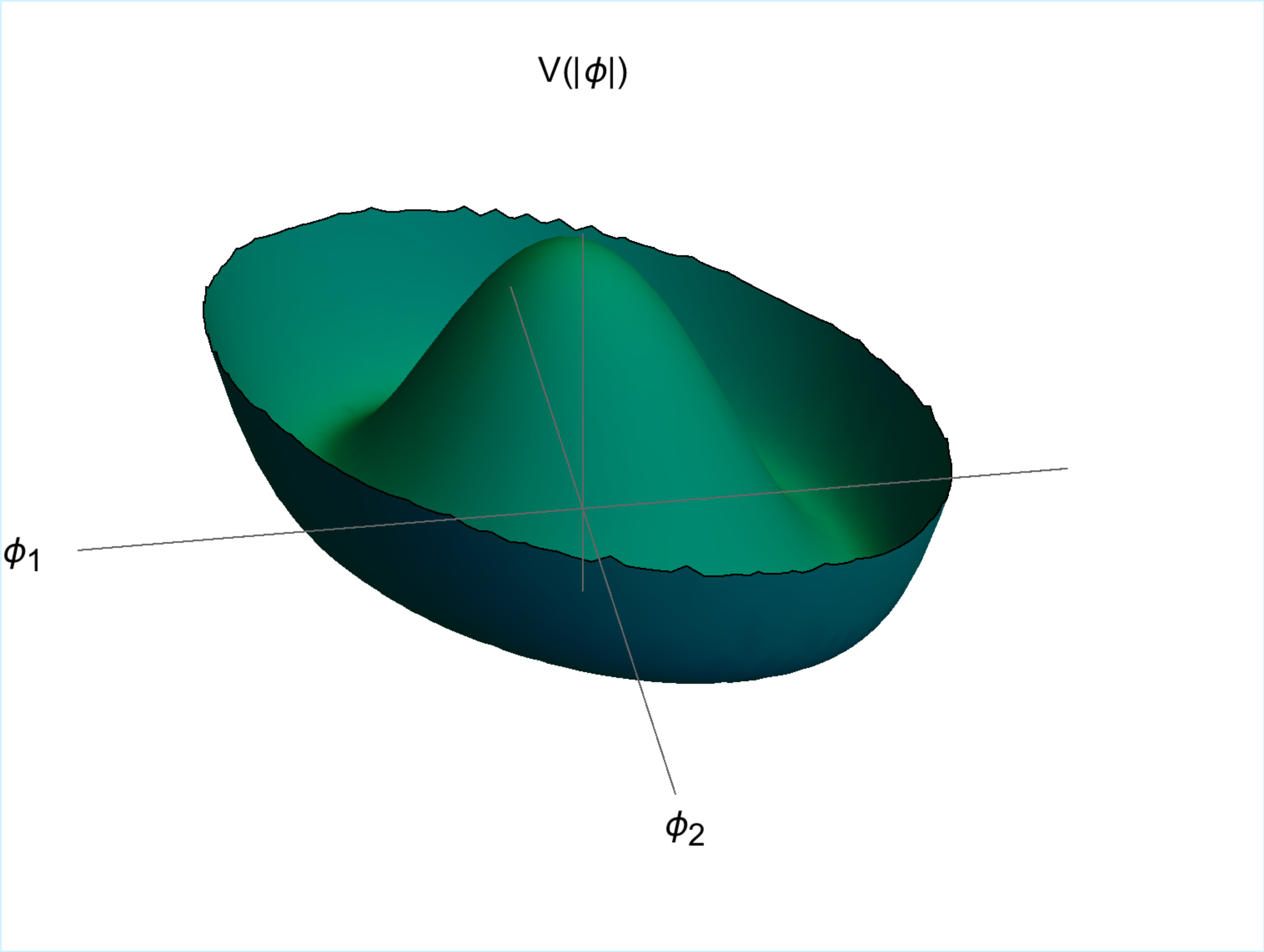
- Perfect simultaneous multi-thimble calculations
- Application to real time dynamics
- Thimbles in gauge theories

Backup Slides

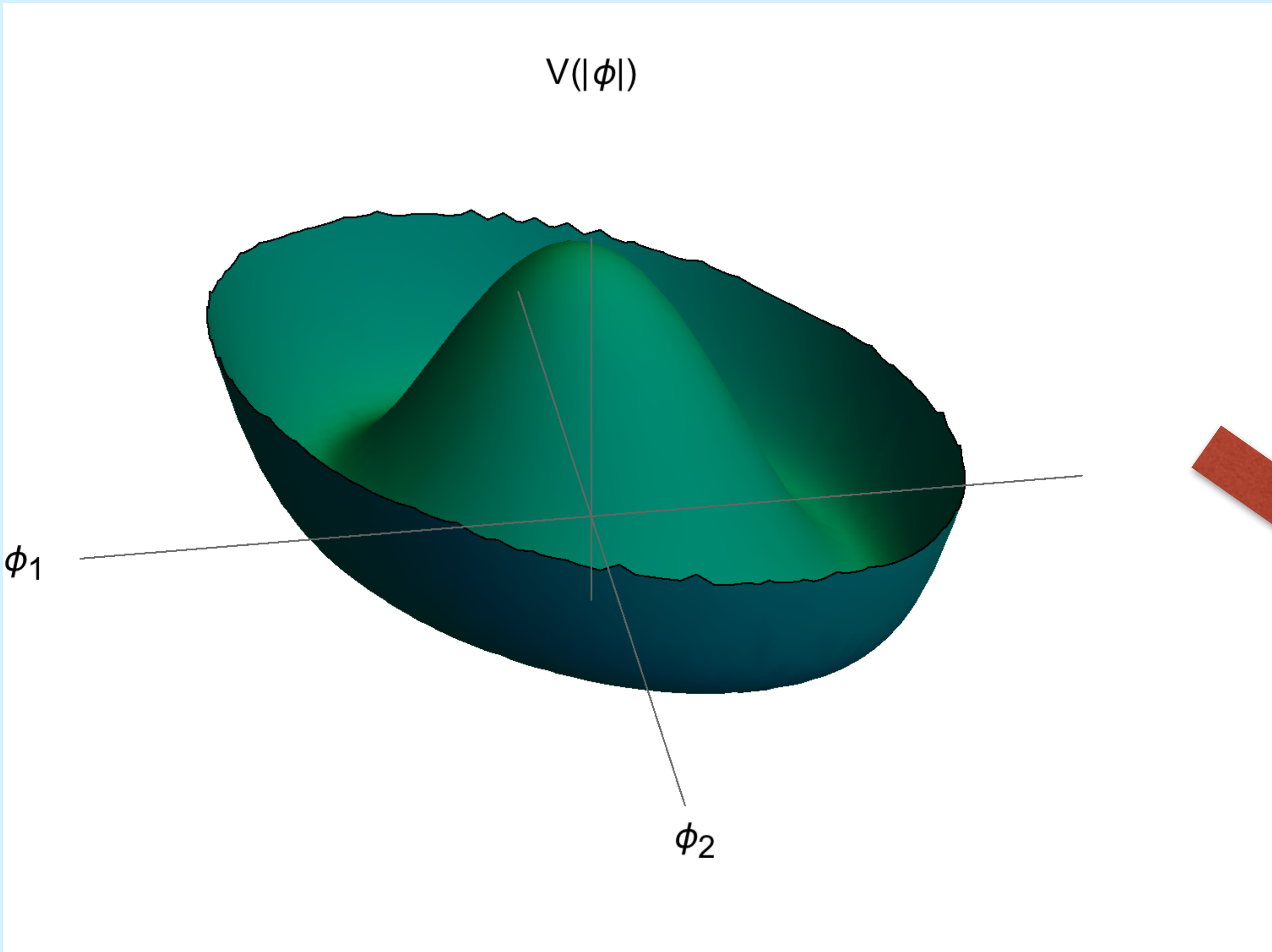
$$\mu > \mu_{crit}$$

In continuum $\mu_c = m$

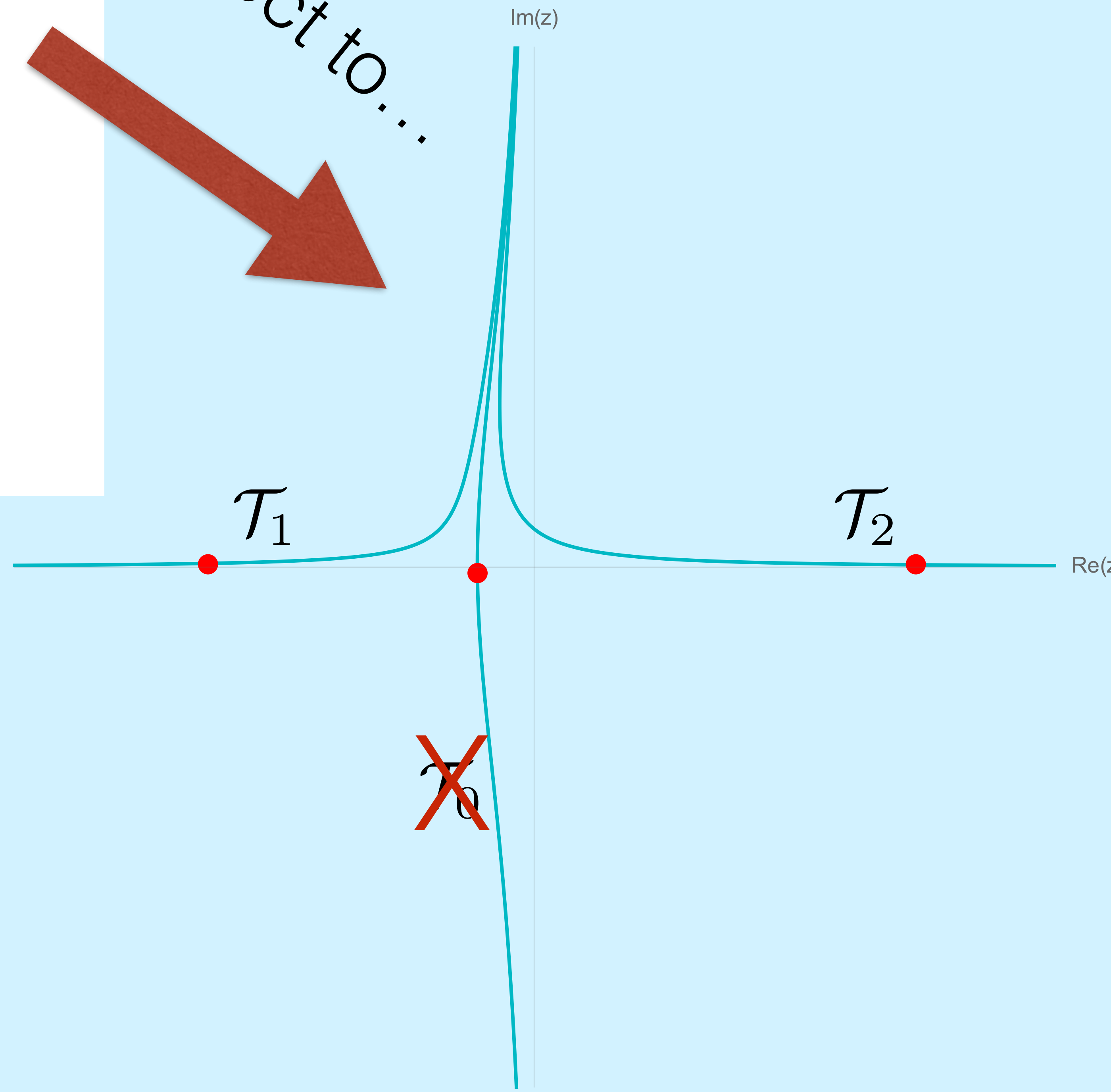
On lattice $\cosh(\mu_c) - 1 = \frac{m^2}{2}$



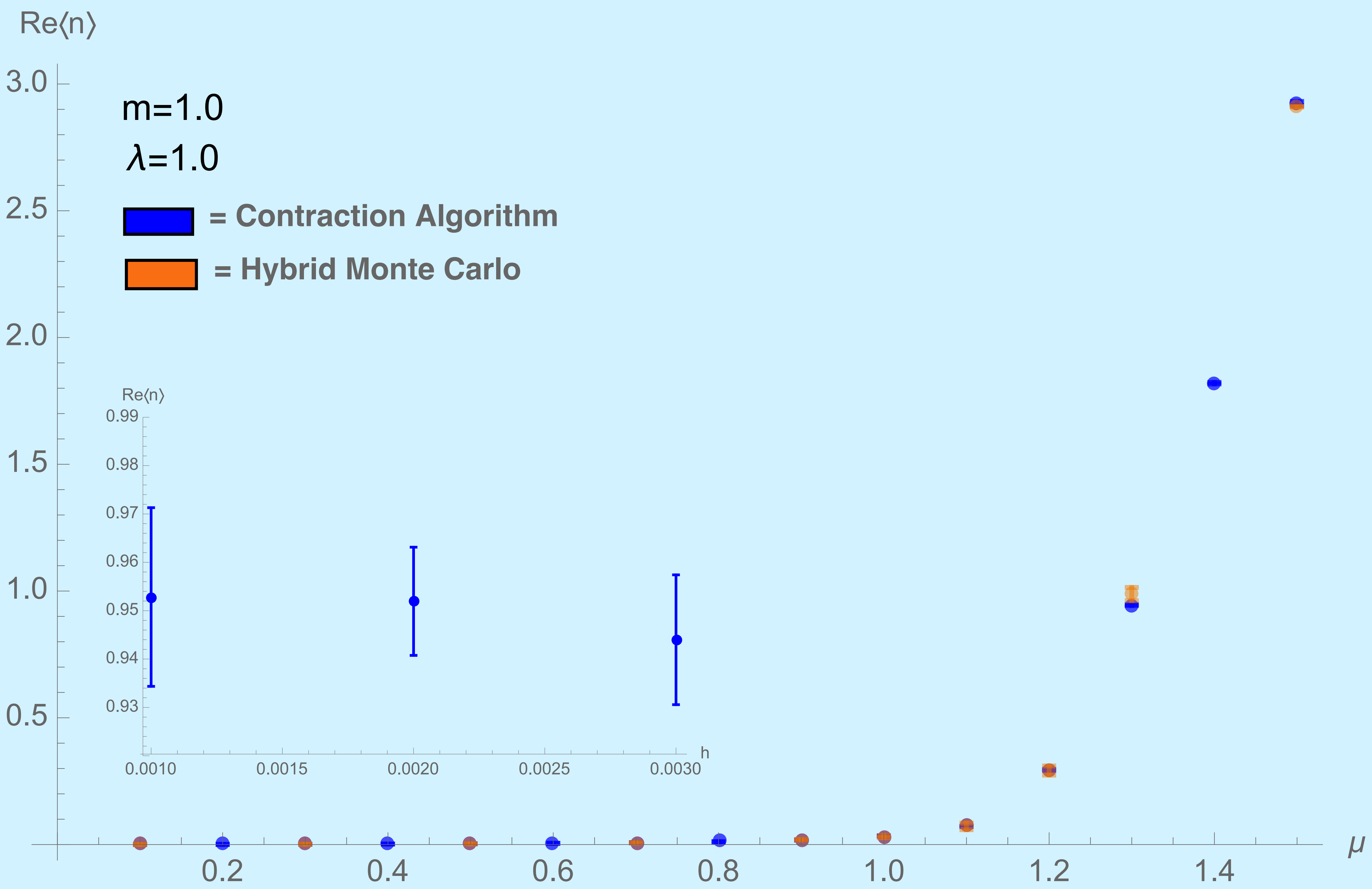
Thimbles of…



Project to…



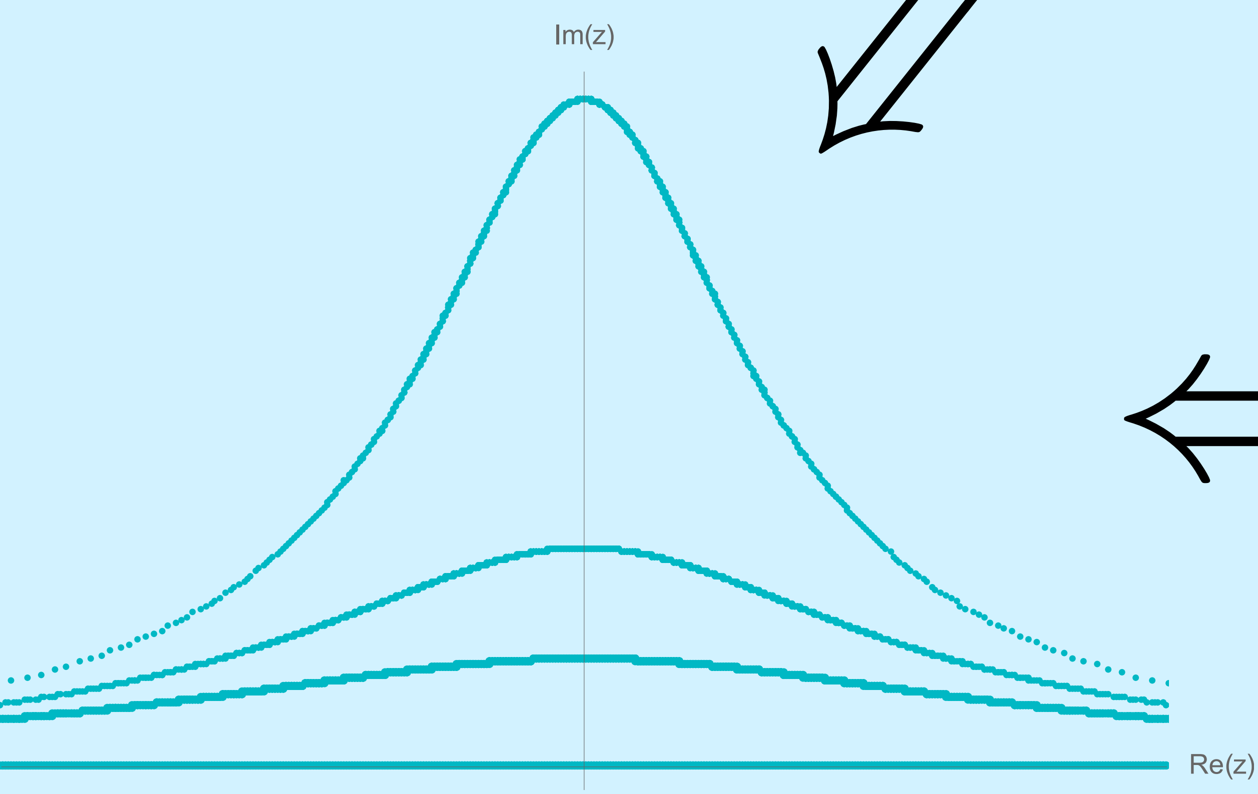
Charge: Tangent Plane

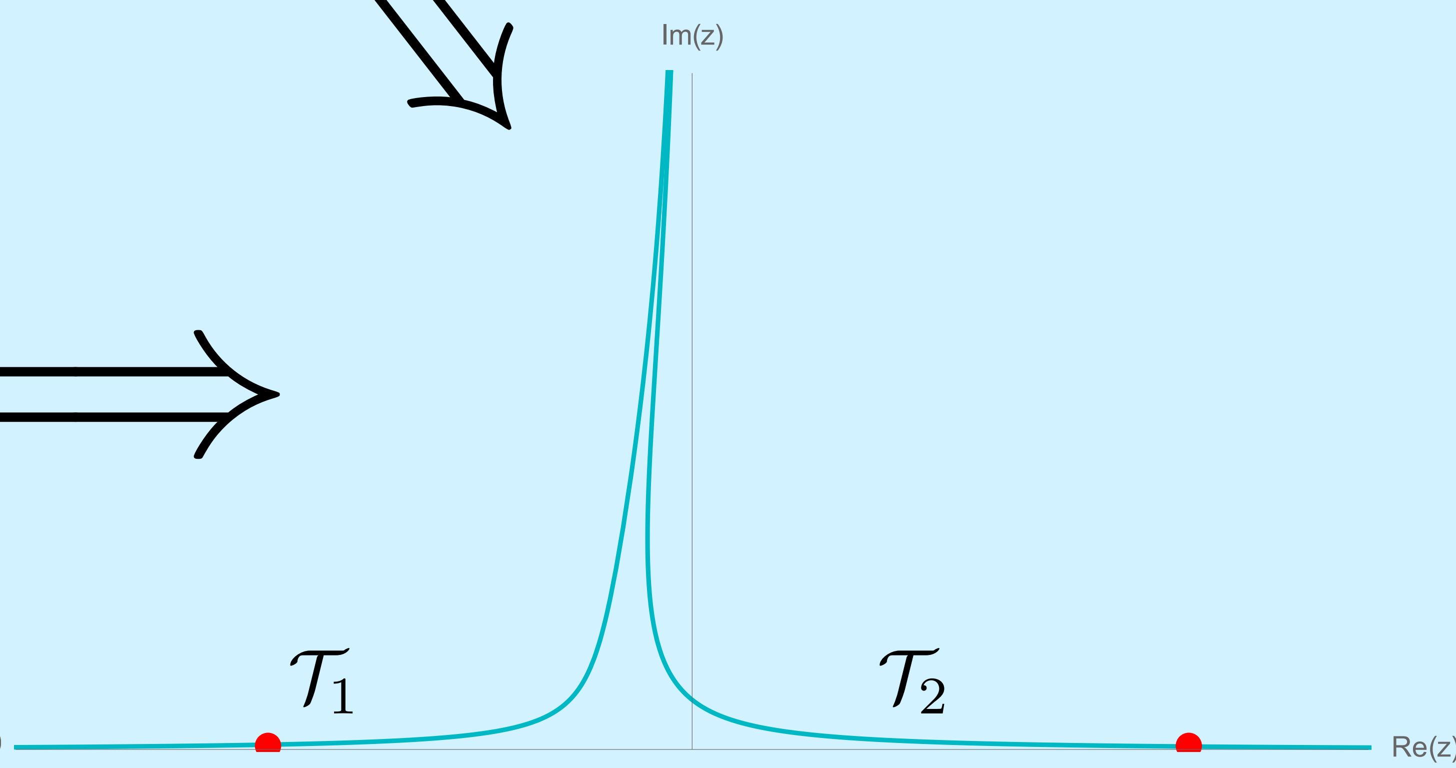


[2] H. Fujii, D. Honda, M. Kato, Y. Kikukawa, S. Komatsu, and T. Sano. Hybrid Monte Carlo on Lefschetz thimbles- A study of the residual sign problem. JHEP, 10:147, 2013.

Equivalent Surfaces

$$\int_{\mathbb{R}^n} \mathrm{e}^{-S}(\phi)\mathcal{O}(\phi)d^n\phi$$





Multi-Thimble

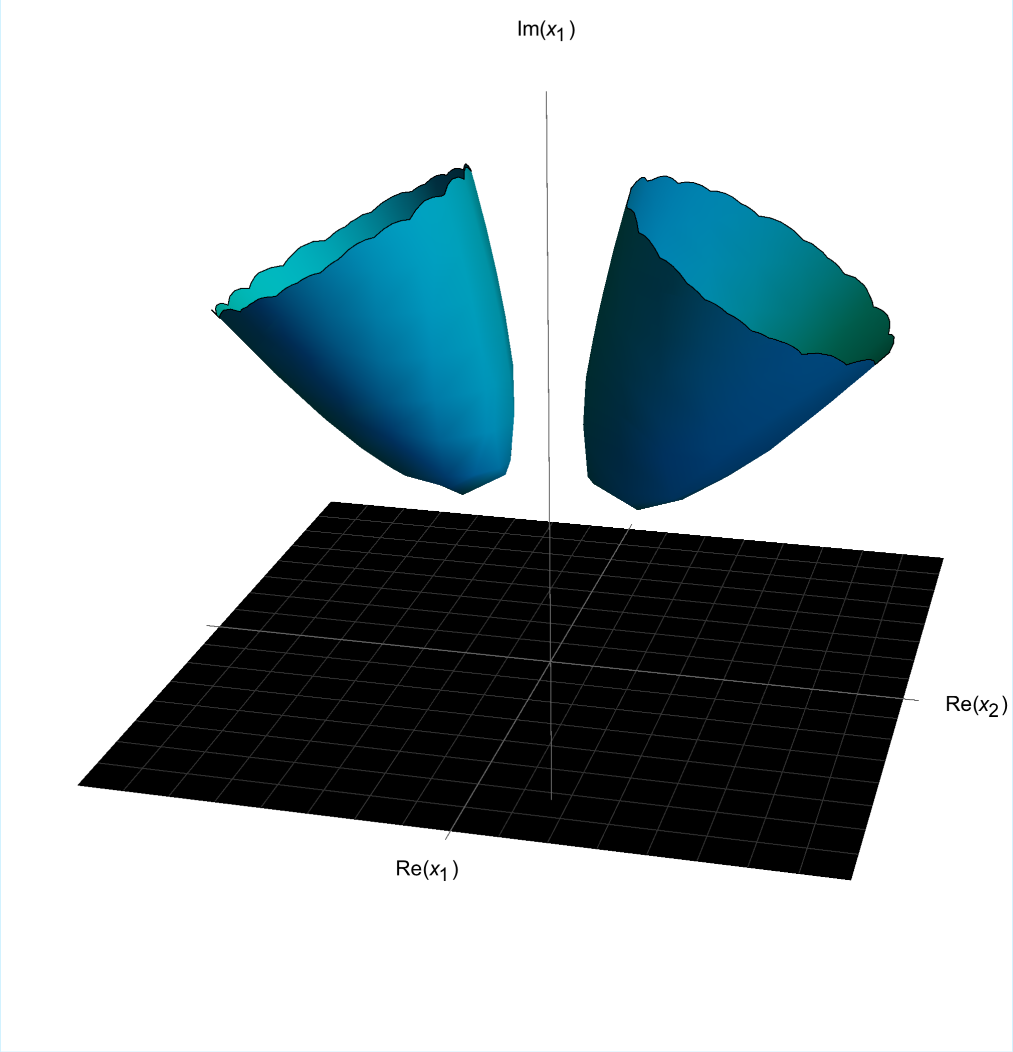
$$\langle \mathcal{O} \rangle = \frac{n_1 \mathrm{e}^{-iS_I(\phi_1)} \int_{\mathcal{T}_1} \mathrm{e}^{-S_R(\phi)} \mathcal{O}(\phi) d\phi + n_2 \mathrm{e}^{-iS_I(\phi_2)} \int_{\mathcal{T}_2} \mathrm{e}^{-S_R(\phi)} \mathcal{O}(\phi) d\phi}{n_1 \mathrm{e}^{-iS_I(\phi_1)} \int_{\mathcal{T}_1} \mathrm{e}^{-S_R(\phi)} d\phi + n_2 \mathrm{e}^{-iS_I(\phi_2)} \int_{\mathcal{T}_2} \mathrm{e}^{-S_R(\phi)} d\phi}$$

$$= \frac{\langle \tilde{\mathcal{O}} \rangle}{\langle \tilde{\mathbb{I}} \rangle}$$

$$\Pr[\phi] = \frac{\mathrm{e}^{-S_R(\phi)}}{Z} \quad Z = \int_{\mathcal{T}_1 \cup \mathcal{T}_2} \mathrm{e}^{-S_R(\phi)}$$

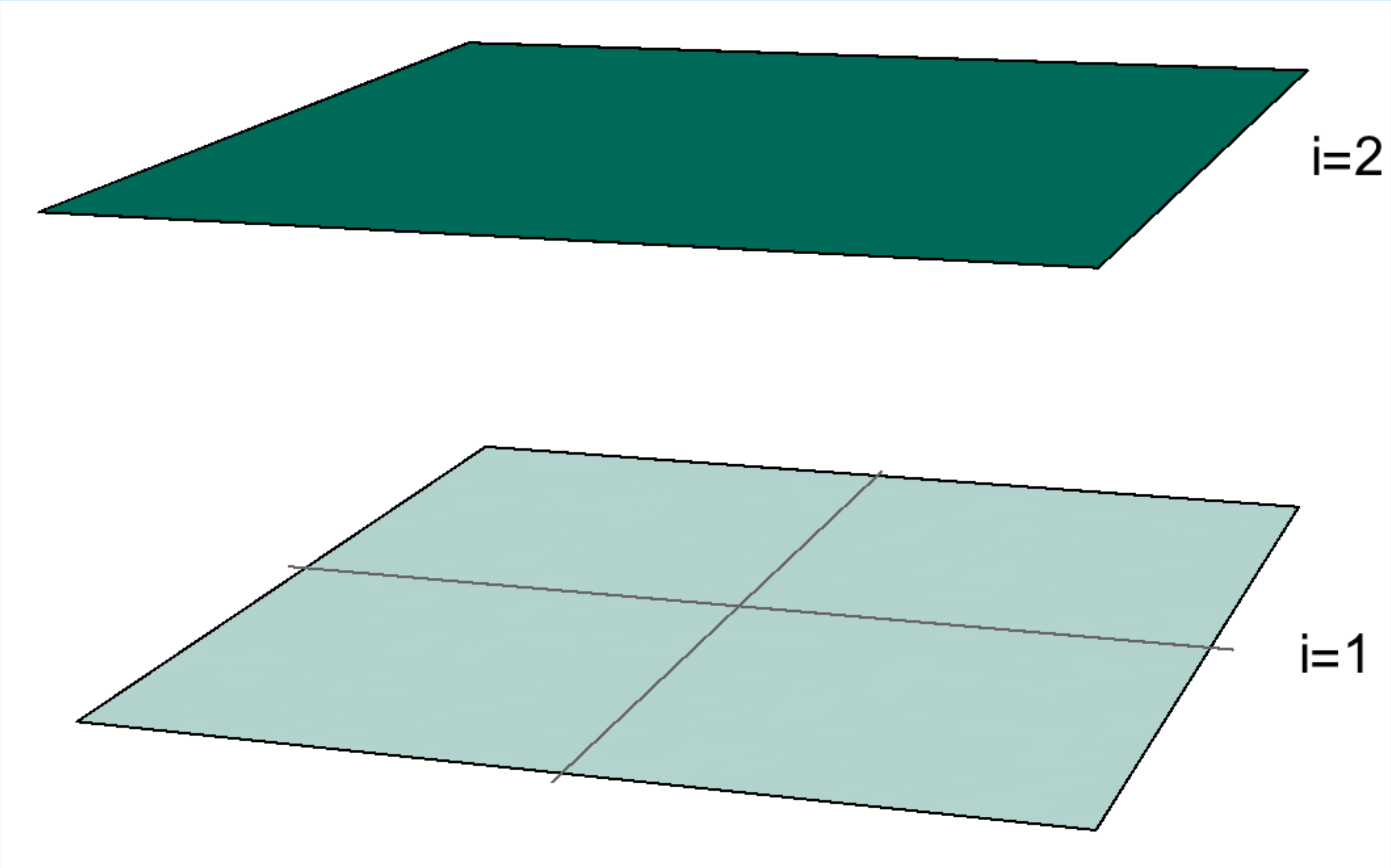
$$\tilde{\mathcal{O}}(\phi) = \begin{cases} n_1 \mathrm{e}^{-iS_I(\phi_1)} \mathcal{O}(\phi) & \phi \in \mathcal{T}_1 \\ n_2 \mathrm{e}^{-iS_I(\phi_2)} \mathcal{O}(\phi) & \phi \in \mathcal{T}_2 \end{cases}$$

$$\tilde{\mathbb{I}}(\phi) = \begin{cases} n_1 \mathrm{e}^{-iS_I(\phi_1)} & \phi \in \mathcal{T}_1 \\ n_2 \mathrm{e}^{-iS_I(\phi_2)} & \phi \in \mathcal{T}_2 \end{cases}$$



Multi-Thimble

$$\langle \tilde{\mathcal{O}} \rangle = \frac{\int\limits_{\mathcal{T}_1 \cup \mathcal{T}_2} \tilde{\mathcal{O}}(\phi) \mathrm{e}^{-S_R(\phi)} d\phi}{\int\limits_{\mathcal{T}_1 \cup \mathcal{T}_2} \mathrm{e}^{-S_R(\phi)} d\phi} = \frac{\int \tilde{\mathcal{O}}(\tilde{\phi}, i) \mathrm{e}^{-S_{eff}(\phi,i)} \mathrm{e}^{i\mathrm{Im}(\ln J)} d\tilde{\phi}}{\int \mathrm{e}^{-S_{eff}(\phi,i)} \mathrm{e}^{i\mathrm{Im}(\ln J)} d\tilde{\phi}}$$



Common set of coordinates
+
integer