

# **HMC on Lefschetz thimbles**

## **-- A study of the residual sign problem**

Y. Kikukawa

in collaboration with

H. Fujii , T. Sano  
M. Kato, S. Komatsu, D. Honda

(the University of Tokyo, Komaba ; Riken)

based on

**arXiv:1309.4371 ; JHEP10(2013)147**

Feb. 20, 2014 @ GSI

# Plan

## 1. Lattice models on Lefschetz thimbles (brief rev.)

- Pahm's result (Morse theory)
- Gradient flow, Critical points, Lefschetz thimbles
- ★ Residual sign problem: extra phase factor / Tangent spaces

## 2. An algorithm of HMC on Lefschetz thimbles

- a. how to parametrize/generate field conf. on the thimble
- b. how to formulate/solve the molecular dynamics on the thimble
- c. how to measure observables : reweighting the residual phase ?

## 3. Test in the $\lambda\varphi^4_\mu$ model

## 4. Summary & Discussions

# Lattice models with complex-valued actions

- QCD with finite chemical potential
- Chiral gauge theories
- Chiral Yukawa theories
- ..., etc.

[  $e^{\mu a}$  a la Hasenfratz and Karsch ]

[ exact chiral gauge symmetry  
thanks to Ginsparg-Wilson rel. ]

[ reflection positivity  
in spite of Ginsparg-Wilson rel. ]

physically well-defined,  
but the state-of-art Monte Carlo methods do not apply straightforwardly

# Approaches to Lattice models with complex-valued actions

highly desirable to have a stochastic method which is based on a sound theoretical basis and applicable to these models

many methods proposed (and many analyses of the sign problem):  
reweighting; histogram; dual variables/worm algorithm;  
Taylor expansion in  $\mu$ ; analytic continuation in  $\mu$  (imaginary  $\mu$ ), etc.

One possible approach is to complexify the lattice models

$$\phi_x \in \mathbb{R} \longrightarrow z_x \in \mathbb{C} \quad U_{x\mu} = e^{iA_{x\mu}^a T^a} \in \text{SU}(3) \longrightarrow e^{iZ_{x\mu}^a T^a} \in \text{SL}(3, \mathbb{C})$$

- complexified Langevin dynamics

Parisi (1983), Klauder (1983), ... (the old and classic approach)

I.-O. Stamatescu et al., Phys. Rev. D75 045007 (2007), etc.

G.Aarts, PRL 102(2009) 131601 ( $\lambda\varphi^4_\mu$ ) D. Sexty, arXiv:1307.7748 (QCD $_\mu$ )

- Path-Integral contours deformed to Lefschetz thimbles

F. Pham (1983); E. Witten, arXiv:1001.2933;

M. Cristoforetti, F. Di Renzo, A. Mukherjee, L. Scorzato (AuroraScience Collaboration)  
Phys. Rev. D 86, 074506 (2012), arXiv:1205.3996

Phys. Rev. D88, 051501 (2013), arXiv:1303.7204; 051502, arXiv:1308.0233 ;

G.Aarts Phys. Rev. D88, 094501 (2013), arXiv:1308.4811

# Approaches to Lattice models with complex-valued actions

highly desirable to have a stochastic method which is based on a sound theoretical basis and applicable to these models

many methods proposed (and many analyses of the sign problem):  
reweighting; histogram; dual variables/worm algorithm;  
Taylor expansion in  $\mu$ ; analytic continuation in  $\mu$  (imaginary  $\mu$ ), etc.

One possible approach is to complexify the lattice models

$$\phi_x \in \mathbb{R} \longrightarrow z_x \in \mathbb{C} \quad U_{x\mu} = e^{iA_{x\mu}^a T^a} \in \text{SU}(3) \longrightarrow e^{iZ_{x\mu}^a T^a} \in \text{SL}(3, \mathbb{C})$$

- complexified Langevin dynamics

Parisi (1983), Klauder (1983), ... (the old and classic approach)

I.-O. Stamatescu et al., Phys. Rev. D75 045007 (2007), etc.

G.Aarts, PRL 102(2009) 131601 ( $\lambda\varphi^4_\mu$ ) D. Sexty, arXiv:1307.7748 (QCD $_\mu$ )

- Path-Integral contours deformed to Lefschetz thimbles  
F. Pham (1983); E. Witten, arXiv:1001.2933;  
M. Cristoforetti, F. Di Renzo, A. Mukherjee, L. Scorzato (AuroraScience)  
Phys. Rev. D 86, 074506 (2012), arXiv:1205.3996  
Phys. Rev. D88, 051501 (2013), arXiv:1303.7204; 051502, arXiv:1308.0233 ;  
G.Aarts Phys. Rev. D88, 094501 (2013), arXiv:1308.4811

cf. July 1, 2010  
Journal Club @ Komaba  
by D. Honda  
Im(S)= const.!, HMC?! ;-)

# Lattice models on Lefschetz thimbles

$$x \in \mathcal{C}_{\mathbb{R}} (\subseteq \mathbb{R}^n) \longrightarrow x + iy = z \in \mathbb{C}^n$$

$$S[x] \rightarrow S[x + iy] = S[z]$$

$$Z = \int_{\mathcal{C}_{\mathbb{R}}} \mathcal{D}[x] \exp\{-S[x]\} = \int_{\mathcal{C}} \mathcal{D}[z] \exp\{-S[z]\} \quad (\mathcal{D}[x] = d^n x)$$

the contour of path-integration is selected by using the result of Morse theory [ F. Pham (1983) ]

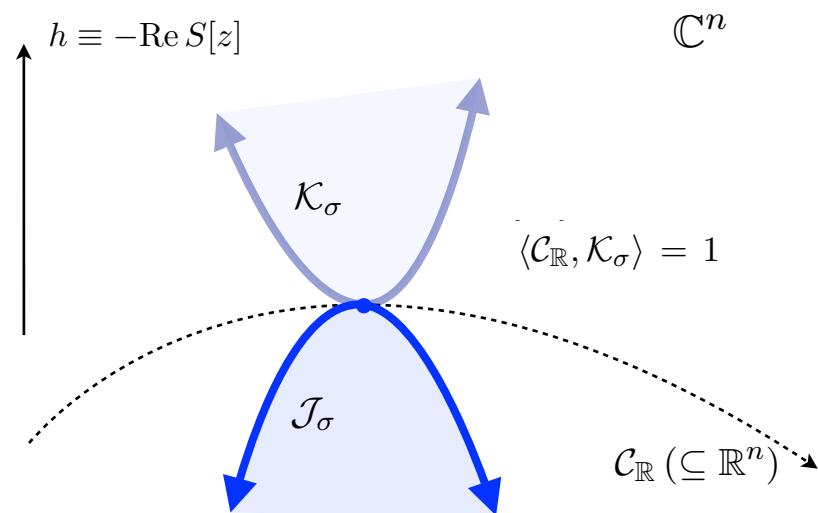
$$\mathcal{C}_{\mathbb{R}} = \sum_{\sigma \in \Sigma} n_{\sigma} \mathcal{J}_{\sigma}, \quad n_{\sigma} = \langle \mathcal{C}_{\mathbb{R}}, \mathcal{K}_{\sigma} \rangle$$

$$h \equiv -\text{Re } S[z]$$

$$\frac{d}{dt} z(t) = \frac{\partial \bar{S}[\bar{z}]}{\partial \bar{z}}, \quad \frac{d}{dt} \bar{z}(t) = \frac{\partial S[z]}{\partial z}, \quad t \in \mathbb{R}$$

**critical points  $z_{\sigma}$ :**  $\left. \frac{\partial S[z]}{\partial z} \right|_{z=z_{\sigma}} = 0$

**Lefschetz thimble  $\mathcal{J}_{\sigma}(\mathcal{K}_{\sigma})$**  (n-dim. real mfd.)  
 =the union of all down(up)ward flows which trace back to  $z_{\sigma}$  in the limit t goes to  $-\infty$



$$\langle \mathcal{J}_{\sigma}, \mathcal{K}_{\tau} \rangle = \delta_{\sigma\tau} \text{ (intersection numbers)}$$

# Lattice models on Lefschetz thimbles

$$x \in \mathcal{C}_{\mathbb{R}} (\subseteq \mathbb{R}^n) \longrightarrow x + iy = z \in \mathbb{C}^n$$

$$S[x] \rightarrow S[x + iy] = S[z]$$

$$Z = \int_{\mathcal{C}_{\mathbb{R}}} \mathcal{D}[x] \exp\{-S[x]\} = \int_{\mathcal{C}} \mathcal{D}[z] \exp\{-S[z]\} \quad ( \mathcal{D}[x] = d^n x )$$

the contour of path-integration is selected by using the result of Morse theory [ *F. Pham (1983)* ]

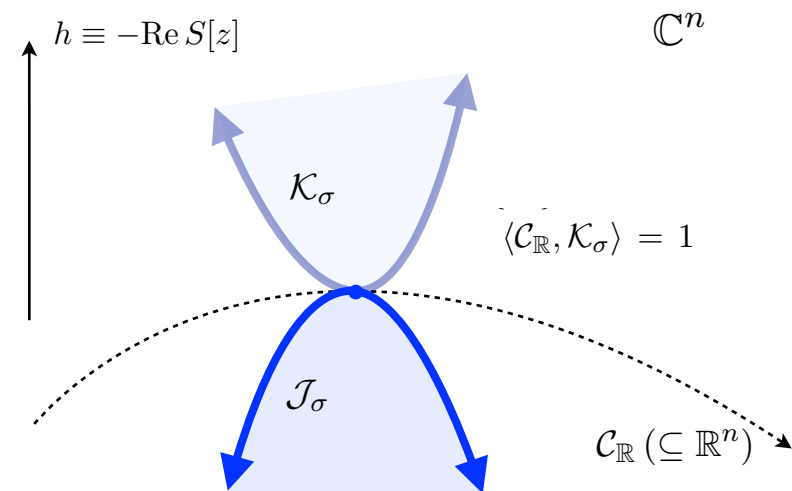
$$\mathcal{C}_{\mathbb{R}} = \sum_{\sigma \in \Sigma} n_{\sigma} \mathcal{J}_{\sigma}, \quad n_{\sigma} = \langle \mathcal{C}_{\mathbb{R}}, \mathcal{K}_{\sigma} \rangle$$

$$h \equiv -\text{Re } S[z]$$

$$\frac{d}{dt} z(t) = \frac{\partial \bar{S}[\bar{z}]}{\partial \bar{z}}, \quad \frac{d}{dt} \bar{z}(t) = \frac{\partial S[z]}{\partial z}, \quad t \in \mathbb{R}$$

$$\frac{d}{dt} h = -\frac{1}{2} \left\{ \frac{\partial S[z]}{\partial z} \cdot \frac{d}{dt} z(t) + \frac{\partial \bar{S}[\bar{z}]}{\partial \bar{z}} \cdot \frac{d}{dt} \bar{z}(t) \right\} = - \left| \frac{\partial S[z]}{\partial z} \right|^2 \leq 0$$

$$\frac{d}{dt} \text{Im } S[z] = \frac{1}{2i} \left\{ \frac{\partial S[z]}{\partial z} \cdot \frac{d}{dt} z(t) - \frac{\partial \bar{S}[\bar{z}]}{\partial \bar{z}} \cdot \frac{d}{dt} \bar{z}(t) \right\} = 0 \quad !$$



# Partition function

$$Z = \sum_{\sigma \in \Sigma} n_{\sigma} \exp\{-S[z_{\sigma}]\} Z_{\sigma}, \quad n_{\sigma} = \langle \mathcal{C}_{\mathbb{R}}, \mathcal{K}_{\sigma} \rangle$$

$$Z_{\sigma} = \int_{\mathcal{J}_{\sigma}} \mathcal{D}[z] \exp\{-\text{Re}(S[z] - S[z_{\sigma}])\}$$

## Observables

$$\langle O[z] \rangle = \frac{1}{Z} \sum_{\sigma \in \Sigma} n_{\sigma} \exp\{-S[z_{\sigma}]\} Z_{\sigma} \langle O[z] \rangle_{\mathcal{J}_{\sigma}}$$

$$\langle O[z] \rangle_{\mathcal{J}_{\sigma}} = \frac{1}{Z_{\sigma}} \int_{\mathcal{J}_{\sigma}} \mathcal{D}[z] \exp\{-\text{Re}(S[z] - S[z_{\sigma}])\} O[z]$$

$$\langle \mathcal{C}_{\mathbb{R}}, \mathcal{K}_{\sigma} \rangle = 0$$

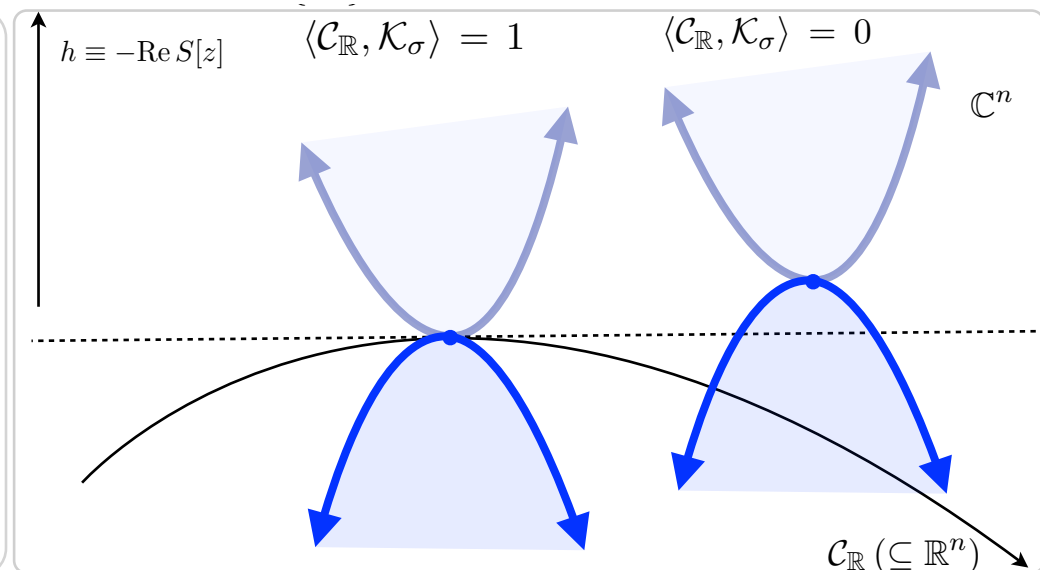
$\{z_{\sigma}\}$  satisfying  $-\text{Re}S[z_{\sigma}] > \max\{-\text{Re}S[x]\} (x \in \mathcal{C}_{\mathbb{R}})$

$$\langle \mathcal{C}_{\mathbb{R}}, \mathcal{K}_{\sigma} \rangle = 1$$

$\{z_{\sigma}\}$  in the original cycle  $\mathcal{C}_{\mathbb{R}}$

the relative weights proportional to  $\exp(-S[z_{\sigma}])$

$$z_{\text{vac}} \in \mathcal{C}_{\mathbb{R}} \quad -\text{Re}S[z_{\text{vac}}] = \max\{-\text{Re}S[x]\} (x \in \mathcal{C}_{\mathbb{R}})$$





# Observables

$$\langle O[z] \rangle = \frac{1}{Z} \sum_{\sigma \in \Sigma} n_{\sigma} \exp\{-S[z_{\sigma}]\} Z_{\sigma} \langle O[z] \rangle_{\mathcal{J}_{\sigma}}$$

$$\langle O[z] \rangle_{\mathcal{J}_{\sigma}} = \frac{1}{Z_{\sigma}} \int_{\mathcal{J}_{\sigma}} \mathcal{D}[z] \exp\{-\text{Re}(S[z] - S[z_{\sigma}])\} O[z]$$

# Observables

$$\langle O[z] \rangle = \frac{1}{Z} \sum_{\sigma \in \Sigma} n_{\sigma} \exp\{-S[z_{\sigma}]\} Z_{\sigma} \langle O[z] \rangle_{\mathcal{J}_{\sigma}}$$

$$\langle O[z] \rangle_{\mathcal{J}_{\sigma}} = \frac{1}{Z_{\sigma}} \int_{\mathcal{J}_{\sigma}} \mathcal{D}[z] \exp\{-\text{Re}(S[z] - S[z_{\sigma}])\} O[z]$$

It is not straightforward to compute the sum, in general

$$Z_{\sigma} = 1/\sqrt{\det K}$$

$$K_{ij} \equiv \partial_i \partial_j S[z]|_{z=z_{\sigma}}$$

in the saddle point approximation

# Observables

$$\langle O[z] \rangle = \frac{1}{Z} \sum_{\sigma \in \Sigma} n_{\sigma} \exp\{-S[z_{\sigma}]\} Z_{\sigma} \langle O[z] \rangle_{\mathcal{J}_{\sigma}}$$

It is not straightforward to compute the sum, in general

$$\langle O[z] \rangle_{\mathcal{J}_{\sigma}} = \frac{1}{Z_{\sigma}} \int_{\mathcal{J}_{\sigma}} \mathcal{D}[z] \exp\{-\text{Re}(S[z] - S[z_{\sigma}])\} O[z]$$

$$Z_{\sigma} = 1/\sqrt{\det K}$$

$$K_{ij} \equiv \partial_i \partial_j S[z]|_{z=z_{\sigma}}$$

in the saddle point approximation

The functional measure should be specified by **the tangent spaces** of the thimble  
It may give rise to **an extra phase factor !**  
>> **residual sign problem**

if  $\{U_z^{\alpha}\}$  is an orthonormal basis of the tangent space

$$\delta z = U_z^{\alpha} \delta \xi^{\alpha} \quad |\delta z|^2 = \delta \xi^2$$

$$d^n z|_{\mathcal{J}_{\sigma}} = d^n \delta \xi \det U_z$$

$$e^{i\phi_z} = \det U_z = \frac{\det V_z}{|\det V_z|}$$

# Observables

$$\langle O[z] \rangle = \frac{1}{Z} \sum_{\sigma \in \Sigma} n_{\sigma} \exp\{-S[z_{\sigma}]\} Z_{\sigma} \langle O[z] \rangle_{\mathcal{J}_{\sigma}}$$

It is not straightforward to compute the sum, in general

$$\langle O[z] \rangle_{\mathcal{J}_{\sigma}} = \frac{1}{Z_{\sigma}} \int_{\mathcal{J}_{\sigma}} \mathcal{D}[z] \exp\{-\text{Re}(S[z] - S[z_{\sigma}])\} O[z]$$

$$Z_{\sigma} = 1/\sqrt{\det K}$$

$$K_{ij} \equiv \partial_i \partial_j S[z]|_{z=z_{\sigma}}$$

in the saddle point approximation

Since  $\text{Im}(S)$  stays constant, this part may be evaluated by **MC**, but with the residual phase factor **reweighted**

The functional measure should be specified by **the tangent spaces** of the thimble  
It may give rise to **an extra phase factor!**  
>> **residual sign problem**

if  $\{U_z^{\alpha}\}$  is an orthonormal basis of the tangent space

$$\delta z = U_z^{\alpha} \delta \xi^{\alpha} \quad |\delta z|^2 = \delta \xi^2$$

$$d^n z|_{\mathcal{J}_{\sigma}} = d^n \delta \xi \det U_z$$

$$e^{i\phi_z} = \det U_z = \frac{\det V_z}{|\det V_z|}$$

# Observables

$$\langle O[z] \rangle = \frac{1}{Z} \sum_{\sigma \in \Sigma} n_{\sigma} \exp\{-S[z_{\sigma}]\} Z_{\sigma} \langle O[z] \rangle_{\mathcal{J}_{\sigma}}$$

It is not straightforward to compute the sum, in general

$$\langle O[z] \rangle_{\mathcal{J}_{\sigma}} = \frac{1}{Z_{\sigma}} \int_{\mathcal{J}_{\sigma}} \mathcal{D}[z] \exp\{-\text{Re}(S[z] - S[z_{\sigma}])\} O[z]$$

$$Z_{\sigma} = 1/\sqrt{\det K}$$

$$K_{ij} \equiv \partial_i \partial_j S[z]|_{z=z_{\sigma}}$$

in the saddle point approximation

Since  $\text{Im}(S)$  stays constant, this part may be evaluated by **MC**, but with the residual phase factor **reweighted**

The functional measure should be specified by **the tangent spaces** of the thimble  
It may give rise to **an extra phase factor!**  
>> **residual sign problem**

a possible approximation :  
**take a single thimble**  $\mathcal{J}_{\text{vac}}$

$$\langle O[z] \rangle = \langle O[z] \rangle_{\mathcal{J}_{\text{vac}}}$$

(AuroraScience Collaboration)

if  $\{U_z^{\alpha}\}$  is an orthonormal basis of the tangent space

$$\delta z = U_z^{\alpha} \delta \xi^{\alpha} \quad |\delta z|^2 = \delta \xi^2$$

$$d^n z |_{\mathcal{J}_{\sigma}} = d^n \delta \xi \det U_z$$

$$e^{i\phi_z} = \det U_z = \frac{\det V_z}{|\det V_z|}$$

# Geometric properties of Lefschetz thimbles

## a) Tangent spaces of Lefschetz thimbles

basis of tangent vectors  $\{V_z^\alpha\} (\alpha = 1, \dots, n)$

at a generic point  $z$  on  $\mathcal{J}_\sigma$

$$\frac{d}{dt} V_{zi}^\alpha(t) = \bar{\partial}_i \bar{\partial}_j \bar{S}[\bar{z}] \bar{V}_{zj}^\alpha(t) \quad (\alpha = 1, \dots, n)$$

$$\{V_z \partial + \bar{V}_z \bar{\partial}\} V'_z - \{V'_z \partial + \bar{V}'_z \bar{\partial}\} V_z = 0$$

$$g \equiv \bar{\partial} \bar{S}[\bar{z}]$$

$$\{g \partial + \bar{g} \bar{\partial}\} V_z^\alpha - \{V_z^\alpha \partial + \bar{V}_z^\alpha \bar{\partial}\} g = 0$$

In the vicinity of critical point  $z_\sigma$

linearized flow equation and its solution:

$$\frac{d}{dt} (z_i(t) - z_{\sigma i}) = \bar{K}_{ij} (\bar{z}_j(t) - \bar{z}_{\sigma j}), \quad K_{ij} \equiv \partial_i \partial_j S[z]|_{z=z_\sigma}$$

$$z_i(t) - z_{\sigma i} = v_i^\alpha \exp(\kappa^\alpha (t - t_0)) \xi_0^\alpha, \quad \xi_0^\alpha \in \mathbb{R} \quad (\alpha = 1, \dots, n)$$

$$v_i^\alpha K_{ij} v_j^\beta = \kappa^\alpha \delta^{\alpha\beta}$$

$$\kappa^\alpha \geq 0 \quad (\alpha = 1, \dots, n)$$

$$v_i^\alpha (\alpha = 1, \dots, n) \text{ are orthonormal}$$

$\{v^\alpha\} (\alpha = 1, \dots, n)$  spans the tangent space  $T_{z_\sigma}$

$$\bar{V}_{zi}^\alpha V_{zi}^\beta - \bar{V}_{zi}^\beta V_{zi}^\alpha = 0 \quad (\alpha, \beta = 1, \dots, n)$$

$$V_z^\alpha = U_z^\beta E^{\beta\alpha} \quad \{U_z^\alpha\} \text{ is an orthonormal basis}$$

$E$  is a real upper triangle matrix

$$\frac{d}{dt} \text{Im}\{\bar{V}_z^\alpha(t) V_z^\beta(t)\}$$

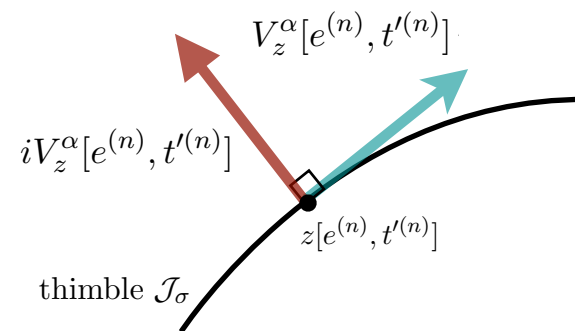
$$= \text{Im}\{V_z^\alpha \partial^2 S[z] V_z^\beta(t) + \bar{V}_z^\alpha \bar{\partial}^2 \bar{S}[\bar{z}] \bar{V}_z^\beta(t)\} = 0$$

## b) Normal directions of thimbles

the set of normal vectors

$$\{iU_z^\alpha\} \text{ or } \{iV_z^\alpha\} (\alpha = 1, \dots, n)$$

$$\text{Re}\{(-i)\bar{V}_{zi}^\alpha V_{zi}^\beta\} = 0$$



## c) Parametrization of points z on thimbles

Asymptotic solutions of Flow equations

$$z(t) \simeq z_\sigma + v^\alpha \exp(\kappa^\alpha t) e^\alpha; \quad e^\alpha e^\alpha = n$$

$$V_z^\alpha(t) \simeq v^\alpha \exp(\kappa^\alpha t),$$

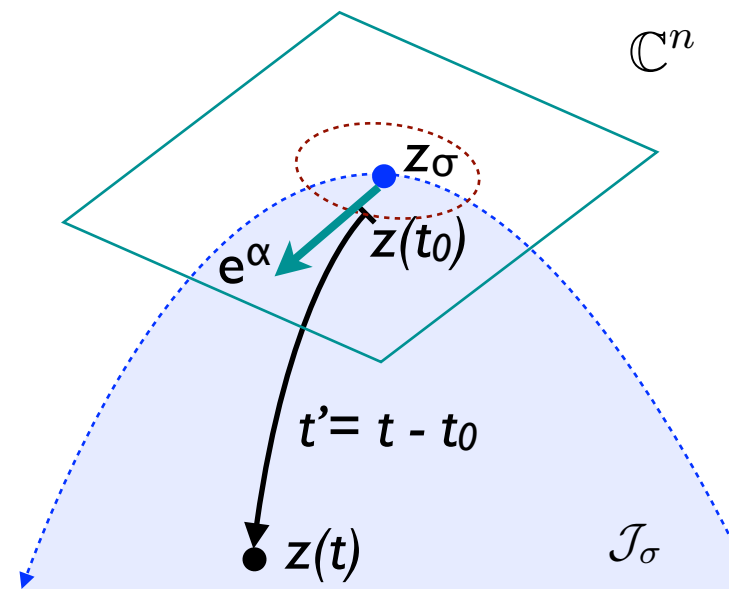
the **direction** of the flow :  $e^\alpha$  ( $\alpha = 1, \dots, n; \|e\|^2 = n$ )

the **time** of the flow :  $t' = t - t_0$

$$z[e, t'] : (e^\alpha, t') \rightarrow z \in \mathcal{J}_\sigma$$

$$z[e, t'] = z(t)|_{t=t'+t_0}$$

$$\delta z[e, t'] = V_z^\alpha[e, t'] (\delta e^\alpha + \kappa^\alpha e^\alpha \delta t')$$



# Algorithm of HMC on Lefschetz thimbles

**the saddle-point structures !**

a) To generate a thimble

use the parameterization  $z[e, t'] : (e^\alpha, t') \rightarrow z \in \mathcal{J}_\sigma$

solve the flow eqs. for **both  $\mathbf{z}[e, t']$  &  $\mathbf{V}_z^\alpha[e, t']$**  by 4th-order RK

b) To formulate / solve the molecular dynamics

introduce a dynamical system constrained to the thimble

use 2nd-order constraint-preserving symmetric integrator

c) To measure observables

try to reweight the residual sign factors

$$\langle O[z] \rangle_{\mathcal{J}_\sigma} = \frac{\langle e^{i\phi_z} O[z] \rangle'_{\mathcal{J}_\sigma}}{\langle e^{i\phi_z} \rangle'_{\mathcal{J}_\sigma}}$$

where  $\langle o[z] \rangle'_{\mathcal{J}_\sigma} = \frac{1}{N_{\text{conf}}} \sum_{k=1}^{N_{\text{conf}}} o[z^{(k)}]$

$$e^{i\phi_z} = \det U_z = \frac{\det V_z}{|\det V_z|}$$

$\{\langle e^{i\phi_z} \rangle'_{\mathcal{J}_\sigma}\} (\sigma \in \Sigma)$  **should not be vanishingly small**



# Algorithm of HMC on Lefschetz thimbles

**the saddle-point structures !**

a) To generate a thimble

use the parameterization  $z[e, t'] : (e^\alpha, t') \rightarrow z \in \mathcal{J}_\sigma$

solve the flow eqs. for **both  $\mathbf{z}[e, t']$  &  $\mathbf{V}_z^\alpha[e, t']$**  by 4th-order RK

**numerically very demanding !**

b) To formulate / solve the molecular dynamics

introduce a dynamical system constrained to the thimble

use 2nd-order constraint-preserving symmetric integrator

c) To measure observables

try to reweight the residual sign factors

$$\langle O[z] \rangle_{\mathcal{J}_\sigma} = \frac{\langle e^{i\phi_z} O[z] \rangle'_{\mathcal{J}_\sigma}}{\langle e^{i\phi_z} \rangle'_{\mathcal{J}_\sigma}}$$

where  $\langle o[z] \rangle'_{\mathcal{J}_\sigma} = \frac{1}{N_{\text{conf}}} \sum_{k=1}^{N_{\text{conf}}} o[z^{(k)}]$

$$e^{i\phi_z} = \det U_z = \frac{\det V_z}{|\det V_z|}$$

$\{\langle e^{i\phi_z} \rangle'_{\mathcal{J}_\sigma}\} (\sigma \in \Sigma)$  **should not be vanishingly small**

# Algorithm of HMC on Lefschetz thimbles

**the saddle-point structures !**

a) To generate a thimble

use the parameterization  $z[e, t'] : (e^\alpha, t') \rightarrow z \in \mathcal{J}_\sigma$

solve the flow eqs. for **both  $\mathbf{z}[e, t']$  &  $\mathbf{V}_z^\alpha[e, t']$**  by 4th-order RK

**numerically very demanding !**

b) To formulate / solve the molecular dynamics

introduce a dynamical system constrained to the thimble

use 2nd-order constraint-preserving symmetric integrator

c) To measure observables

try to reweight the residual sign factors

$$\langle O[z] \rangle_{\mathcal{J}_\sigma} = \frac{\langle e^{i\phi_z} O[z] \rangle'_{\mathcal{J}_\sigma}}{\langle e^{i\phi_z} \rangle'_{\mathcal{J}_\sigma}}$$

where  $\langle o[z] \rangle'_{\mathcal{J}_\sigma} = \frac{1}{N_{\text{conf}}} \sum_{k=1}^{N_{\text{conf}}} o[z^{(k)}]$

$$e^{i\phi_z} = \det U_z = \frac{\det V_z}{|\det V_z|}$$

$\{\langle e^{i\phi_z} \rangle'_{\mathcal{J}_\sigma}\} (\sigma \in \Sigma)$  **should not be vanishingly small**

**A possible sign problem !    Need a careful and systematic study !**

## b) To formulate/solve Molecular Dynamics on the thimble

### Constrained dynamical system

Equations of motion:

$$\dot{z}_i = w_i,$$

$$\dot{w}_i = -\bar{\partial}_i \bar{S}[\bar{z}] - iV_{zi}^\alpha \lambda^\alpha \quad \lambda^\alpha \in \mathbb{R} \quad (\alpha = 1, \dots, n)$$

Constraints:

$$z_i = z_i[e, t'] \quad w_i = V_{zi}^\alpha[e, t'] w^\alpha, \quad w^\alpha \in \mathbb{R}$$

A conserved Hamiltonian:

$$H = \frac{1}{2} \bar{w}_i w_i + \frac{1}{2} \{S[z] + \bar{S}[\bar{z}]\}$$

$$\begin{aligned} \dot{H} &= \frac{1}{2} \{\dot{w}_i w_i + \bar{w}_i \dot{w}_i\} + \frac{1}{2} \{\partial_i S[z] \dot{z}_i + \bar{\partial}_i \bar{S}[\bar{z}] \dot{\bar{z}}_i\} \\ &= \frac{1}{2} \{(+i\bar{V}_{zi}^\alpha \lambda^\alpha) w_i + \bar{w}_i (-iV_{zi}^\alpha \lambda^\alpha)\} \\ &= \frac{i}{2} \lambda^\alpha w^\beta \left\{ \bar{V}_{zi}^\alpha V_{zi}^\beta - \bar{V}_{zi}^\beta V_{zi}^\alpha \right\} = 0. \end{aligned}$$

## b) To formulate/solve Molecular Dynamics on the thimble

### Second-order constraint-preserving symmetric integrator

$$z^n = z[e^{(n)}, t'^{(n)}],$$

$$w^n = V_z^\alpha[e^{(n)}, t'^{(n)}] w^{\alpha(n)}, \quad w^{\alpha(n)} \in \mathbb{R}.$$

$$w^{n+1/2} = w^n - \frac{1}{2} \Delta\tau \bar{\partial} \bar{S}[\bar{z}^n] - \frac{1}{2} \Delta\tau i V_z^\alpha[e^{(n)}, t'^{(n)}] \lambda_{[r]}^\alpha,$$

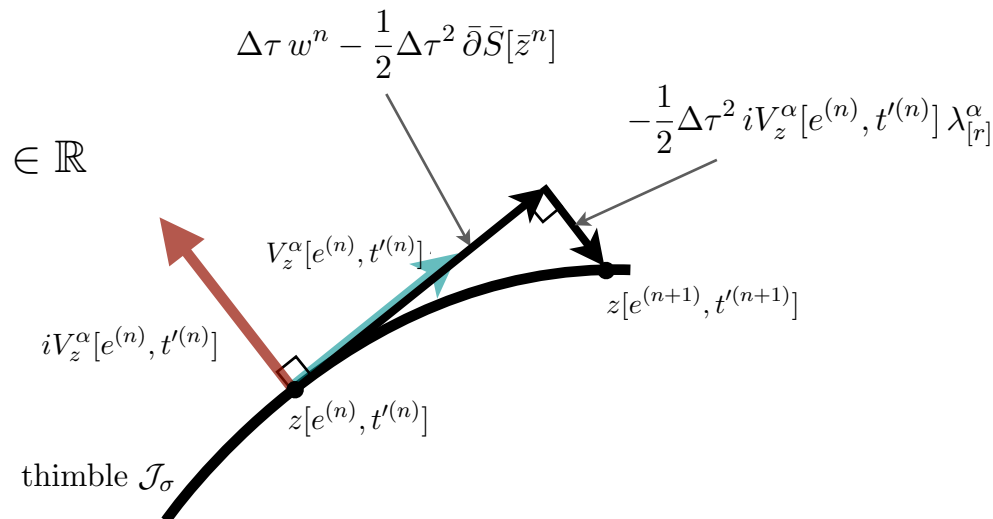
$$z^{n+1} = z^n + \Delta\tau w^{n+1/2},$$

$$w^{n+1} = w^{n+1/2} - \frac{1}{2} \Delta\tau \bar{\partial} \bar{S}[\bar{z}^{n+1}] - \frac{1}{2} \Delta\tau i V_z^\alpha[e^{(n+1)}, t'^{(n+1)}] \lambda_{[v]}^\alpha$$

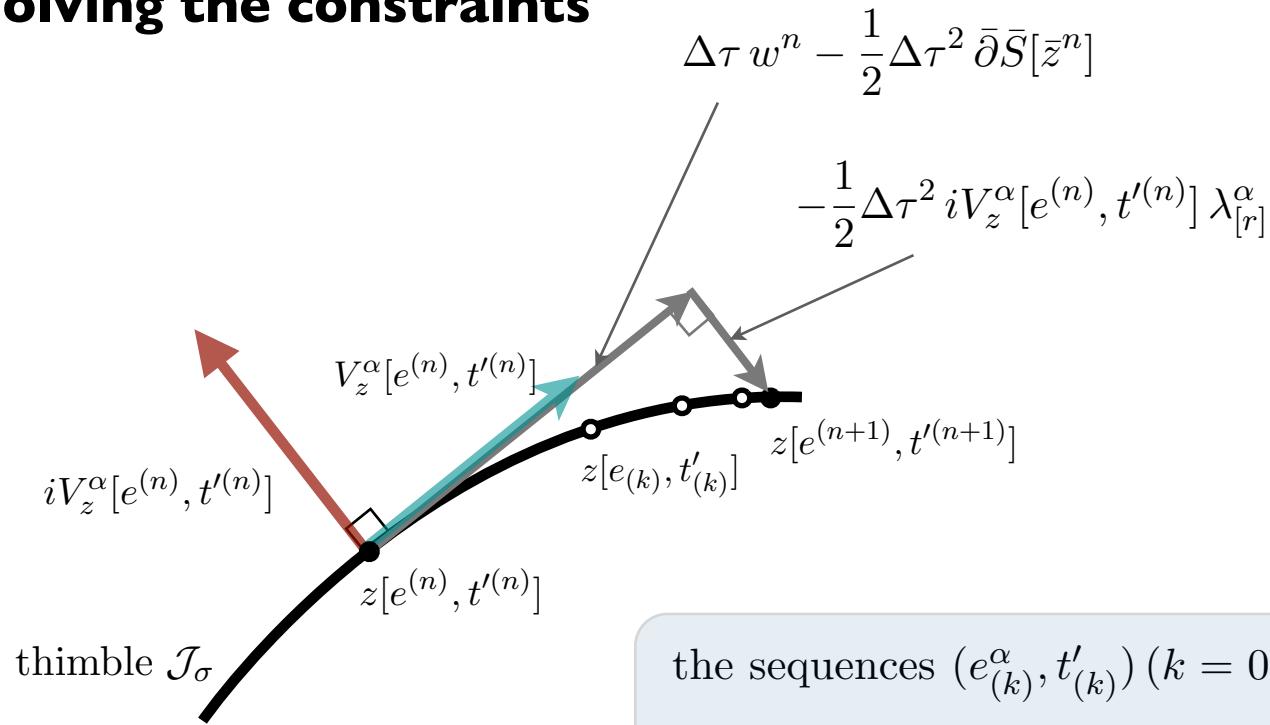
$\lambda_{[r]}^\alpha$  and  $\lambda_{[v]}^\alpha$  are fixed by

$$z^{n+1} = z[e^{(n+1)}, t'^{(n+1)}],$$

$$w^{n+1} = V_z^\alpha[e^{(n+1)}, t'^{(n+1)}] w^{\alpha(n+1)}, \quad w^{\alpha(n+1)} \in \mathbb{R}$$



# Solving the constraints

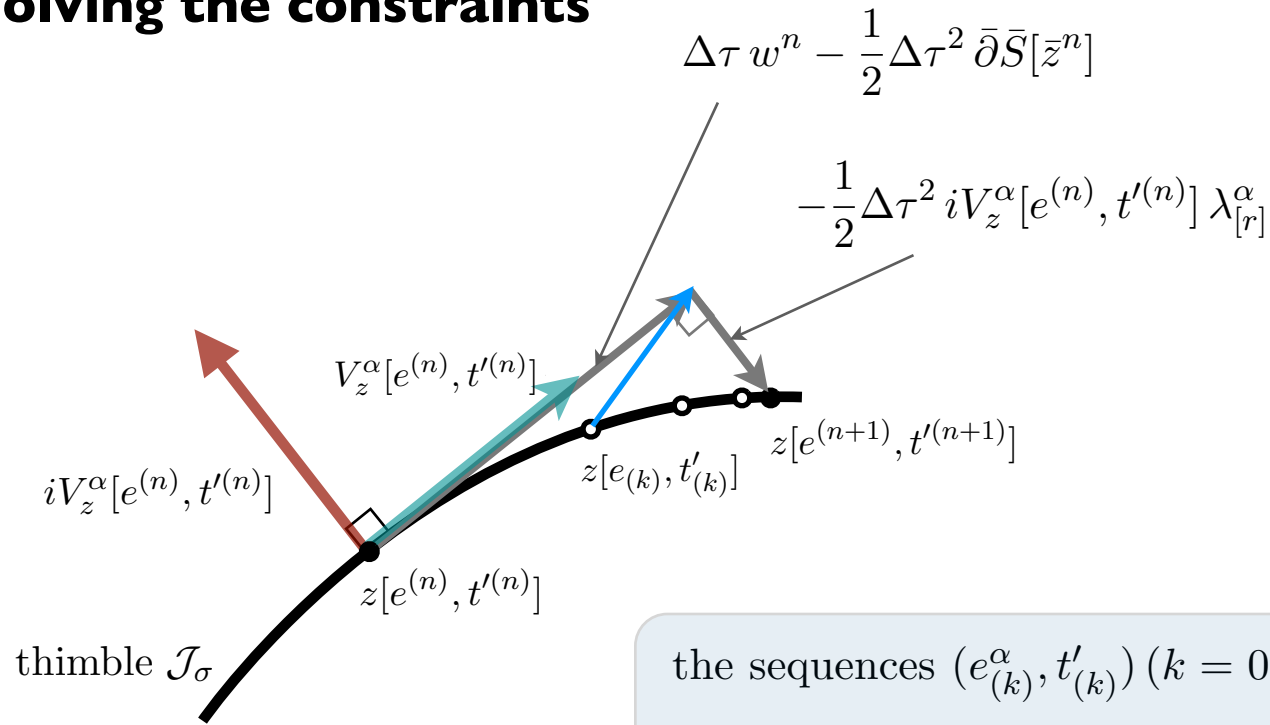


the sequences  $(e_{(k)}^\alpha, t'_{(k)})$  ( $k = 0, 1, \dots$ ) with  $(e_{(0)}^\alpha, t'_{(0)}) = (e^{\alpha(n)}, t'^{(n)})$

$$\Delta e_{(k)}^\alpha = e_{(k+1)}^\alpha - e_{(k)}^\alpha, \quad \sum_{\alpha=1} \Delta e_{(k)}^\alpha e^{\alpha(n)} = 0,$$

$$\Delta t'_{(k)} = t'_{(k+1)} - t'_{(k)},$$

# Solving the constraints

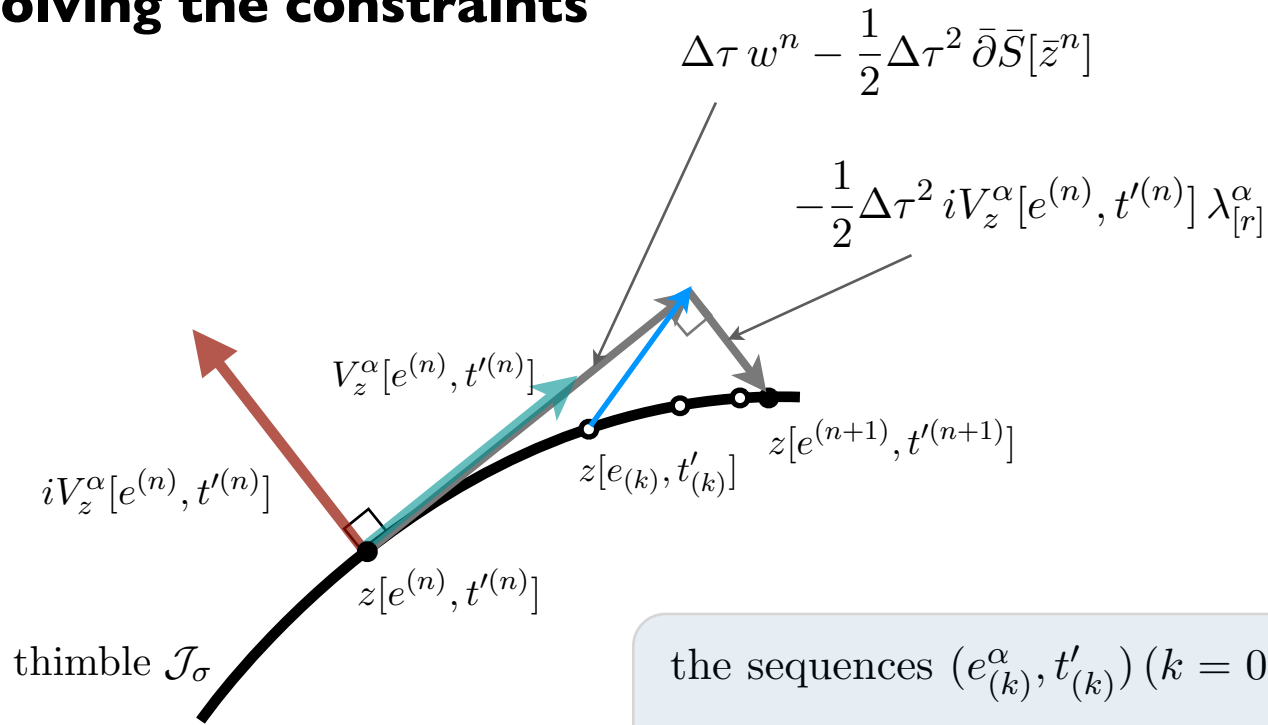


the sequences  $(e_{(k)}^\alpha, t'_{(k)})$  ( $k = 0, 1, \dots$ ) with  $(e_{(0)}^\alpha, t'_{(0)}) = (e^{\alpha(n)}, t'^{(n)})$

$$\Delta e_{(k)}^\alpha = e_{(k+1)}^\alpha - e_{(k)}^\alpha, \quad \sum_{\alpha=1} \Delta e_{(k)}^\alpha e^{\alpha(n)} = 0,$$

$$\Delta t'_{(k)} = t'_{(k+1)} - t'_{(k)},$$

# Solving the constraints



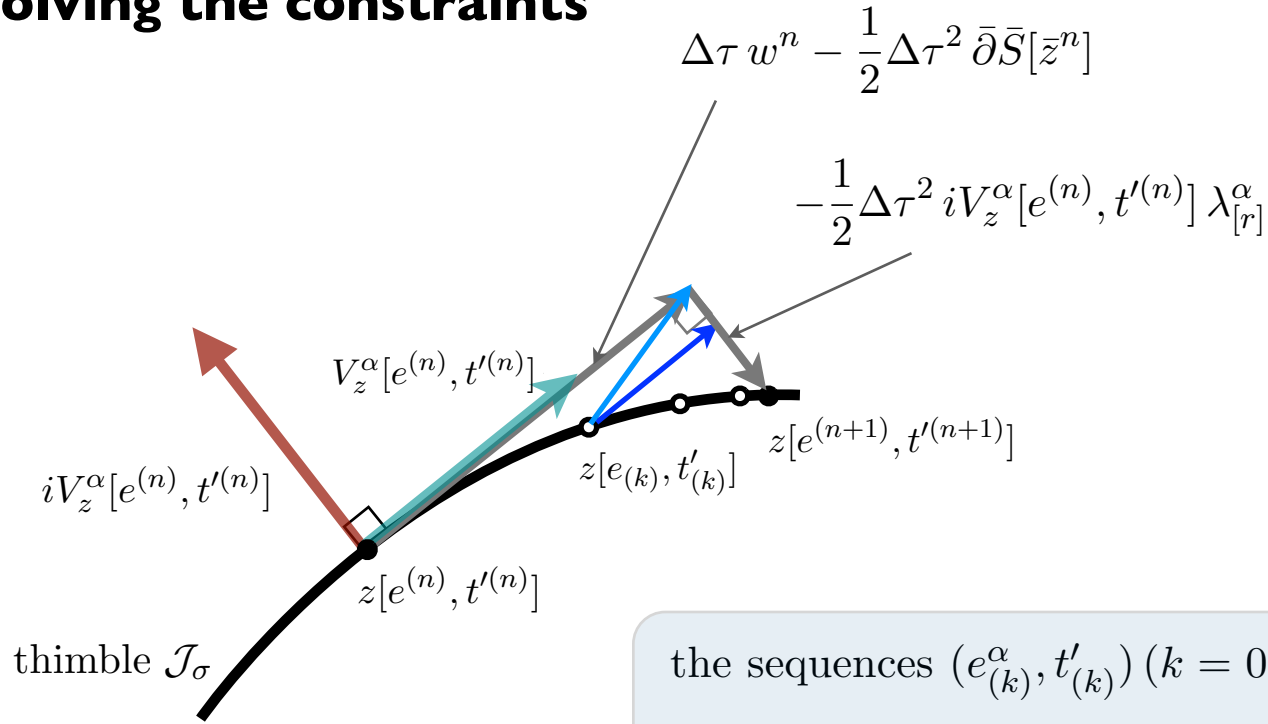
the sequences  $(e_{(k)}^\alpha, t'_{(k)})$  ( $k = 0, 1, \dots$ ) with  $(e_{(0)}^\alpha, t'_{(0)}) = (e^{\alpha(n)}, t'^{(n)})$

$$\Delta e_{(k)}^\alpha = e_{(k+1)}^\alpha - e_{(k)}^\alpha, \quad \sum_{\alpha=1} \Delta e_{(k)}^\alpha e^{\alpha(n)} = 0,$$

$$\Delta t'_{(k)} = t'_{(k+1)} - t'_{(k)},$$

$$\Delta z_{(k)}[e^{(n)}, t'^{(n)}] \equiv z_i[e^{(n)}, t'^{(n)}] + \Delta\tau w_i^n - \frac{1}{2}\Delta\tau^2 \bar{\partial}_i \bar{S}[\bar{z}^n] - z_i[e^{(k)}, t'^{(k)}]$$

# Solving the constraints



the sequences  $(e_{(k)}^\alpha, t'_{(k)})$  ( $k = 0, 1, \dots$ ) with  $(e_{(0)}^\alpha, t'_{(0)}) = (e^{\alpha(n)}, t'^{(n)})$

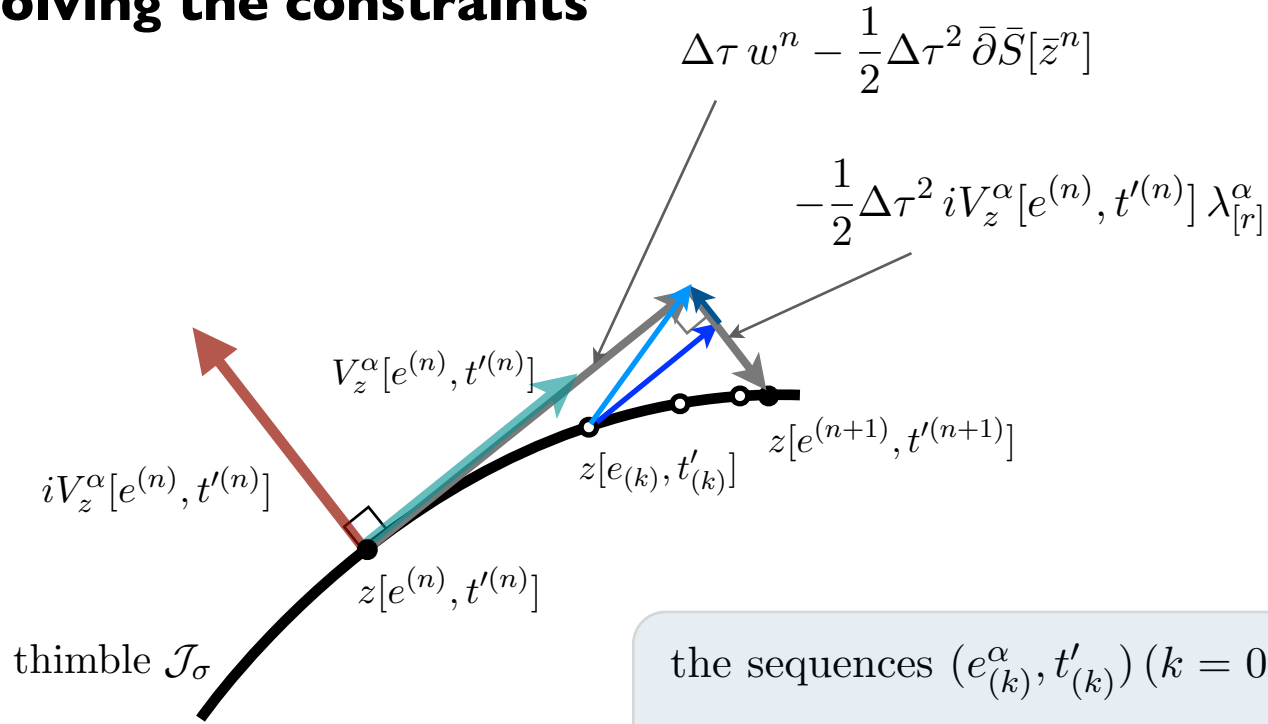
$$\Delta e_{(k)}^\alpha = e_{(k+1)}^\alpha - e_{(k)}^\alpha, \quad \sum_{\alpha=1} \Delta e_{(k)}^\alpha e^{\alpha(n)} = 0,$$

$$\Delta t'_{(k)} = t'_{(k+1)} - t'_{(k)},$$

$$\Delta z_{(k)}[e^{(n)}, t'^{(n)}] \equiv z_i[e^{(n)}, t'^{(n)}] + \Delta\tau w_i^n - \frac{1}{2}\Delta\tau^2 \bar{\partial}_i \bar{S}[\bar{z}^n] - z_i[e_{(k)}, t'_{(k)}]$$



# Solving the constraints



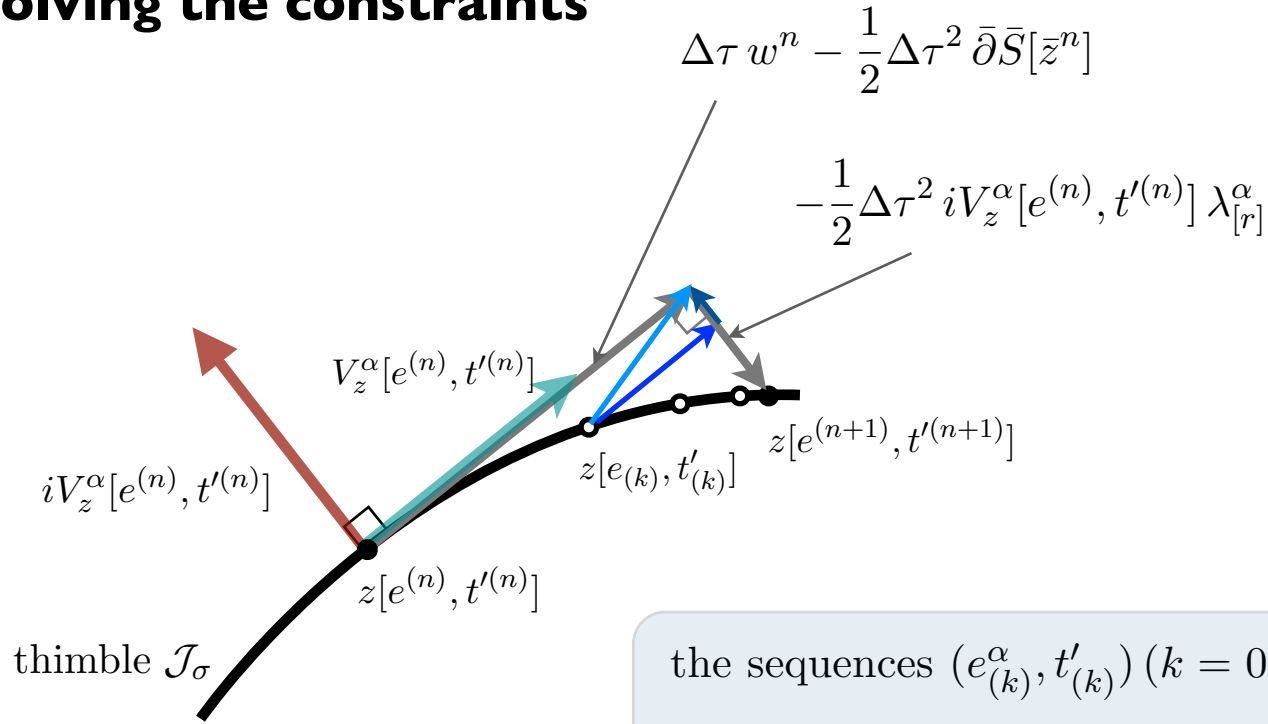
the sequences  $(e_{(k)}^\alpha, t'_{(k)})$  ( $k = 0, 1, \dots$ ) with  $(e_{(0)}^\alpha, t'_{(0)}) = (e^{\alpha(n)}, t'^{(n)})$

$$\Delta e_{(k)}^\alpha = e_{(k+1)}^\alpha - e_{(k)}^\alpha, \quad \sum_{\alpha=1} \Delta e_{(k)}^\alpha e^{\alpha(n)} = 0,$$

$$\Delta t'_{(k)} = t'_{(k+1)} - t'_{(k)},$$

$$\Delta z_{(k)}[e^{(n)}, t'^{(n)}] \equiv z_i[e^{(n)}, t'^{(n)}] + \Delta\tau w_i^n - \frac{1}{2}\Delta\tau^2 \bar{\partial}_i \bar{S}[\bar{z}^n] - z_i[e_{(k)}, t'_{(k)}]$$

# Solving the constraints



the sequences  $(e_{(k)}^\alpha, t'_{(k)})$  ( $k = 0, 1, \dots$ ) with  $(e_{(0)}^\alpha, t'_{(0)}) = (e^{\alpha(n)}, t'^{(n)})$

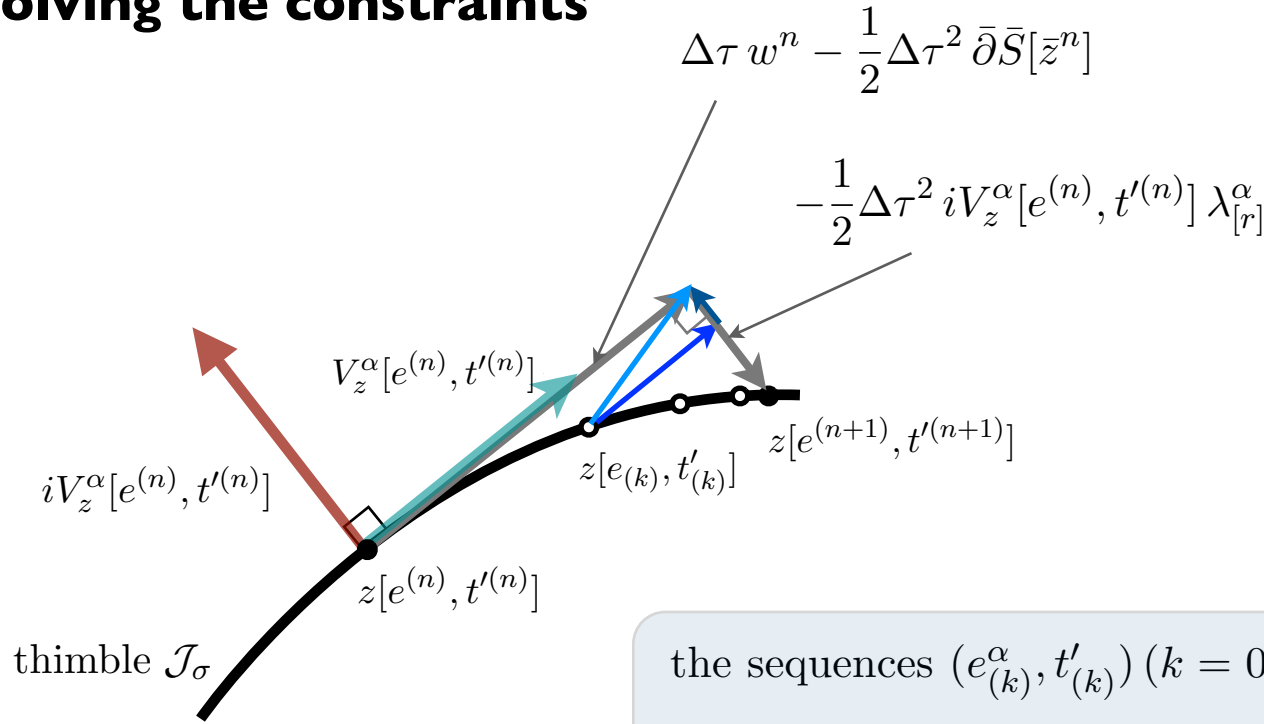
$$\Delta e_{(k)}^\alpha = e_{(k+1)}^\alpha - e_{(k)}^\alpha, \quad \sum_{\alpha=1} \Delta e_{(k)}^\alpha e^{\alpha(n)} = 0,$$

$$\Delta t'_{(k)} = t'_{(k+1)} - t'_{(k)},$$

$$\Delta z_{(k)}[e^{(n)}, t'^{(n)}] \equiv z_i[e^{(n)}, t'^{(n)}] + \Delta\tau w_i^n - \frac{1}{2}\Delta\tau^2 \bar{\partial}_i \bar{S}[\bar{z}^n] - z_i[e^{(k)}, t'^{(k)}]$$

$$\Delta z_{(k)}[e^{(n)}, t'^{(n)}]_{\parallel} = V_z^\alpha[e^{(n)}, t'^{(n)}] \left( \Delta e_{(k)}^\alpha + e^{\alpha(n)} \kappa^\alpha \Delta t'_{(k)} \right)$$

# Solving the constraints



the sequences  $(e_{(k)}^\alpha, t'_{(k)})$  ( $k = 0, 1, \dots$ ) with  $(e_{(0)}^\alpha, t'_{(0)}) = (e^{\alpha(n)}, t'^{(n)})$

$$\Delta e_{(k)}^\alpha = e_{(k+1)}^\alpha - e_{(k)}^\alpha, \quad \sum_{\alpha=1} \Delta e_{(k)}^\alpha e^{\alpha(n)} = 0,$$

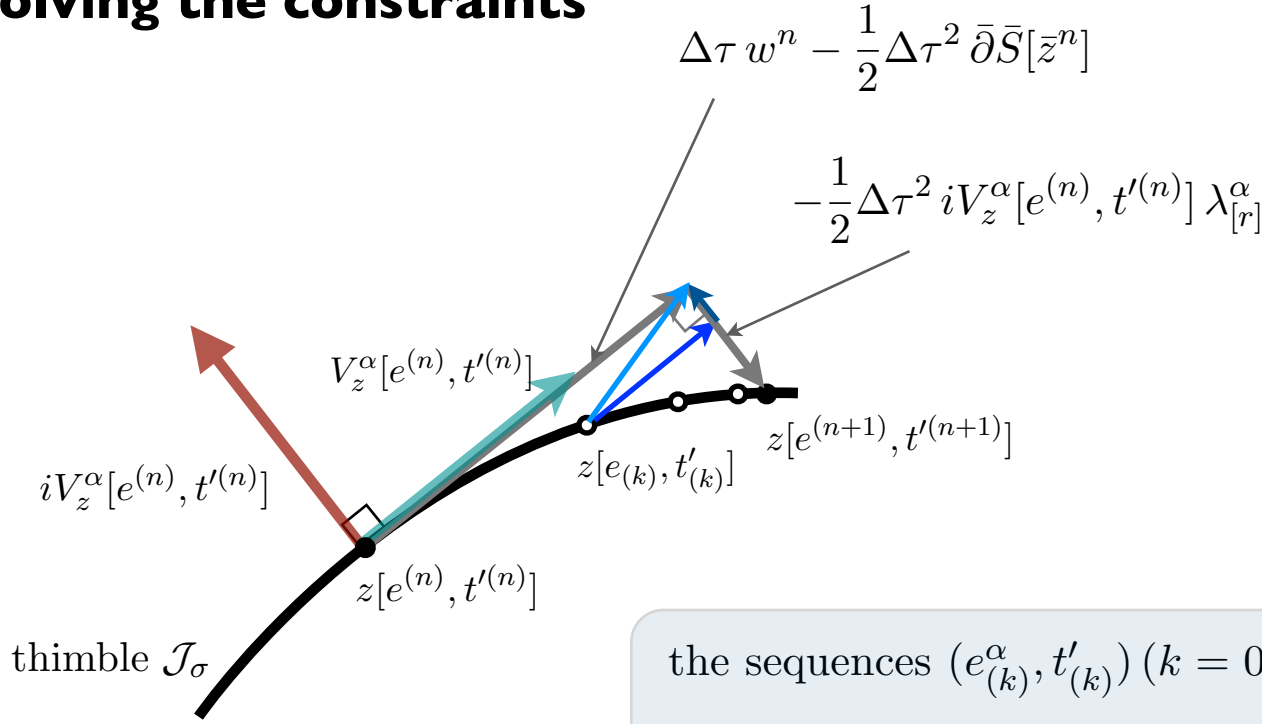
$$\Delta t'_{(k)} = t'_{(k+1)} - t'_{(k)},$$

$$\Delta z_{(k)}[e^{(n)}, t'^{(n)}] \equiv z_i[e^{(n)}, t'^{(n)}] + \Delta\tau w_i^n - \frac{1}{2}\Delta\tau^2 \bar{\partial}_i \bar{S}[\bar{z}^n] - z_i[e^{(k)}, t'_{(k)}]$$

$$\Delta z_{(k)}[e^{(n)}, t'^{(n)}]_{||} = V_z^\alpha[e^{(n)}, t'^{(n)}] \left( \Delta e_{(k)}^\alpha + e^{\alpha(n)} \kappa^\alpha \Delta t'_{(k)} \right)$$

$$\Delta z_{(k)}[e^{(n)}, t'^{(n)}]_{\perp} = iV_z^\alpha[e^{(n)}, t'^{(n)}] \left( \frac{1}{2}\Delta\tau^2 \lambda_{[r]}^\alpha \right)$$

# Solving the constraints



the sequences  $(e_{(k)}^\alpha, t'_{(k)})$  ( $k = 0, 1, \dots$ ) with  $(e_{(0)}^\alpha, t'_{(0)}) = (e^{(n)}, t'^{(n)})$

$$\Delta e_{(k)}^\alpha = e_{(k+1)}^\alpha - e_{(k)}^\alpha, \quad \sum_{\alpha=1} \Delta e_{(k)}^\alpha e^{\alpha(n)} = 0,$$

$$\Delta t'_{(k)} = t'_{(k+1)} - t'_{(k)},$$

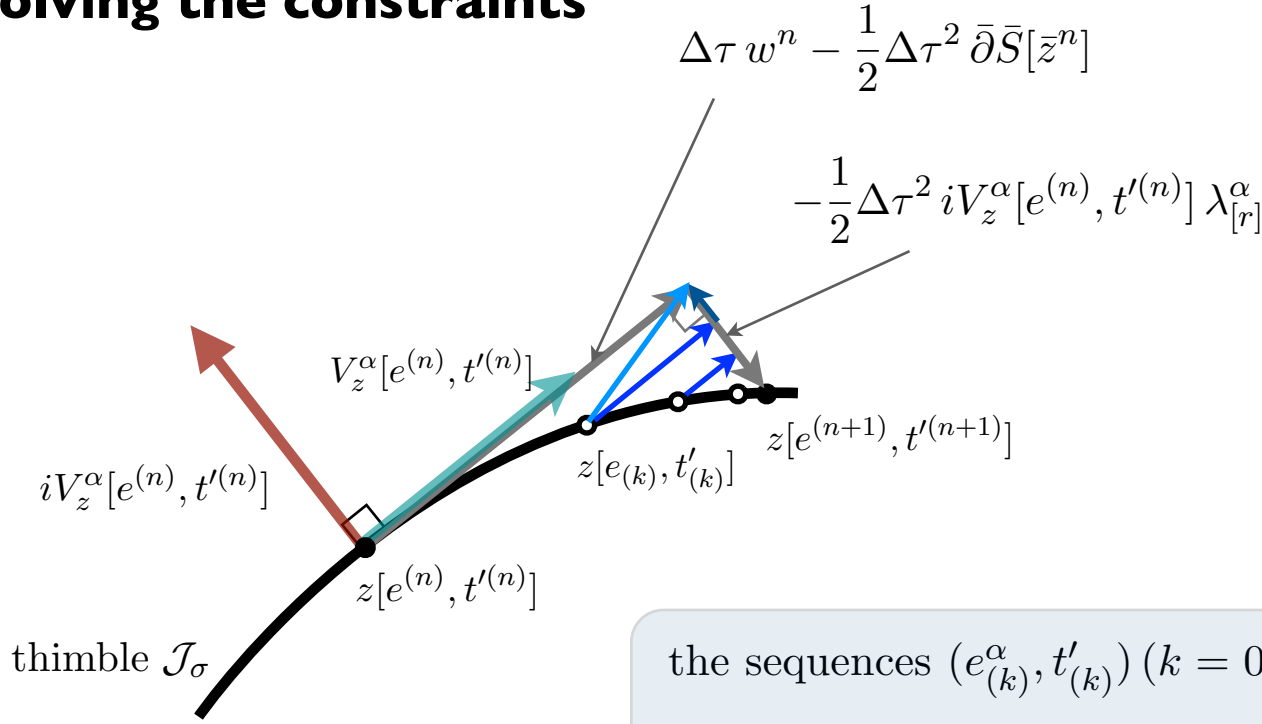
$$\Delta z_{(k)}[e^{(n)}, t'^{(n)}] \equiv z_i[e^{(n)}, t'^{(n)}] + \Delta\tau w_i^n - \frac{1}{2}\Delta\tau^2 \bar{\partial}_i \bar{S}[\bar{z}^n] - z_i[e_{(k)}, t'_{(k)}]$$

$$\Delta z_{(k)}[e^{(n)}, t'^{(n)}]_{||} = V_z^\alpha[e^{(n)}, t'^{(n)}] \left( \Delta e_{(k)}^\alpha + e^{\alpha(n)} \kappa^\alpha \Delta t'_{(k)} \right)$$

$$\Delta z_{(k)}[e^{(n)}, t'^{(n)}]_{\perp} = iV_z^\alpha[e^{(n)}, t'^{(n)}] \left( \frac{1}{2}\Delta\tau^2 \lambda_{[r](k)}^\alpha \right)$$

$$\left\| V_z^\alpha[e^{(n)}, t'^{(n)}] \left( \Delta e_{(k)}^\alpha + e^{\alpha(n)} \kappa^\alpha \Delta t'_{(k)} \right) \right\|^2 \leq n \epsilon'^2$$

# Solving the constraints



the sequences  $(e_{(k)}^\alpha, t'_{(k)})$  ( $k = 0, 1, \dots$ ) with  $(e_{(0)}^\alpha, t'_{(0)}) = (e^{(n)}, t'^{(n)})$

$$\Delta e_{(k)}^\alpha = e_{(k+1)}^\alpha - e_{(k)}^\alpha, \quad \sum_{\alpha=1} \Delta e_{(k)}^\alpha e^{\alpha(n)} = 0,$$

$$\Delta t'_{(k)} = t'_{(k+1)} - t'_{(k)},$$

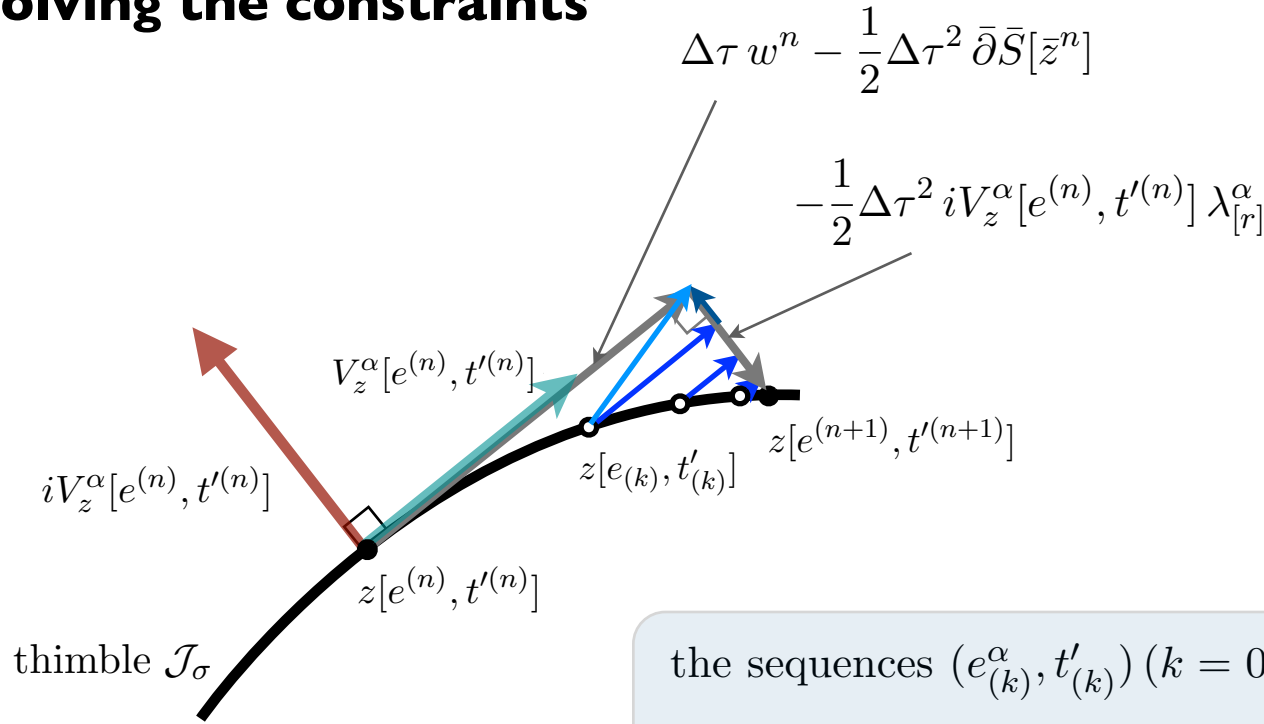
$$\Delta z_{(k)}[e^{(n)}, t'^{(n)}] \equiv z_i[e^{(n)}, t'^{(n)}] + \Delta\tau w_i^n - \frac{1}{2} \Delta\tau^2 \bar{\partial}_i \bar{S}[\bar{z}^n] - z_i[e_{(k)}, t'_{(k)}]$$

$$\Delta z_{(k)}[e^{(n)}, t'^{(n)}]_{\parallel} = V_z^\alpha[e^{(n)}, t'^{(n)}] \left( \Delta e_{(k)}^\alpha + e^{\alpha(n)} \kappa^\alpha \Delta t'_{(k)} \right)$$

$$\Delta z_{(k)}[e^{(n)}, t'^{(n)}]_{\perp} = iV_z^\alpha[e^{(n)}, t'^{(n)}] \left( \frac{1}{2} \Delta\tau^2 \lambda_{[r](k)}^\alpha \right)$$

$$\left\| V_z^\alpha[e^{(n)}, t'^{(n)}] \left( \Delta e_{(k)}^\alpha + e^{\alpha(n)} \kappa^\alpha \Delta t'_{(k)} \right) \right\|^2 \leq n \epsilon'^2$$

# Solving the constraints



the sequences  $(e_{(k)}^\alpha, t'_{(k)})$  ( $k = 0, 1, \dots$ ) with  $(e_{(0)}^\alpha, t'_{(0)}) = (e^{(n)}, t'^{(n)})$

$$\Delta e_{(k)}^\alpha = e_{(k+1)}^\alpha - e_{(k)}^\alpha, \quad \sum_{\alpha=1} \Delta e_{(k)}^\alpha e^{\alpha(n)} = 0,$$

$$\Delta t'_{(k)} = t'_{(k+1)} - t'_{(k)},$$

$$\Delta z_{(k)}[e^{(n)}, t'^{(n)}] \equiv z_i[e^{(n)}, t'^{(n)}] + \Delta\tau w_i^n - \frac{1}{2} \Delta\tau^2 \bar{\partial}_i \bar{S}[\bar{z}^n] - z_i[e_{(k)}, t'_{(k)}]$$

$$\Delta z_{(k)}[e^{(n)}, t'^{(n)}]_{\parallel} = V_z^\alpha[e^{(n)}, t'^{(n)}] \left( \Delta e_{(k)}^\alpha + e^{\alpha(n)} \kappa^\alpha \Delta t'_{(k)} \right)$$

$$\Delta z_{(k)}[e^{(n)}, t'^{(n)}]_{\perp} = iV_z^\alpha[e^{(n)}, t'^{(n)}] \left( \frac{1}{2} \Delta\tau^2 \lambda_{[r](k)}^\alpha \right)$$

$$\left\| V_z^\alpha[e^{(n)}, t'^{(n)}] \left( \Delta e_{(k)}^\alpha + e^{\alpha(n)} \kappa^\alpha \Delta t'_{(k)} \right) \right\|^2 \leq n \epsilon'^2$$

## the constraints to be solved

$$z[e^{(n+1)}, t'^{(n+1)}] - z[e^{(n)}, t'^{(n)}] = \Delta\tau w^n - \frac{1}{2}\Delta\tau^2 \bar{\partial}\bar{S}[\bar{z}^n] - \frac{1}{2}\Delta\tau^2 iV_z^\alpha[e^{(n)}, t'^{(n)}] \lambda_{[r]}^\alpha$$

the sequences  $(e_{(k)}^\alpha, t'_{(k)})$  ( $k = 0, 1, \dots$ ) with  $(e_{(0)}^\alpha, t'_{(0)}) = (e^{\alpha(n)}, t'^{(n)})$

$$\Delta e_{(k)}^\alpha = e_{(k+1)}^\alpha - e_{(k)}^\alpha, \quad \sum_{\alpha=1} \Delta e_{(k)}^\alpha e^{\alpha(n)} = 0,$$

$$\Delta t'_{(k)} = t'_{(k+1)} - t'_{(k)},$$

where

$$\begin{aligned} \Delta e_{(k)}^\alpha + e^{\alpha(n)} \kappa^\alpha \Delta t'_{(k)} &= \text{Re} \left[ \{V_z^{-1}[e^{(n)}, t'^{(n)}]\}_i^\alpha \times \right. \\ &\quad \left. (z_i[e^{(n)}, t'^{(n)}] + \Delta\tau w_i^n - \frac{1}{2}\Delta\tau^2 \bar{\partial}_i \bar{S}[\bar{z}^n] - z_i[e_{(k)}, t'_{(k)}]) \right] \\ \frac{1}{2}\Delta\tau^2 \lambda_{[r]}^\alpha &= \text{Im} \left[ \{V_z^{-1}[e^{(n)}, t'^{(n)}]\}_i^\alpha (z_i[e^{(n)}, t'^{(n)}] - z_i[e_{(k)}, t'_{(k)}]) \right] \end{aligned}$$

stopping cond. :

$$\left\| V_z^\alpha[e^{(n)}, t'^{(n)}] (\Delta e_{(k)}^\alpha + e^{\alpha(n)} \kappa^\alpha \Delta t'_{(k)}) \right\|^2 \leq n \epsilon'^2$$

$$\frac{1}{2}\Delta\tau \lambda_{[v]}^\alpha = \text{Im} \left[ \{V_z^{-1}[e^{(n+1)}, t'^{(n+1)}]\}_i^\alpha (w_i^{n+1/2} - \frac{1}{2}\Delta\tau \bar{\partial}_i \bar{S}[\bar{z}^{n+1}]) \right]$$

## a HMC update

A hybrid Monte Carlo update then consists of the following steps for a given trajectory length  $\tau_{\text{traj}}$  and a number of steps  $n_{\text{step}}$ :

1. Set the initial field configuration  $z_i$ :

$$\{e^{\alpha(0)}, t'^{(0)}\} = \{e^\alpha, t'\}, \quad z^0 = z[e, t'].$$

2. Refresh the momenta  $w_i$  by generating  $n$  pairs of unit gaussian random numbers  $(\xi_i, \eta_i)$ , setting tentatively  $w_i = \xi_i + i\eta_i$ , and chopping the non-tangential parts:

$$w^0 = V_z^\alpha \text{Re}[\{V_z^{-1}\}_j^\alpha (\xi_j + i\eta_j)] = U_z^\alpha \text{Re}[\{U_z^{-1}\}_j^\alpha (\xi_j + i\eta_j)].$$

3. Repeat  $n_{\text{step}}$  times of the second order symmetric integration the step size  $\Delta\tau = \tau_{\text{traj}}/n_{\text{step}}$ .
4. Accept or reject by  $\Delta H = H[w^{n_{\text{step}}}, z^{n_{\text{step}}}] - H[w^0, z^0]$ .

As for the initialization procedure, one may generate unit gaussian random numbers  $\eta^\alpha (\alpha = 1, \dots, n)$ , set

$$e^\alpha = \eta^\alpha \sqrt{\frac{n}{\sum_{\beta=1}^n \eta^\beta \eta^\beta}}, \quad t' = -t_0,$$

and then prepare  $z[e, t']$ ,  $\{V_z^\alpha[e, t']\}$ , and the inverse matrix  $V_z^{-1}[e, t']$ .



# Test in the $\lambda\varphi^4_\mu$ model

Complex Langevin simulation

G.Aarts, PRL 102:131601, 2009, arXiv:0810.2089

Dual variables / worm algorithm

C. Gattringer and T. Kolber, NP B869 (2013) 56, arXiv:1206.2954

$$\varphi(x) = (\phi_1(x) + i\phi_2(x))/\sqrt{2}$$

$$\phi_a(x) \in \mathbb{R} \quad (a = 1, 2)$$

$$\phi_a(x) \rightarrow z_a(x) \in \mathbb{C} \quad (a = 1, 2)$$

$$S[z] = \sum_{x \in \mathbb{L}^4} \left\{ + \frac{1}{2} z_a(x) z_a(x) + \frac{\lambda_0}{4} (z_a(x) z_a(x))^2 - K_0 \sum_{k=1}^3 z_a(x) z_a(x + \hat{k}) - K_0 z_a(x) z_b(x + \hat{0}) [\delta_{ab} \cosh(\mu) - i\epsilon_{ab} \sinh(\mu)] \right\}.$$

$$\text{where } K_0 = \frac{1}{(2D+\kappa)}, \lambda_0 = K_0^2 \lambda$$

$K=1.0, \lambda=1.0, \mu=0.0 \sim 1.8$

$L=4$  (, ... 12)

# Test in the $\lambda\varphi^4_\mu$ model

Complex Langevin simulation

G.Aarts, PRL 102:131601, 2009, arXiv:0810.2089

Dual variables / worm algorithm

C. Gattringer and T. Kolber, NP B869 (2013) 56, arXiv:1206.2954

$$\varphi(x) = (\phi_1(x) + i\phi_2(x))/\sqrt{2}$$

$$\phi_a(x) \in \mathbb{R} \quad (a = 1, 2)$$

$$\phi_a(x) \rightarrow z_a(x) \in \mathbb{C} \quad (a = 1, 2)$$

$$S[z] = \sum_{x \in \mathbb{L}^4} \left\{ +\frac{1}{2} z_a(x) z_a(x) + \frac{\lambda_0}{4} (z_a(x) z_b(x) z_c(x) z_d(x)) \right. \\ \left. - K_0 z_a(x) z_b(x + \hat{0}) [\delta_{ab} \cos \varphi(x)] \right\}$$

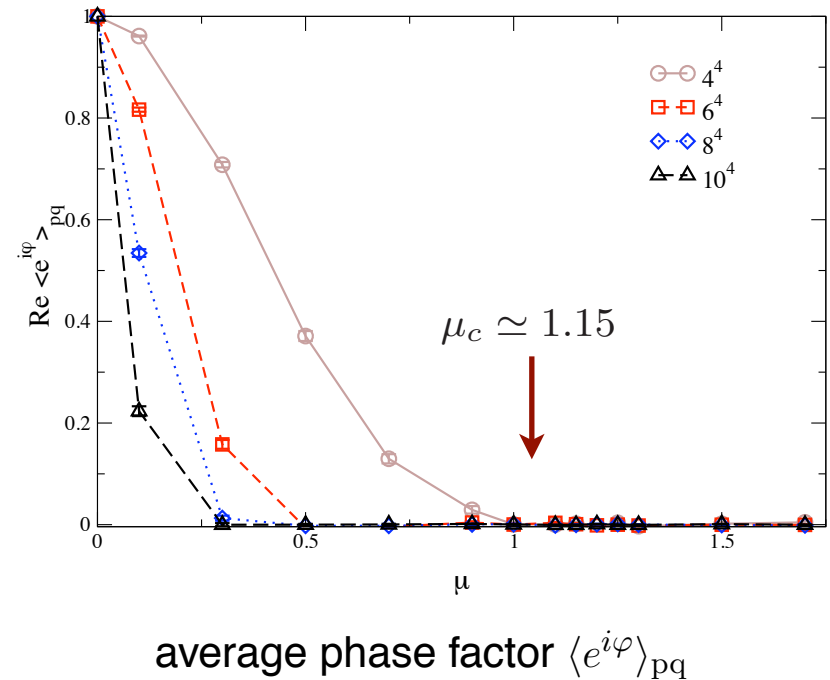
where  $K_0 = \frac{1}{(2D+\kappa)}$ ,  $\lambda_0 = K_0^2 \lambda$

$K=1.0$ ,  $\lambda=1.0$ ,  $\mu=0.0 \sim 1.8$

$L=4$  (, ... 12)

## HOW SEVERE IS THE SIGN PROBLEM?

AVERAGE PHASE FACTOR



G.Aarts, PRL 102:131601, 2009, arXiv:0810.2089

# Test in the $\lambda\varphi^4_\mu$ model (cont'd)

## critical points with constant field $\mathbf{z}_a(\mathbf{x})=\mathbf{z}_a$

$$\left. \frac{\partial S[z]}{\partial z_a(x)} \right|_{z_a(x)=z_a} = (1 - 6K_0 - 2K_0 \cosh(\mu)) z_a + \lambda_0(z_1^2 + z_2^2)z_a = 0 \quad (a = 1, 2).$$

critical value of  $\mu$  (classical)  $\tilde{\mu}_c = \ln \left[ \left( \frac{1 - 6K_0}{2K_0} \right) + \sqrt{\left( \frac{1 - 6K_0}{2K_0} \right)^2 - 1} \right]$

$$\mu_c \sim 0.962 \text{ for } K=1.0, \lambda=1.0$$

1. For  $\mu \leq \tilde{\mu}_c$ ,

(a)  $z_1 = z_2 = 0$  ;  $S[z] = 0$ ,

(b)  $z_1 = i\phi_0 \cos \theta$ ,  $z_2 = i\phi_0 \sin \theta$  ;  $S[z] = -L^4 \frac{\lambda_0}{4} \phi_0^4$ ,

where  $\phi_0 = \sqrt{\frac{+(1-6K_0-2K_0 \cosh(\mu))}{\lambda_0}}$ .

2. For  $\mu > \tilde{\mu}_c$ ,

(a)  $z_1 = z_2 = 0$  ;  $S[z] = 0$ ,

(b)  $z_1 = \phi_0 \cos \theta$ ,  $z_2 = \phi_0 \sin \theta$  ;  $S[z] = -L^4 \frac{\lambda_0}{4} \phi_0^4$ ,

where  $\phi_0 = \sqrt{\frac{-(1-6K_0-2K_0 \cosh(\mu))}{\lambda_0}}$ .

← the thimble 1-(a)

← the thimble 2-(a)

← the thimble 2-(b)

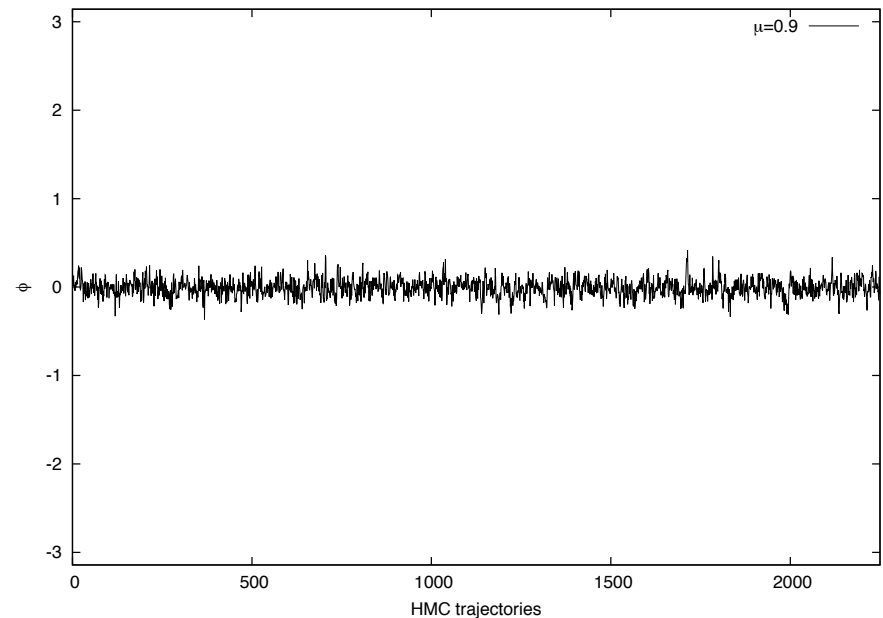
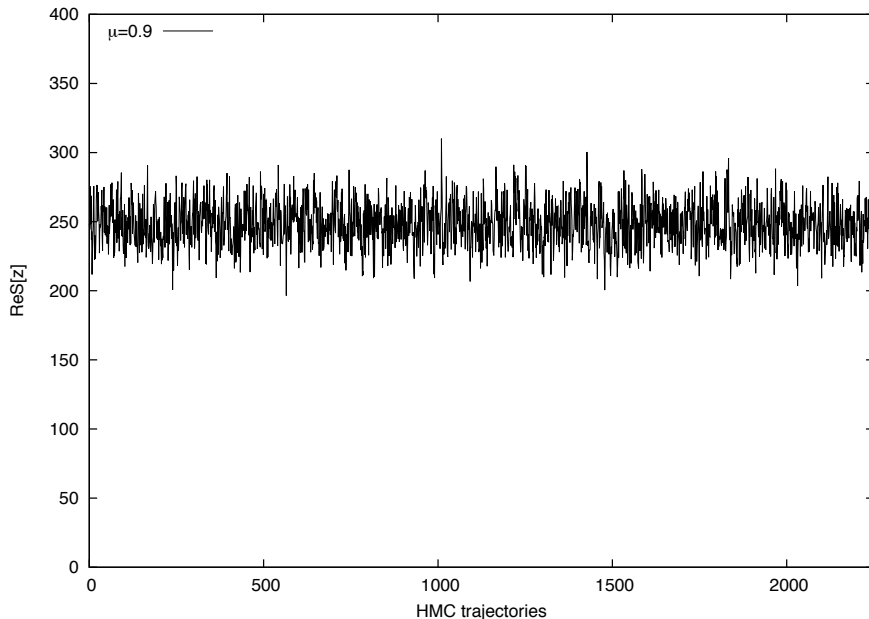
# HMC on the thimble I-(a)

$$\mu < \tilde{\mu}_c$$

simulation parameters :

	Parameters	Resulting conditions
Thimble (Solving flow eqs.)	$t_0 = -5.0$ $n_{\text{lefs}} = 100$ $h = t'/n_{\text{lefs}} \simeq 0.05$	$ \text{Re}(S[z(t_0)] - S[z_{\text{vac}}])  \lesssim 1.0$ $ \text{Im}S[z]  \lesssim 1.0 \times 10^{-4}$ $\ \bar{\partial}\bar{S} - V^\alpha \kappa^\alpha e^\alpha\ ^2/2V \leq 1.0 \times 10^{-4}$
Molecular Dynamics (Solving constraint)	$\tau_{\text{traj}} = 1.0$ $n_{\text{step}} = 20$ $\Delta\tau = 0.05$ $\epsilon' = 1.0 \times 10^{-3}$	scale variable range : $t' \in [4.9, 5.1]$ $\Delta H \lesssim 0.1$ acceptance rate $\simeq 0.99$ number of iterations : $l \lesssim 4$
Auto-corr. time		$\tau_{\text{int}} \simeq 2$ for $\text{Re}S[z]$ $\tau_{\text{int}} \simeq 3$ for $\phi_z$

HMC histories ( $\mu = 0.9$ )

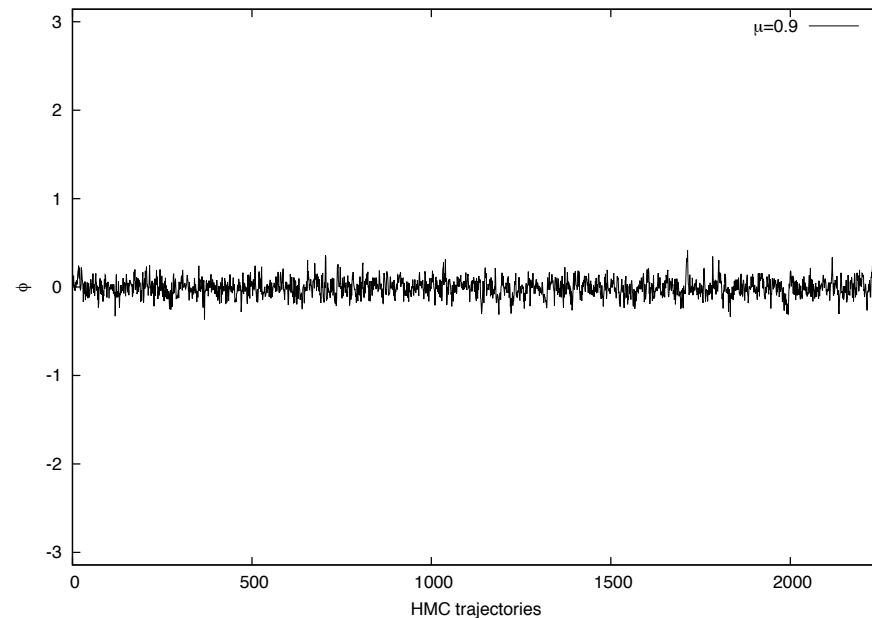
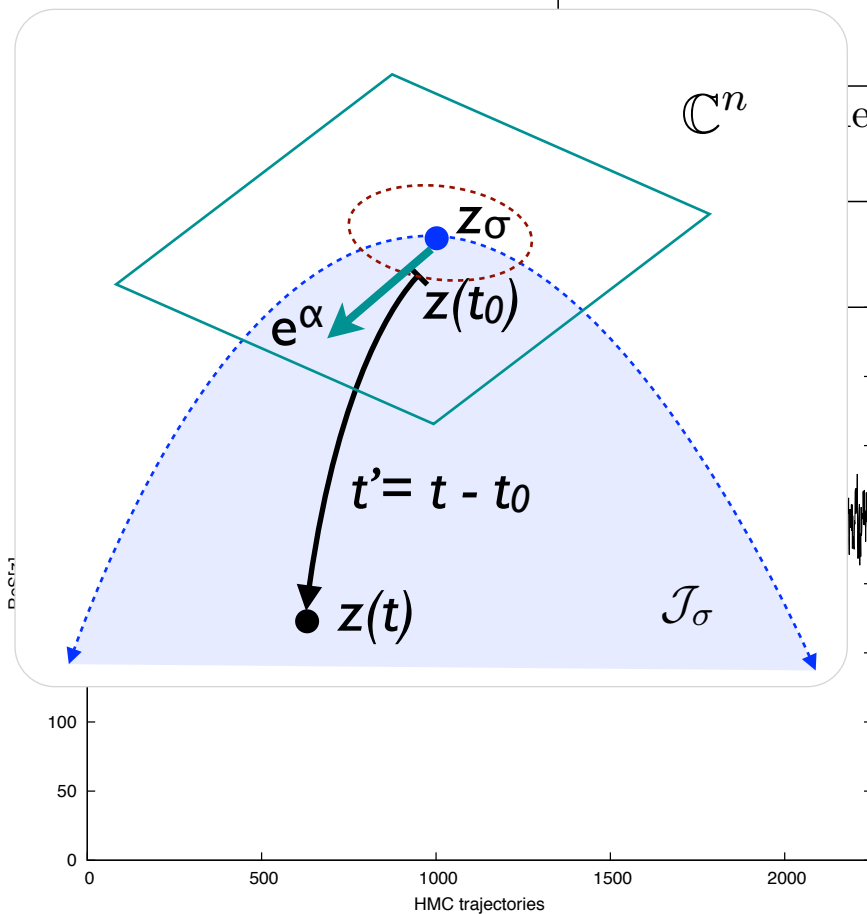


# HMC on the thimble I-(a)

$$\mu < \tilde{\mu}_c$$

simulation parameters :

	Parameters	Resulting conditions
Thimble (Solving flow eqs.)	$t_0 = -5.0$ $n_{\text{lefs}} = 100$ $h = t'/n_{\text{lefs}} \simeq 0.05$	$ \text{Re}(S[z(t_0)] - S[z_{\text{vac}}])  \lesssim 1.0$ $ \text{Im}S[z]  \lesssim 1.0 \times 10^{-4}$ $\ \bar{\partial}\bar{S} - V^\alpha \kappa^\alpha e^\alpha\ ^2/2V \leq 1.0 \times 10^{-4}$
Molecular Dynamics (Solving constraint)	$\tau_{\text{traj}} = 1.0$ $n_{\text{step}} = 20$ $\Delta\tau = 0.05$ $\epsilon' = 1.0 \times 10^{-3}$	scale variable range : $t' \in [4.9, 5.1]$ $\Delta H \lesssim 0.1$ acceptance rate $\simeq 0.99$ number of iterations : $l \lesssim 4$
		$\tau_{\text{int}} \simeq 2$ for $\text{Re}S[z]$ $\tau_{\text{int}} \simeq 3$ for $\phi_z$



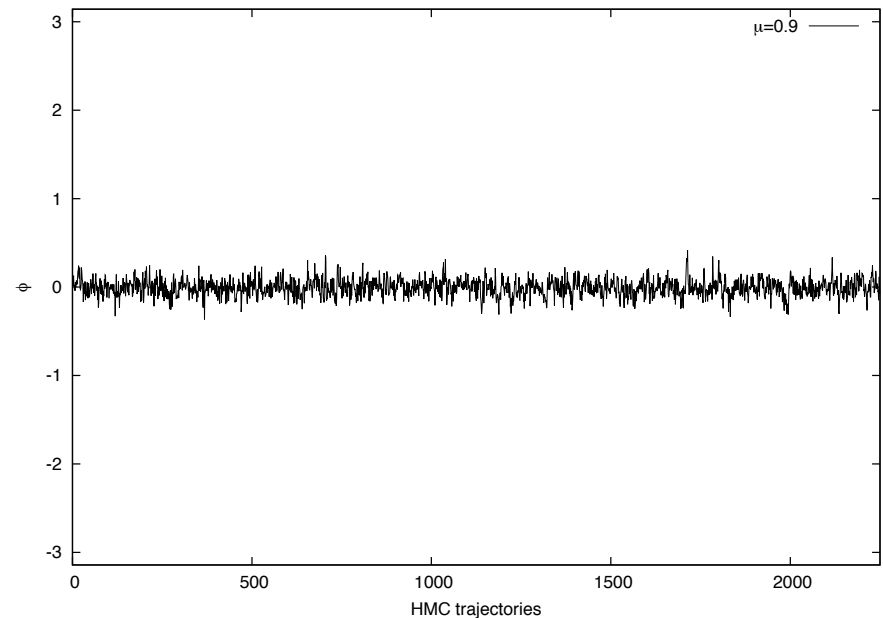
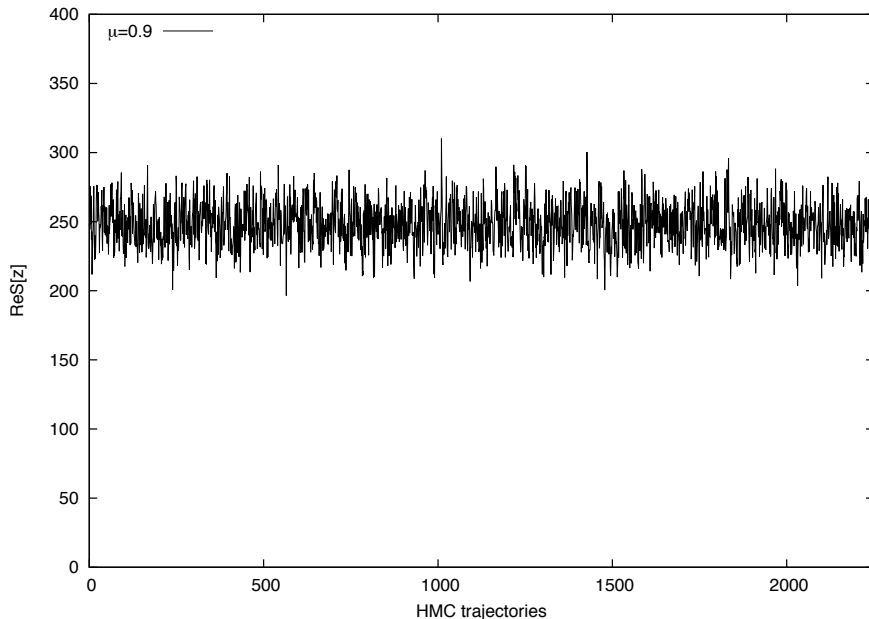
# HMC on the thimble I-(a)

$$\mu < \tilde{\mu}_c$$

simulation parameters :

	Parameters	Resulting conditions
Thimble (Solving flow eqs.)	$t_0 = -5.0$ $n_{\text{lefs}} = 100$ $h = t'/n_{\text{lefs}} \simeq 0.05$	$ \text{Re}(S[z(t_0)] - S[z_{\text{vac}}])  \lesssim 1.0$ $ \text{Im}S[z]  \lesssim 1.0 \times 10^{-4}$ $\ \bar{\partial}\bar{S} - V^\alpha \kappa^\alpha e^\alpha\ ^2/2V \leq 1.0 \times 10^{-4}$
Molecular Dynamics (Solving constraint)	$\tau_{\text{traj}} = 1.0$ $n_{\text{step}} = 20$ $\Delta\tau = 0.05$ $\epsilon' = 1.0 \times 10^{-3}$	scale variable range : $t' \in [4.9, 5.1]$ $\Delta H \lesssim 0.1$ acceptance rate $\simeq 0.99$ number of iterations : $l \lesssim 4$
Auto-corr. time		$\tau_{\text{int}} \simeq 2$ for $\text{Re}S[z]$ $\tau_{\text{int}} \simeq 3$ for $\phi_z$

HMC histories ( $\mu = 0.9$ )



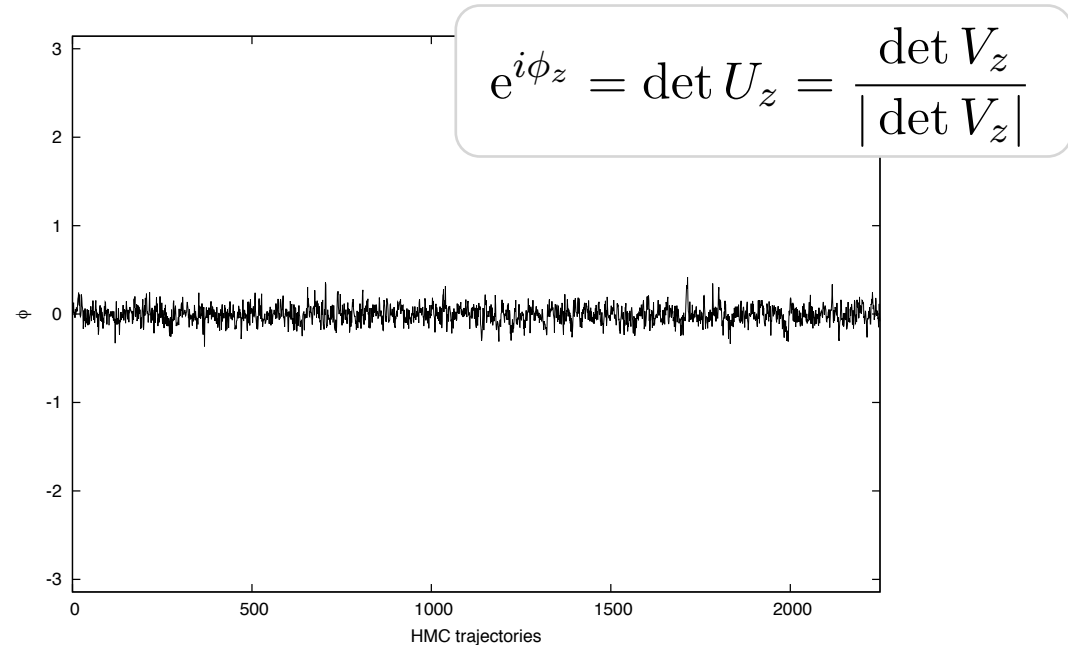
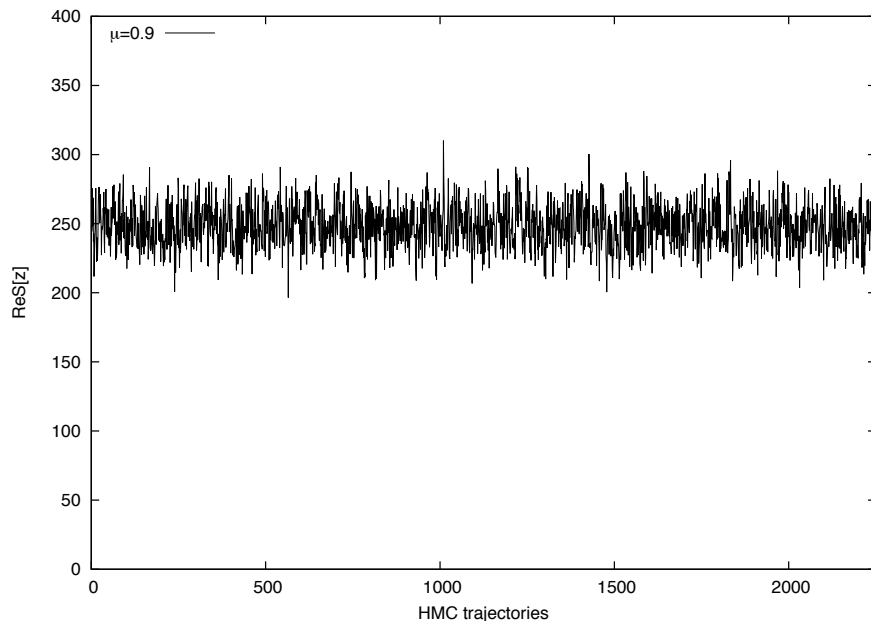
# HMC on the thimble I-(a)

$$\mu < \tilde{\mu}_c$$

simulation parameters :

	Parameters	Resulting conditions
Thimble (Solving flow eqs.)	$t_0 = -5.0$ $n_{\text{lefs}} = 100$ $h = t'/n_{\text{lefs}} \simeq 0.05$	$ \text{Re}(S[z(t_0)] - S[z_{\text{vac}}])  \lesssim 1.0$ $ \text{Im}S[z]  \lesssim 1.0 \times 10^{-4}$ $\ \bar{\partial}\bar{S} - V^\alpha \kappa^\alpha e^\alpha\ ^2/2V \leq 1.0 \times 10^{-4}$
Molecular Dynamics (Solving constraint)	$\tau_{\text{traj}} = 1.0$ $n_{\text{step}} = 20$ $\Delta\tau = 0.05$ $\epsilon' = 1.0 \times 10^{-3}$	scale variable range : $t' \in [4.9, 5.1]$ $\Delta H \lesssim 0.1$ acceptance rate $\simeq 0.99$ number of iterations : $l \lesssim 4$
Auto-corr. time		$\tau_{\text{int}} \simeq 2$ for $\text{Re}S[z]$ $\tau_{\text{int}} \simeq 3$ for $\phi_z$

HMC histories ( $\mu = 0.9$ )



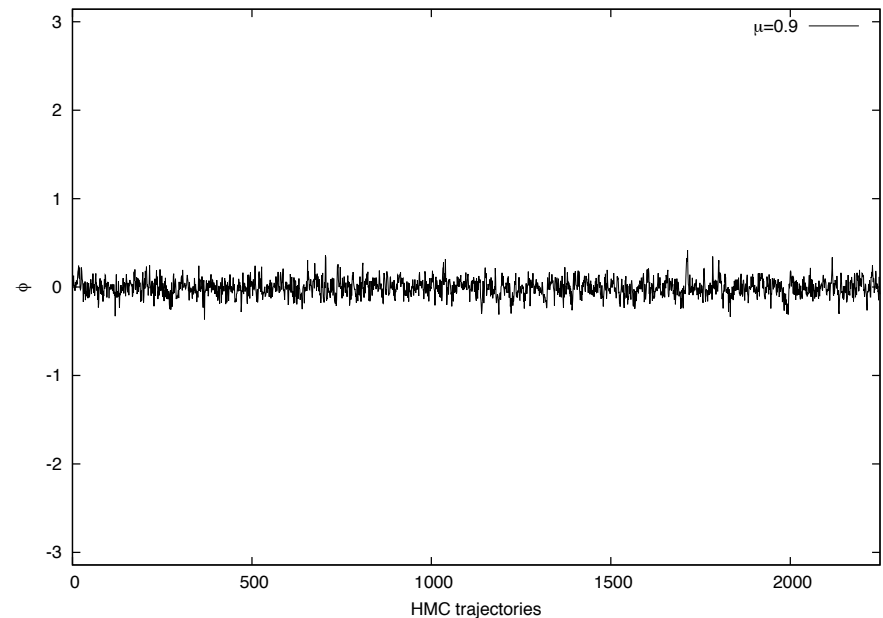
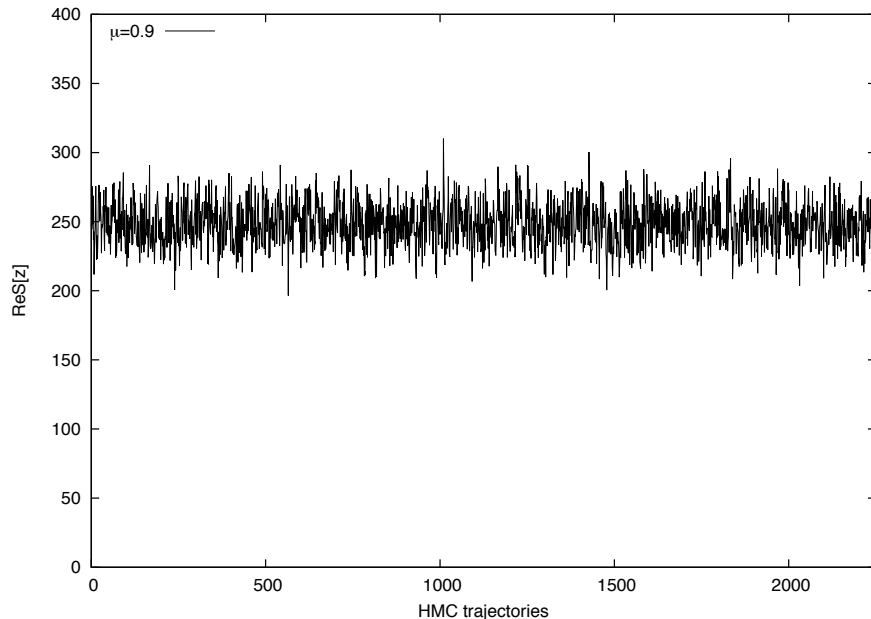
# HMC on the thimble I-(a)

$$\mu < \tilde{\mu}_c$$

simulation parameters :

	Parameters	Resulting conditions
Thimble (Solving flow eqs.)	$t_0 = -5.0$ $n_{\text{lefs}} = 100$ $h = t'/n_{\text{lefs}} \simeq 0.05$	$ \text{Re}(S[z(t_0)] - S[z_{\text{vac}}])  \lesssim 1.0$ $ \text{Im}S[z]  \lesssim 1.0 \times 10^{-4}$ $\ \bar{\partial}\bar{S} - V^\alpha \kappa^\alpha e^\alpha\ ^2/2V \leq 1.0 \times 10^{-4}$
Molecular Dynamics (Solving constraint)	$\tau_{\text{traj}} = 1.0$ $n_{\text{step}} = 20$ $\Delta\tau = 0.05$ $\epsilon' = 1.0 \times 10^{-3}$	scale variable range : $t' \in [4.9, 5.1]$ $\Delta H \lesssim 0.1$ acceptance rate $\simeq 0.99$ number of iterations : $l \lesssim 4$
Auto-corr. time		$\tau_{\text{int}} \simeq 2$ for $\text{Re}S[z]$ $\tau_{\text{int}} \simeq 3$ for $\phi_z$

HMC histories ( $\mu = 0.9$ )





# HMC on the thimble I-(a)

$$\mu < \tilde{\mu}_c$$

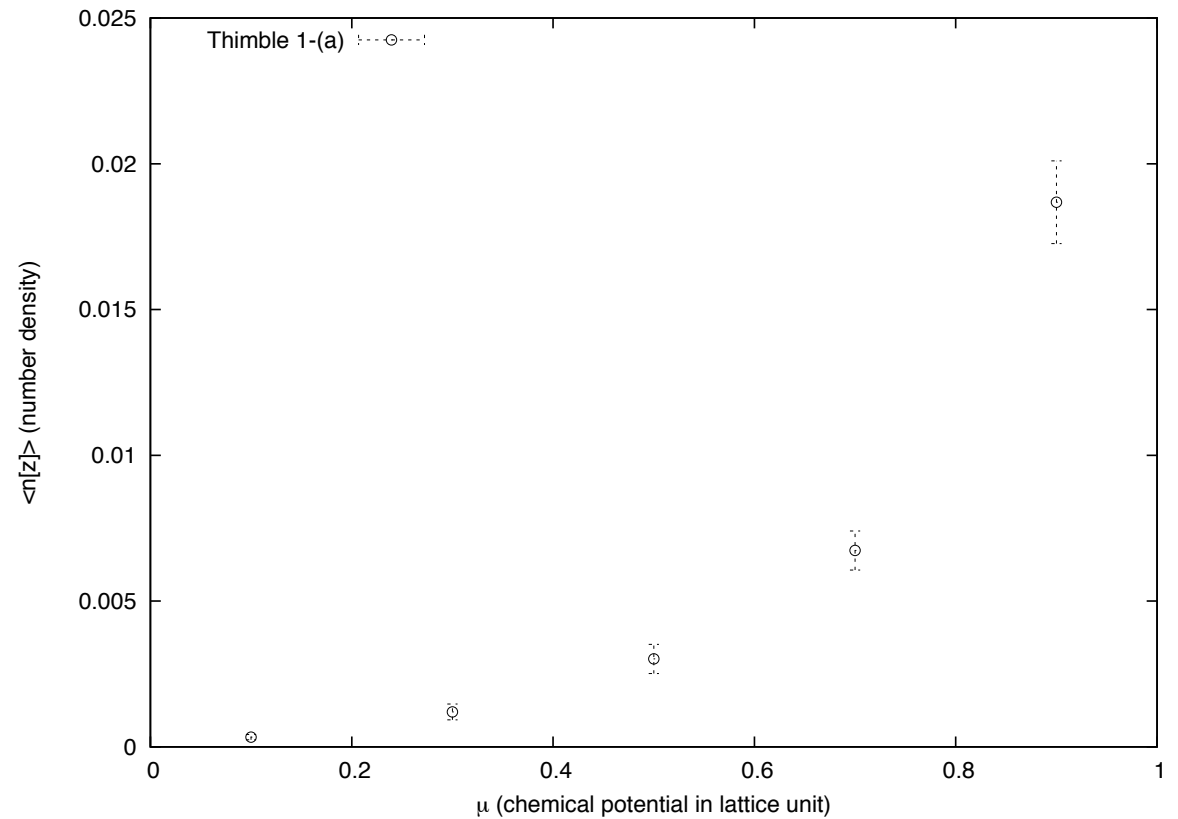
generated 4,250 traj.

sampling 300 conf. with the separation of 10

residual phase :

$\mu$	$\langle e^{i\phi_z} \rangle'_{\mathcal{J}_{\text{vac}}}$
0.1	$(9.99\text{e-}01, -1.15\text{e-}03) \pm (5.7\text{e-}02, 7.4\text{e-}04)$
0.3	$(9.99\text{e-}01, -1.03\text{e-}03) \pm (5.7\text{e-}02, 2.1\text{e-}03)$
0.5	$(9.98\text{e-}01, -2.68\text{e-}03) \pm (5.7\text{e-}02, 3.3\text{e-}03)$
0.7	$(9.97\text{e-}01, 5.24\text{e-}04) \pm (5.7\text{e-}02, 4.3\text{e-}03)$
0.9	$(9.94\text{e-}01, -7.40\text{e-}03) \pm (5.7\text{e-}02, 5.9\text{e-}03)$

number density :



$$e^{i\phi_z} = \det U_z = \frac{\det V_z}{|\det V_z|}$$

$$n[z] = \frac{1}{L^4} \sum_x K_0 z_a(x) z_b(x + \hat{0}) [\delta_{ab} \sinh(\mu) - i\epsilon_{ab} \cosh(\mu)]$$

# HMC on the thimble 2-(b) $\mu > \tilde{\mu}_c$

**Critical region of real dimension one :**  $\theta \in [0, 2\pi]$

$$z_a(x; t) \simeq R_{ab}(\theta) \left\{ \delta_{b1} \phi_0 + \sum_{\beta=1}^{2V-1} v_b(x)^\beta \exp(\kappa^\beta t) e^\beta \right\} \quad (t \ll 0)$$

$$\delta z_a(x; t) = V_a(x; t)^0 (\phi_0 \sqrt{V} \delta\theta) + \sum_{\beta=1}^{2V-1} V_b(x; t)^\beta (\delta e^\beta + \kappa^\beta e^\beta \delta t)$$

**zero mode**

$$\kappa^0 = 0$$

$$v_a(x)^0 = \delta_{a2} / \sqrt{V}$$

**Critical fluctuation : lowest mode**  $\kappa^1 = 2\lambda_0 \phi_0^2$   
 $v_a(x)^1 = \delta_{a1} / \sqrt{V}$

**gets very light !** ( $\mu \gtrsim \tilde{\mu}_c$ )

$$z_a(x; t) \simeq R_{ab}(\theta) \left\{ \delta_{b1} \frac{\phi_0}{\sqrt{1 - \frac{2}{\sqrt{V}\phi_0} e^1 \exp(\kappa^1 t)}} + \sum_{\beta=2}^{2V-1} v_b(x)^\beta \exp(\kappa^\beta t) e^\beta \right\}$$

$$\sum_{\beta=2}^{2V-1} e^\beta e^\beta = 2V-2$$

$$V_a(x; t)^0 \simeq R_{ab}(\theta) v_b(x)^0 \frac{1}{\sqrt{1 - \frac{2}{\sqrt{V}\phi_0} e^1 \exp(\kappa^1 t)}},$$

$$V_a(x; t)^1 \simeq R_{ab}(\theta) v_b(x)^1 \frac{\exp(\kappa^1 t)}{\left(1 - \frac{2}{\sqrt{V}\phi_0} e^1 \exp(\kappa^1 t)\right)^{3/2}},$$

$$V_a(x; t)^\beta \simeq R_{ab}(\theta) v_b(x)^\beta \exp(\kappa^\beta t) \quad (\beta = 2, \dots, 2V-1)$$

the *global* flow mode  $z_a(x; t) = z_a(t)$

$$\begin{aligned} \frac{d}{dt} z_a(t) &= \bar{\partial}_{ax} \bar{S}[\bar{z}] \Big|_{z_a(x;t)=z_a(t)} \\ &= \lambda_0 (\bar{z}_b(t) \bar{z}_b(t) - \phi_0^2) \bar{z}_a(t) \end{aligned}$$

# HMC on the thimble 2-(b) $\mu > \tilde{\mu}_c$

simulation parameters :

	Parameters	Resulting conditions
Thimble	$t_0 = -3.0$ $n_{\text{lefs}} = 100$ $h = t'/n_{\text{lefs}} \simeq 0.03$	$ \text{Re}(S[z(t_0)] - S[z_{\text{vac}}])  \lesssim 2.0 \times 10^1$ $ \text{Im}(S[z] - S[z_{\text{vac}}])  \lesssim 5.0 \times 10^{-2}$ $\ \bar{\partial}\bar{S} - V^\alpha \kappa^\alpha e^\alpha\ ^2/2V \leq 3.0 \times 10^{-2}$
MD	$\tau_{\text{traj}} = 0.3$ $n_{\text{step}} = 10, 30 (\mu = 1.0, 1.1)$ $\Delta\tau = 0.03, 0.01 (\mu = 1.0, 1.1)$ $\epsilon' = \sqrt{10} \times 10^{-3}$	$t' \in [2.5, 3.5]$ $\Delta H \lesssim 0.05$ Acceptance rate $\simeq 0.99$ $l \lesssim 4, 6 (\mu = 1.0), 14 (\mu = 1.1)$
Auto-corr. time	(for $\text{Re}S[z]$ ) (for $\phi_z$ )	$\tau_{\text{int}} \simeq 10, 14 (\mu = 1.0, 1.1)$ $\tau_{\text{int}} \simeq 15, 14 (\mu = 1.0), 28 (\mu = 1.1)$

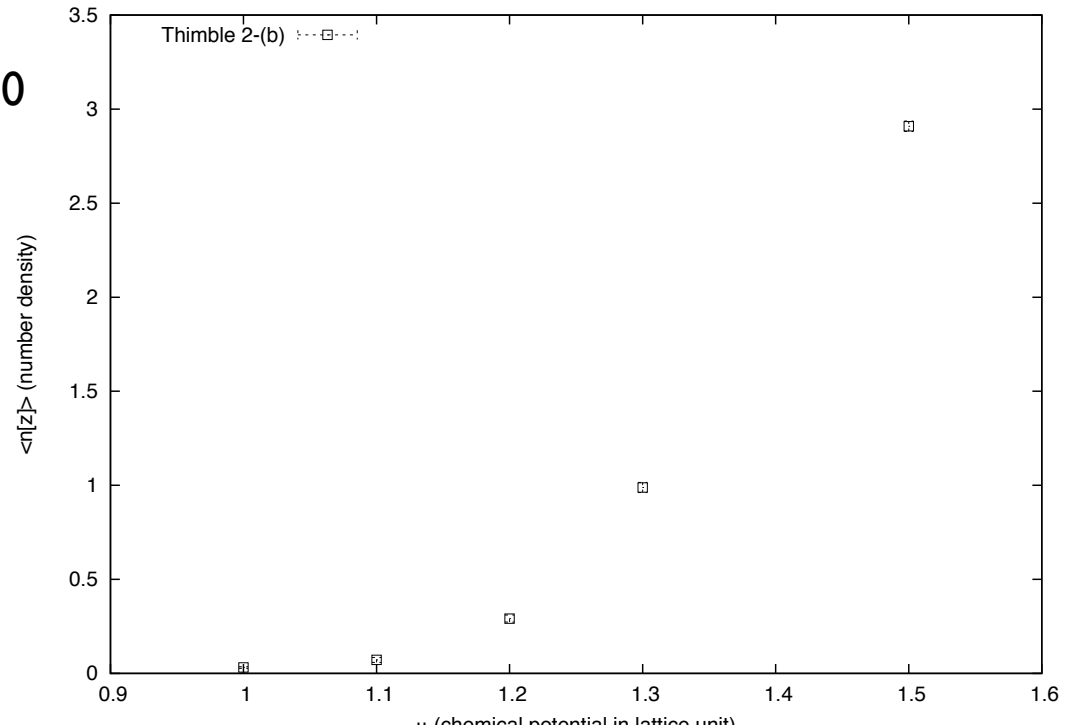
number density :

generated 11,250 traj.

sampling 1,000 conf. with the separation of 10

residual phase averages:

$\mu$	$\langle e^{i\phi_z} \rangle'_{\mathcal{J}_{\text{vac}}}$
1.0	$(9.94\text{e-}01, -8.77\text{e-}03) \pm (3.1\text{e-}02, 3.1\text{e-}03)$
1.1	$(9.94\text{e-}01, -3.21\text{e-}03) \pm (3.1\text{e-}02, 3.4\text{e-}03)$
1.2	$(9.95\text{e-}01, -8.25\text{e-}04) \pm (3.1\text{e-}02, 3.0\text{e-}03)$
1.3	$(9.97\text{e-}01, -3.08\text{e-}03) \pm (3.1\text{e-}02, 2.2\text{e-}03)$
1.5	$(9.99\text{e-}01, -1.06\text{e-}03) \pm (3.1\text{e-}02, 1.0\text{e-}03)$



# HMC on the thimble 2-(b) $\mu > \tilde{\mu}_c$

simulation parameters :

	Parameters	Resulting conditions
Thimble	$t_0 = -3.0$ $n_{\text{lefs}} = 100$ $h = t'/n_{\text{lefs}} \simeq 0.03$	$ \text{Re}(S[z(t_0)] - S[z_{\text{vac}}])  \lesssim 2.0 \times 10^1$ $ \text{Im}(S[z] - S[z_{\text{vac}}])  \lesssim 5.0 \times 10^{-2}$ $\ \bar{\partial}\bar{S} - V^\alpha \kappa^\alpha e^\alpha\ ^2/2V \leq 3.0 \times 10^{-2}$
MD	$\tau_{\text{traj}} = 0.3$ $n_{\text{step}} = 10, 30$ ( $\mu = 1.0, 1.1$ ) $\Delta\tau = 0.03, 0.01$ ( $\mu = 1.0, 1.1$ ) $\epsilon' = \sqrt{10} \times 10^{-3}$	$t' \in [2.5, 3.5]$ $\Delta H \lesssim 0.05$ Acceptance rate $\simeq 0.99$ $l \lesssim 4, 6$ ( $\mu = 1.0$ ), $14$ ( $\mu = 1.1$ )
Auto-corr. time	(for $\text{Re}S[z]$ ) (for $\phi_z$ )	$\tau_{\text{int}} \simeq 10, 14$ ( $\mu = 1.0, 1.1$ ) $\tau_{\text{int}} \simeq 15, 14$ ( $\mu = 1.0$ ), $28$ ( $\mu = 1.1$ )

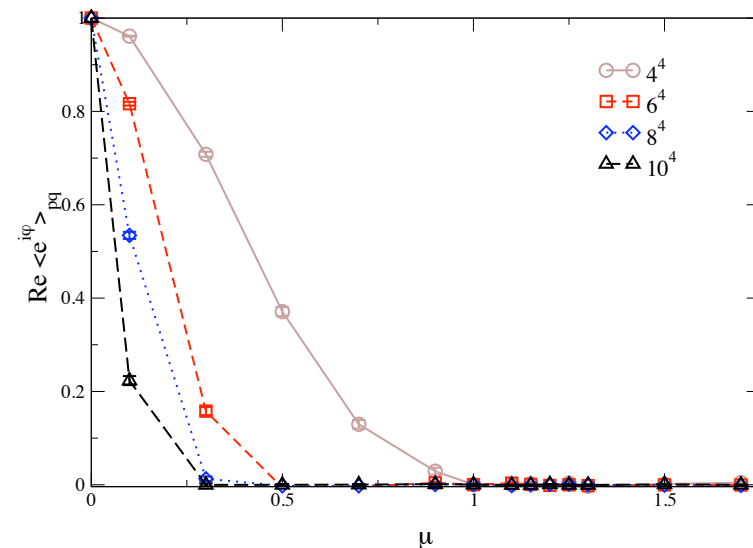
generated 11,250 traj.  
sampling 1,000 conf. with the separation of 10

residual phase averages:

$\mu$	$\langle e^{i\phi_z} \rangle'_{\mathcal{J}_{\text{vac}}}$
1.0	$(9.94\text{e-}01, -8.77\text{e-}03) \pm (3.1\text{e-}02, 3.1\text{e-}03)$
1.1	$(9.94\text{e-}01, -3.21\text{e-}03) \pm (3.1\text{e-}02, 3.4\text{e-}03)$
1.2	$(9.95\text{e-}01, -8.25\text{e-}04) \pm (3.1\text{e-}02, 3.0\text{e-}03)$
1.3	$(9.97\text{e-}01, -3.08\text{e-}03) \pm (3.1\text{e-}02, 2.2\text{e-}03)$
1.5	$(9.99\text{e-}01, -1.06\text{e-}03) \pm (3.1\text{e-}02, 1.0\text{e-}03)$

## HOW SEVERE IS THE SIGN PROBLEM?

AVERAGE PHASE FACTOR



average phase factor  $\langle e^{i\phi} \rangle_{\text{pq}}$

# HMC on the thimble 2-(b) $\mu > \tilde{\mu}_c$

simulation parameters :

	Parameters	Resulting conditions
Thimble	$t_0 = -3.0$ $n_{\text{lefs}} = 100$ $h = t'/n_{\text{lefs}} \simeq 0.03$	$ \text{Re}(S[z(t_0)] - S[z_{\text{vac}}])  \lesssim 2.0 \times 10^1$ $ \text{Im}(S[z] - S[z_{\text{vac}}])  \lesssim 5.0 \times 10^{-2}$ $\ \bar{\partial}\bar{S} - V^\alpha \kappa^\alpha e^\alpha\ ^2/2V \leq 3.0 \times 10^{-2}$
MD	$\tau_{\text{traj}} = 0.3$ $n_{\text{step}} = 10, 30$ ( $\mu = 1.0, 1.1$ ) $\Delta\tau = 0.03, 0.01$ ( $\mu = 1.0, 1.1$ ) $\epsilon' = \sqrt{10} \times 10^{-3}$	$t' \in [2.5, 3.5]$ $\Delta H \lesssim 0.05$ Acceptance rate $\simeq 0.99$ $l \lesssim 4, 6$ ( $\mu = 1.0$ ), $14$ ( $\mu = 1.1$ )
Auto-corr. time	(for $\text{Re}S[z]$ ) (for $\phi_z$ )	$\tau_{\text{int}} \simeq 10, 14$ ( $\mu = 1.0, 1.1$ ) $\tau_{\text{int}} \simeq 15, 14$ ( $\mu = 1.0$ ), $28$ ( $\mu = 1.1$ )

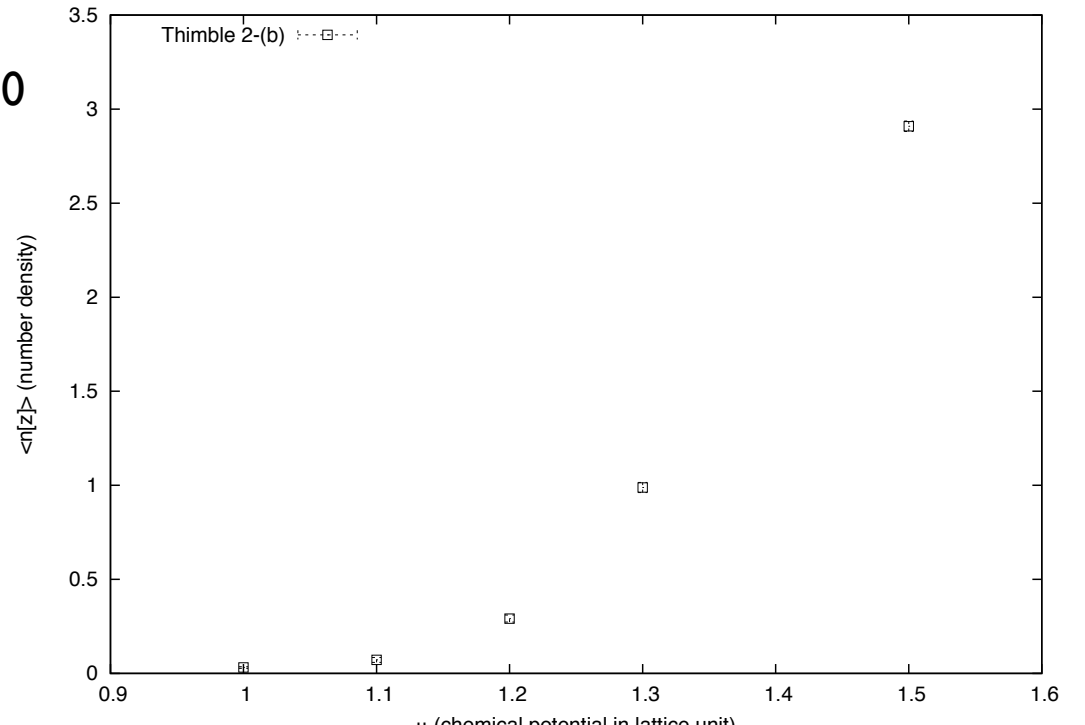
number density :

generated 11,250 traj.

sampling 1,000 conf. with the separation of 10

residual phase averages:

$\mu$	$\langle e^{i\phi_z} \rangle'_{\mathcal{J}_{\text{vac}}}$
1.0	(9.94e-01, -8.77e-03) $\pm$ (3.1e-02, 3.1e-03)
1.1	(9.94e-01, -3.21e-03) $\pm$ (3.1e-02, 3.4e-03)
1.2	(9.95e-01, -8.25e-04) $\pm$ (3.1e-02, 3.0e-03)
1.3	(9.97e-01, -3.08e-03) $\pm$ (3.1e-02, 2.2e-03)
1.5	(9.99e-01, -1.06e-03) $\pm$ (3.1e-02, 1.0e-03)



# Comparison to Complex Langevin simulations

$$\frac{dz(t)}{dt} = -\frac{\partial S[z]}{\partial z} + \eta(t); \quad \langle \eta(t)\eta(t') \rangle = 2\delta(t-t')$$

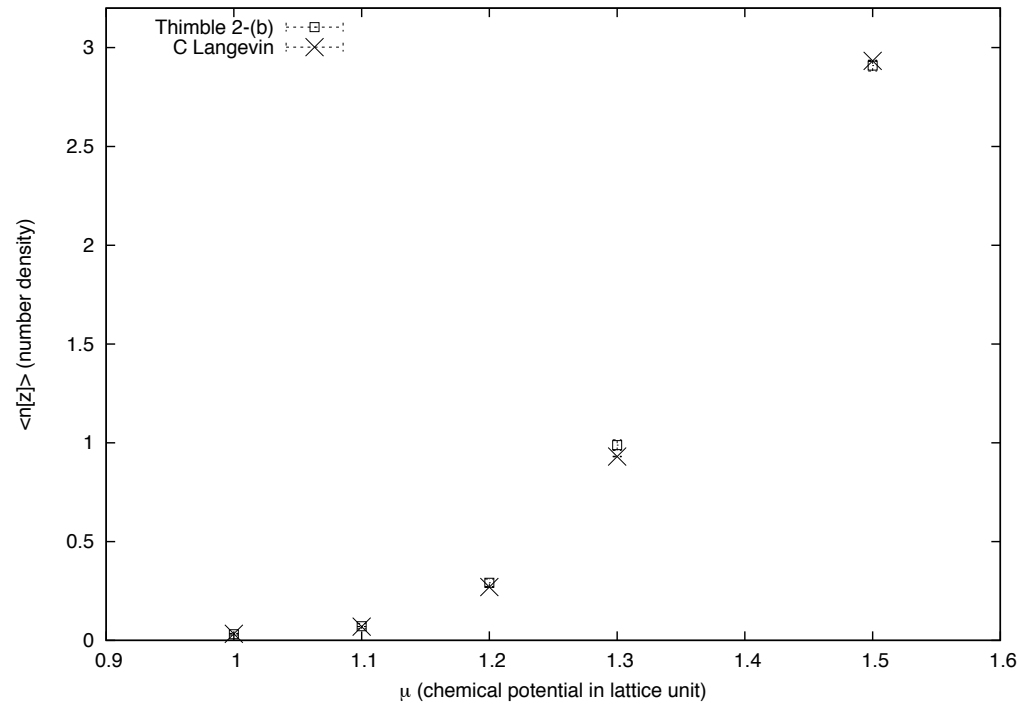
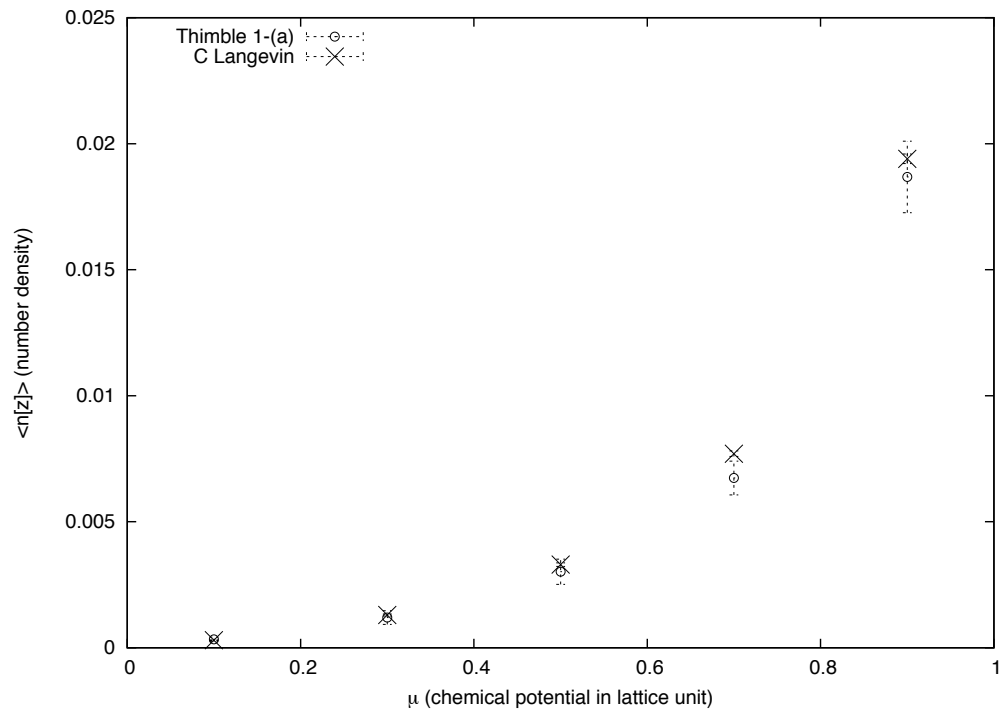
$$\langle \mathcal{O} \rangle = \lim_{t \rightarrow \infty} \frac{1}{t} \int_0^t dt' \mathcal{O}(z(t'))$$

parameters of CL simulations:

step size  $\varepsilon = 5.0 \times 10^{-5}$ , 5,000,000 time steps

sampling 10,000 configurations with the separation of 500

number density :



# Comparison to Complex Langevin simulations

$$\frac{dz(t)}{dt} = -\frac{\partial S[z]}{\partial z} + \eta(t); \quad \langle \eta(t)\eta(t') \rangle = 2\delta(t-t')$$

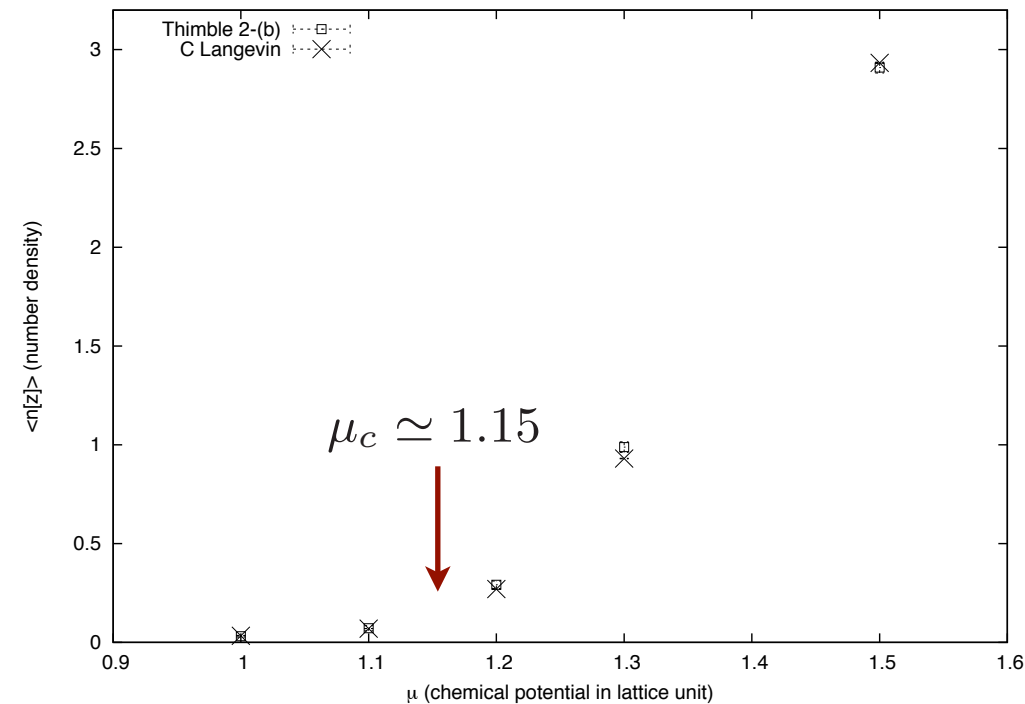
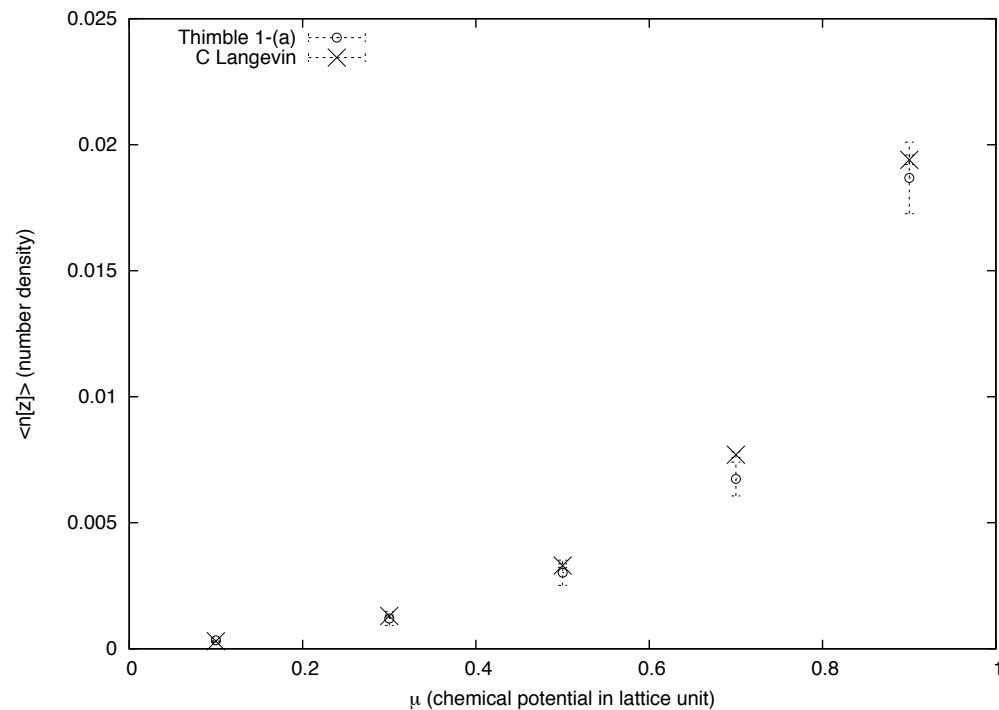
$$\langle \mathcal{O} \rangle = \lim_{t \rightarrow \infty} \frac{1}{t} \int_0^t dt' \mathcal{O}(z(t'))$$

parameters of CL simulations:

step size  $\varepsilon = 5.0 \times 10^{-5}$ , 5,000,000 time steps

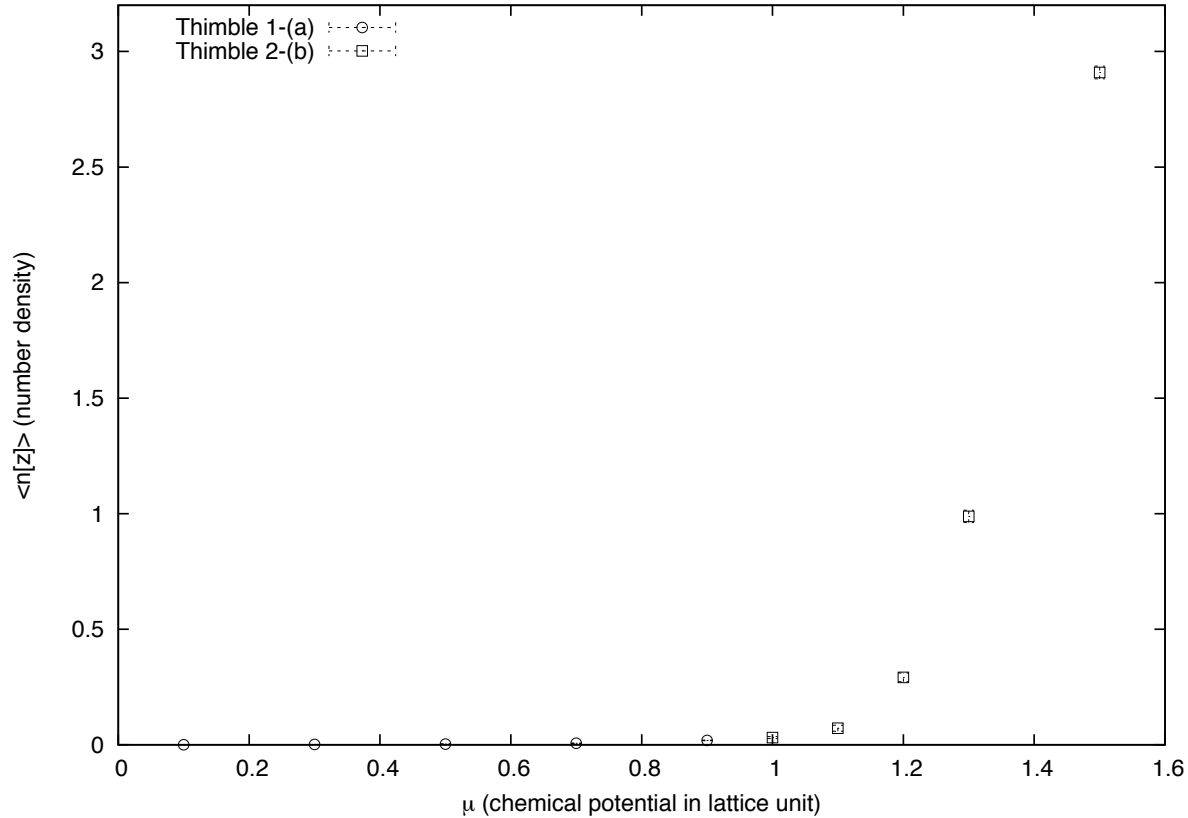
sampling 10,000 configurations with the separation of 500

number density :



# HMC on the thimbles I-(a) & 2-(b)

number density :



$\mu$	$\text{Re} \langle n[z] \rangle_{\mathcal{J}_{\text{vac}}} \text{ (j.-k. error)}$	$\text{Re} \langle e^{i\phi_z} n[z] \rangle'_{\mathcal{J}_{\text{vac}}}$	$\text{Re} \langle n[z] \rangle'_{\mathcal{J}_{\text{vac}}}$
0.1	3.34e-04 (9.2e-05)	3.35e-04	2.15e-04
0.3	1.20e-03 (2.7e-04)	1.19e-03	8.56e-04
0.5	3.02e-03 (5.0e-04)	3.01e-03	2.44e-03
0.7	6.74e-03 (6.7e-04)	6.71e-03	5.91e-03
0.9	1.89e-02 (1.4e-03)	1.85e-02	1.73e-02
1.0	3.14e-02 (4.3e-03)	3.12e-02	3.00e-02
1.1	7.17e-02 (1.3e-02)	7.12e-02	7.01e-02
1.2	2.92e-01 (1.8e-02)	2.90e-01	2.90e-01
1.3	9.88e-01 (2.6e-02)	9.85e-01	9.87e-01
1.5	2.91e-00 (2.7e-02)	2.90e-00	2.90e-00

$\tilde{\mu}_c \simeq 0.962$   
 $\mu_c \simeq 1.15$



# Summary & Discussions

- We have formulated a HMC algorithm which is applicable to lattice models defined on Lefschetz thimbles
- We have tested the algorithm in the  $\lambda\varphi^4_\mu$  model on the lattice  $V=4^4$ 
  - the thimbles associated with the classical vacua
  - the residual phase factors reweighted successfully
  - known results of the number density reproduced (cf. CL, dual v.)
  - Need the careful study of the systematic errors
    - setup of **the asymptotic regions**
    - contributions of **other thimbles, ex. thimble 2-(a), ...**
  - Need the study of the residual sign problem on larger lattices
- Numerical cost per traj.: literally, scales as  $O(V^3 \times n_{\text{step}})$ 
  - solving flow eqs. (all tangent vectors) :  $O(V^2 \times n_{\text{Lefs}})$
  - computing  $V^{-1}$ ,  $\det V$  (residual sign factors) :  $O(V^3)$
- Dynamical fermions :
  - possible applications to  $\text{QCD}_\mu$  cf. D. Sexty, arXiv:1307.7748

# Test in the $\lambda\phi^4_\mu$ model (cont'd)

## critical points with constant field $\mathbf{z}_a(\mathbf{x})=\mathbf{z}_a$

$$\left. \frac{\partial S[z]}{\partial z_a(x)} \right|_{z_a(x)=z_a} = (1 - 6K_0 - 2K_0 \cosh(\mu)) z_a + \lambda_0(z_1^2 + z_2^2)z_a = 0 \quad (a = 1, 2).$$

critical value of  $\mu$  (classical)  $\tilde{\mu}_c = \ln \left[ \left( \frac{1 - 6K_0}{2K_0} \right) + \sqrt{\left( \frac{1 - 6K_0}{2K_0} \right)^2 - 1} \right]$

$$\mu_c \sim 0.962 \text{ for } K=1.0, \lambda=1.0$$

1. For  $\mu \leq \tilde{\mu}_c$ ,

(a)  $z_1 = z_2 = 0 ; S[z] = 0,$

(b)  $z_1 = i\phi_0 \cos \theta, z_2 = i\phi_0 \sin \theta ; S[z] = -L^4 \frac{\lambda_0}{4} \phi_0^4,$

where  $\phi_0 = \sqrt{\frac{+(1-6K_0-2K_0 \cosh(\mu))}{\lambda_0}}.$

2. For  $\mu > \tilde{\mu}_c$ ,

(a)  $z_1 = z_2 = 0 ; S[z] = 0,$

(b)  $z_1 = \phi_0 \cos \theta, z_2 = \phi_0 \sin \theta ; S[z] = -L^4 \frac{\lambda_0}{4} \phi_0^4,$

where  $\phi_0 = \sqrt{\frac{-(1-6K_0-2K_0 \cosh(\mu))}{\lambda_0}}.$

← the thimble 1-(a)

← the thimble 2-(a)

← the thimble 2-(b)

# Summary & Discussions

- We have formulated a HMC algorithm which is applicable to lattice models defined on Lefschetz thimbles
- We have tested the algorithm in the  $\lambda\varphi^4_\mu$  model for  $V=4^4$ 
  - the thimbles associated with the classical vacua
  - the residual phase factors reweighted successfully
  - known results of the number density reproduced (cf. CL, dual v.)
  - Need the careful study of the systematic errors
    - setup of **the asymptotic regions**
    - contributions of **other thimbles, ex. thimble 2-(a), ...**
  - Need the study of the residual sign problem on larger lattices
- Numerical cost per traj.: literally, scales as  $O(V^3 \times n_{\text{step}})$ 
  - solving flow eqs. (all tangent vectors) :  $O(V^2 \times n_{\text{Lefs}})$
  - computing  $V^{-1}$ ,  $\det V$  (residual sign factors) :  $O(V^3)$
- Dynamical fermions :
  - possible applications to  $\text{QCD}_\mu$  cf. D. Sexty, arXiv:1307.7748

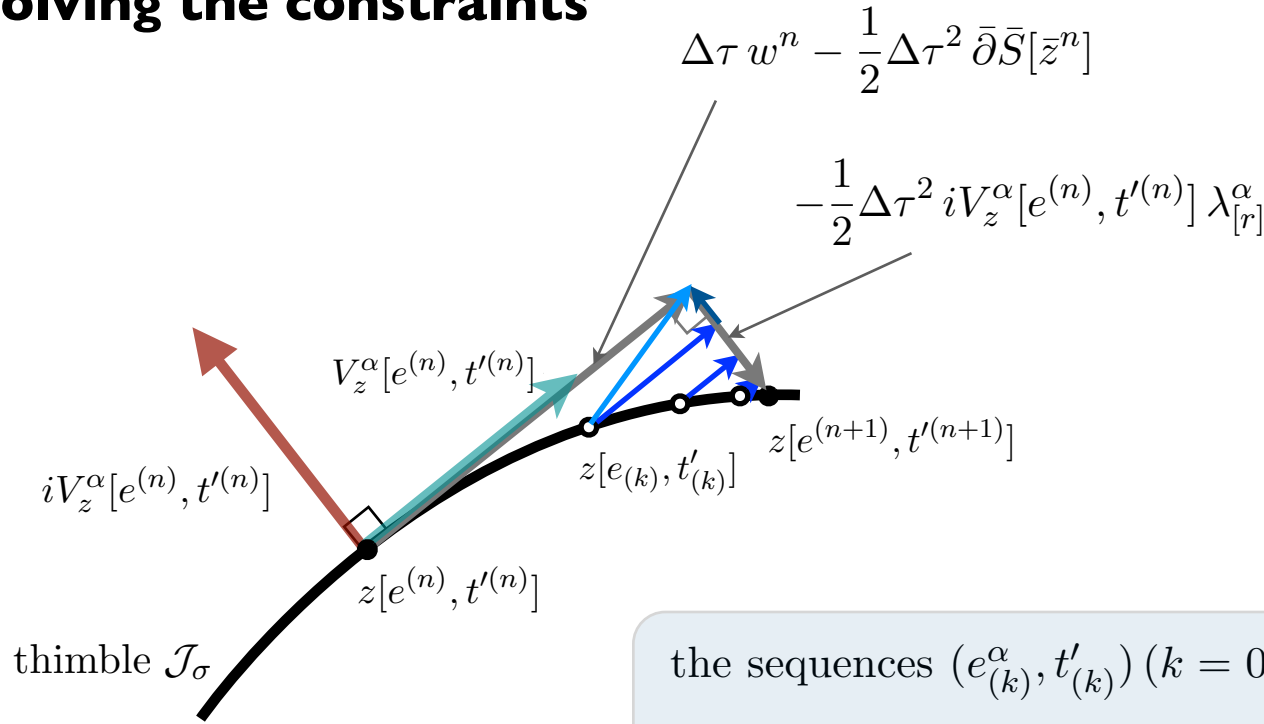
# Summary & Discussions

- We have formulated a HMC algorithm which is applicable to lattice models defined on Lefschetz thimbles
- We have tested the algorithm in the  $\lambda\varphi^4_\mu$  model for  $V=4^4$ 
  - the thimbles associated with the classical vacua
  - the residual phase factors reweighted successfully
  - known results of the number density reproduced (cf. CL, dual v.)
  - Need the careful study of the systematic errors
    - setup of **the asymptotic regions**
    - contributions of **other thimbles, ex. thimble 2-(a), ...**
  - Need the study of the residual sign problem on larger lattices
- Numerical cost per traj.: but, actually  $O(V \times n_{\text{Lefs}} \times n_{\text{step}})$   
solving flow eqs. (~~all~~ tangent vectors) :  $O(\cancel{V^2} \times n_{\text{Lefs}})$   
computing  $\cancel{V}^{-1}$ ,  $\det V$  (residual sign factors) :  $O(V^3)$
- Dynamical fermions :  
possible applications to  $\text{QCD}_\mu$  cf. D. Sexty, arXiv:1307.7748

# Summary & Discussions

- We have formulated a HMC algorithm which is applicable to lattice models defined on Lefschetz thimbles
- We have tested the algorithm in the  $\lambda\varphi^4_\mu$  model for  $V=4^4$ 
  - the thimbles associated with the classical vacua
  - the residual phase factors reweighted successfully
  - known results of the number density reproduced (cf. CL, dual v.)
  - Need the careful study of the systematic errors
    - setup of **the asymptotic regions**
    - contributions of **other thimbles, ex. thimble 2-(a), ...**
  - Need the study of the residual sign problem on larger lattices
- Numerical cost per traj.: but, actually  $O(V \times n_{\text{Lefs}} \times n_{\text{step}})$   
solving flow eqs. (~~all~~ tangent vectors) :  $O(\cancel{V}^2 \times n_{\text{Lefs}}) \times \text{CG} \times V^2(?)$   
computing  ~~$V^{-1}$~~ ,  $\det V$  (residual sign factors) :  $O(V^3)$
- Dynamical fermions : **psuedo fermions** can be implemented  
possible applications to  $\text{QCD}_\mu$  cf. D. Sexty, arXiv:1307.7748

# Solving the constraints



the sequences  $(e_{(k)}^\alpha, t'_{(k)})$  ( $k = 0, 1, \dots$ ) with  $(e_{(0)}^\alpha, t'_{(0)}) = (e^{(n)}, t'^{(n)})$

$$\Delta e_{(k)}^\alpha = e_{(k+1)}^\alpha - e_{(k)}^\alpha, \quad \sum_{\alpha=1} \Delta e_{(k)}^\alpha e^{\alpha(n)} = 0,$$

$$\Delta t'_{(k)} = t'_{(k+1)} - t'_{(k)},$$

$$\Delta z_{(k)}[e^{(n)}, t'^{(n)}] \equiv z_i[e^{(n)}, t'^{(n)}] + \Delta\tau w_i^n - \frac{1}{2} \Delta\tau^2 \bar{\partial}_i \bar{S}[\bar{z}^n] - z_i[e_{(k)}, t'_{(k)}]$$

$$\Delta z_{(k)}[e^{(n)}, t'^{(n)}]_{\parallel} = V_z^\alpha[e^{(n)}, t'^{(n)}] \left( \Delta e_{(k)}^\alpha + e^{\alpha(n)} \kappa^\alpha \Delta t'_{(k)} \right)$$

$$\Delta z_{(k)}[e^{(n)}, t'^{(n)}]_{\perp} = iV_z^\alpha[e^{(n)}, t'^{(n)}] \left( \frac{1}{2} \Delta\tau^2 \lambda_{[r](k)}^\alpha \right)$$

$$\left\| V_z^\alpha[e^{(n)}, t'^{(n)}] \left( \Delta e_{(k)}^\alpha + e^{\alpha(n)} \kappa^\alpha \Delta t'_{(k)} \right) \right\|^2 \leq n \epsilon'^2$$