# HMC on Lefschetz thimbles -- A study of the residual sign problem


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in collaboration with

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based on

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


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# Plan

1. **To define lattice models on Lefschetz thimbles**
   - Morse function, Gradient flow, Lefschetz thimbles
   - ★ extra phase factors / Tangent spaces >> residual sign problem
2. **An algorithm of HMC on Lefschetz thimbles**
   a. to parametrize/generate a thimble
   b. to formulate/solve the molecular dynamics on the thimble
   c. to measure observables by reweighting the residual phase
3. **Test in the $\lambda\varphi^4{}_\mu$ model**
4. **Summary & Discussion**

# Lattice models with complex-valued actions

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

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

## One possible approach based on complexification :

$$\phi_x \in \mathbb{R} \longrightarrow z_x \in \mathbb{C} \qquad U_{x\mu} = \mathrm{e}^{iA^a_{x\mu}T^a} \in \mathrm{SU}(3) \longrightarrow \mathrm{e}^{iZ^a_{x\mu}T^a} \in \mathrm{SL}(3,\mathbb{C})$$

- complexified Langevin dynamics

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

- deformation of path-integration contours to Lefschetz thimbles

**Analytic Continuation of Chern-Simons Theory**
E. Witten, arXiv:1001.2933[hep-lat]

cf. **Vanishing Homologies and the n variable saddle point method**
F. Pham (1983)

**New approach of the sign problem in quantum field theories:**
**High density QCD on a Lefschetz thimble (?)**
AuroraScience Collaboration,
Phys. Rev. D 86, 074506 (2012), arXiv:1205.3996 [hep-lat]

# Lattice models on Lefschetz thimbles

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

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

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

how to choose the contour of Path Integration ?

**Morse theory :**

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

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

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

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

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

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

$\mathcal{J}_\sigma$ the union of all downward flows which trace back to $z_\sigma$ in the limit t --> -∞
**<Lefschetz thimble>** (n-dim. real mfd.)

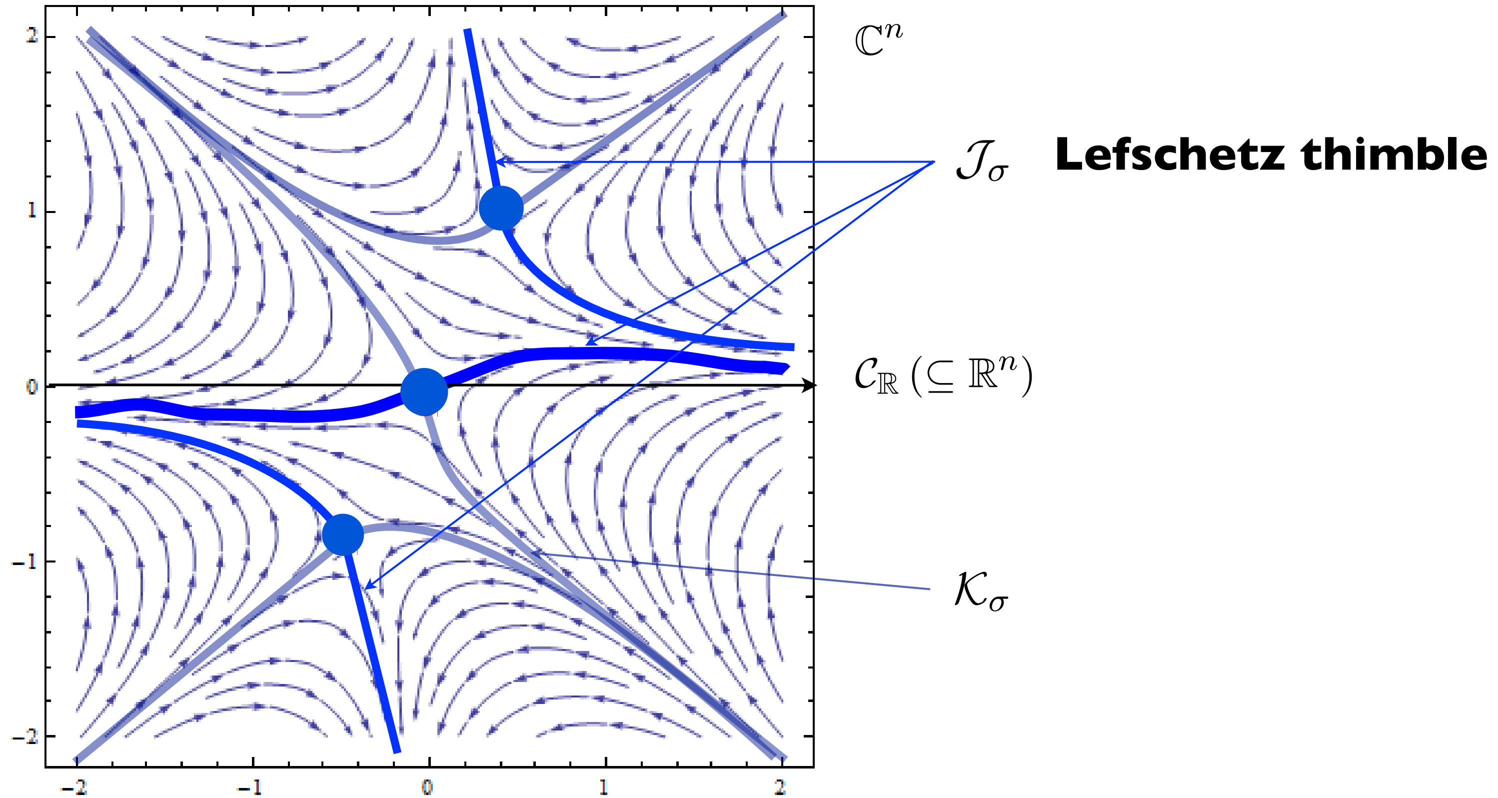
$\mathcal{K}_\sigma$ the union of all upward flows which trace back to $z_\sigma$ in the limit t --> -∞

$$\langle \mathcal{J}_\sigma, \mathcal{K}_\tau \rangle = \delta_{\sigma\tau}$$

(orthogonarity by intersection numbers)

# Simple example (n=1)

$$S[z] = \frac{\kappa}{2} z^2 + \frac{\lambda}{4} z^4 \qquad \kappa \in \mathbb{C}, \lambda > 0$$



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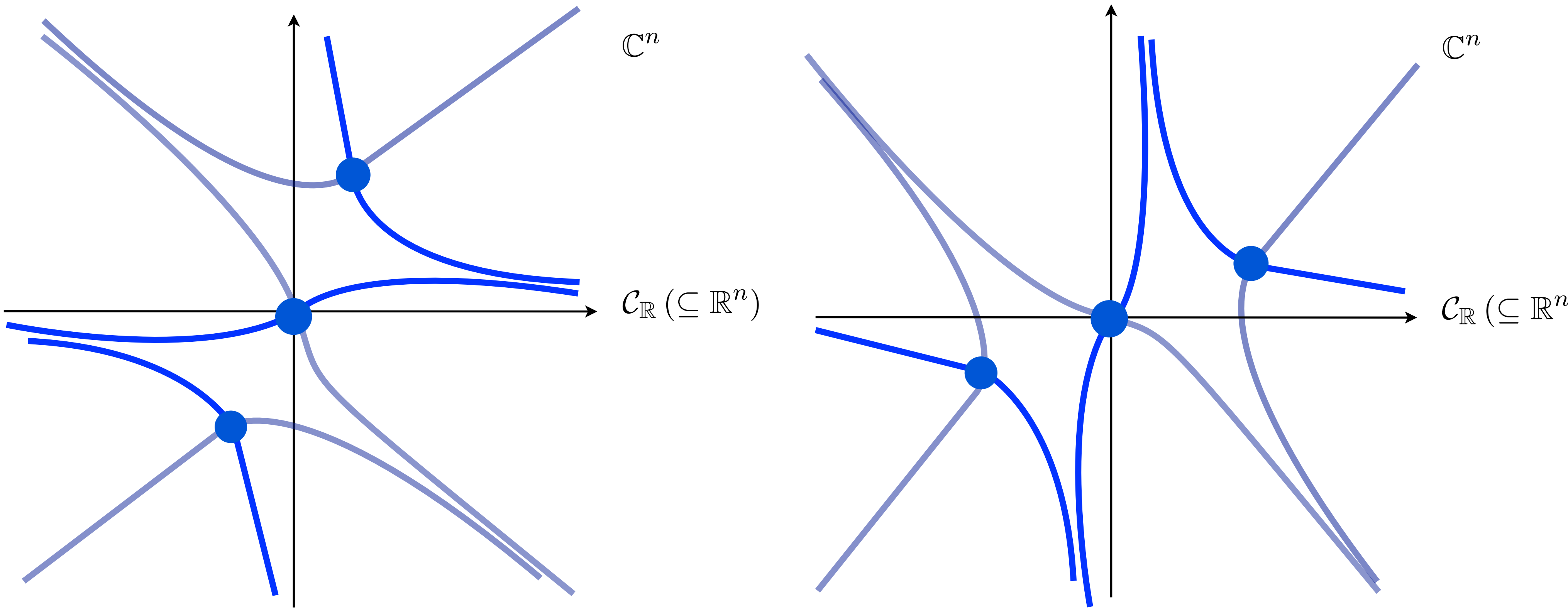

# Partition function

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

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

# Observables

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

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

# Partition function

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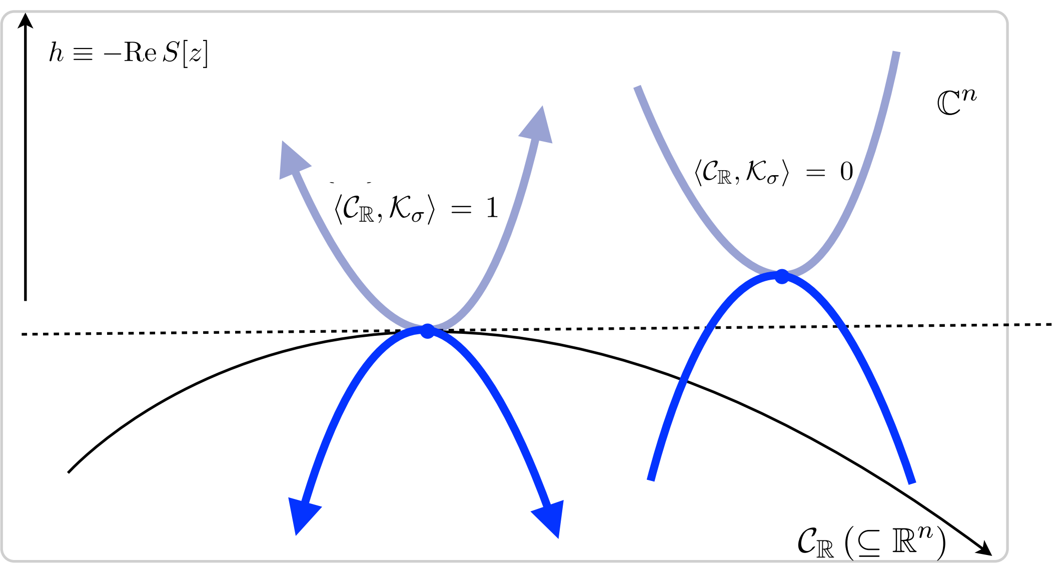



$\langle \mathcal{C}_\mathbb{R}, \mathcal{K}_\sigma\rangle = 0$

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

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

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

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

$z_{\rm vac} \in \mathcal{C}_\mathbb{R} \qquad -\mathrm{Re}\, S[z_{\rm vac}] = \max\{-\mathrm{Re}S[x]\}\ (x \in \mathcal{C}_\mathbb{R})$

## Partition function

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

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

## Observables

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

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

The functional measure should be specified by **the tangent spaces** of the thimble.

# Tangent spaces of Lefschetz thimbles

## In the vicinity of critical point $z_\sigma$

linearized flow equation and its solution:

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

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

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

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

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

$v_i^\alpha(\alpha = 1, \cdots, n)$ are orthonormal

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

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

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

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

$$V_z^\alpha = U_z^\beta E^{\beta\alpha}$$

$\{U_z^\alpha\}$ is an orthonormal basis

$E$ is a real upper triangle matrix

## Residual phase factor

$$\delta z = U_z^\alpha \delta\xi^\alpha \qquad |\delta z|^2 = \delta\xi^2$$

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

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

# Partition function

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

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

# Observables

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

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

The functional measure should be specified by **the tangent spaces** of the thimble.

The functional measure may give rise to **an extra phase factor** !
>> **residual sign problem**

## Partition function

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

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

This part is not straightforward to compute, in general

## Observables

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

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

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

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

in the saddle point approximation

This part may be evaluated by MC, but with the residual phase factor reweighted

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

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

( AuroraScience Collaboration )

# Algorithm of HMC on Lefschetz thimbles

↑

**the saddle-point structures !**

a) To parametrize / generate a thimble

unique parametrization in the asymptotic region close to the critical point / solve the flow eqs. by 4th-order RK

b) To formulate / solve the molecular dynamics

dynamical system constrained to the thimble by the forces in the normal directions / use 2nd-order constraint-preserving symmetric integrator

c) To measure observables

reweighting the residual sign factors

# Algorithm of HMC on Lefschetz thimbles (cont'd)

## a) To parametrize/generate a thimble

### Unique parametrization of z (field conf.) on the thimbles

Asymptotic solutions of gradient flow equations

$$
\begin{aligned}
z(t) &\simeq z_\sigma + v^\alpha \exp(\kappa^\alpha t)\, e^\alpha\,; \qquad e^\alpha e^\alpha = n \\
V_z^\alpha(t) &\simeq v^\alpha \exp(\kappa^\alpha\, t),
\end{aligned}
$$

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

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

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

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

**variation** of z

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

$$\delta \dot{z}_i(t) = \bar{\partial}_i \bar{\partial}_j \bar{S}[\bar{z}]\, \delta z_j(t)$$

$$\delta z(t) \;=\; V_z^\alpha(t)\, \delta c^\alpha$$

$$
\begin{aligned}
\delta z(t) &= v^\alpha\, \exp(\kappa^\alpha\, t)(\delta e^\alpha + e^\alpha \kappa^\alpha \delta t) \\
&= V_z^\alpha(t)(\delta e^\alpha + \kappa^\alpha e^\alpha \delta t) \qquad (t \ll 0)
\end{aligned}
$$

# Algorithm of HMC on Lefschetz thimbles (cont'd)

## a) To parametrize/generate a thimble

**Solve the flow equations by 4th order Runge-Kutta for a given $(e^\alpha, t')$ and $t_0(\ll 0)$ with the initial conditions,**

$$
\begin{aligned}
z_i(t_0) &= z_{\sigma i} + v_i^\alpha \, \exp(\kappa^\alpha t_0)\, e^\alpha \\
V_{zi}^\alpha(t_0) &= v_i^\alpha \, \exp(\kappa^\alpha t_0).
\end{aligned}
$$

$$h = \tau / n_{\text{lefs}}$$

$$
\begin{aligned}
f_1 &= \bar{\partial}\bar{S}[z[t]] \\
f_2 &= \bar{\partial}\bar{S}[z[t] + (h/2) f_1] \\
f_3 &= \bar{\partial}\bar{S}[z[t] + (h/2) f_2] \\
f_4 &= \bar{\partial}\bar{S}[z[t] + h f_3] \\
z(t+h) &= z(t) + \frac{h}{6}\,(f_1 + 2f_2 + 2f_3 + f_4)
\end{aligned}
$$

$$
\begin{aligned}
F_1^\alpha &= \bar{V}^\alpha(t)\bar{\partial}\bar{\partial}\bar{S}[z[t]] \\
F_2^\alpha &= \left\{\bar{V}^\alpha(t) + (h/2)\bar{F}_1^\alpha\right\} \bar{\partial}\bar{\partial}\bar{S}[z[t] + (h/2) f_1] \\
F_3^\alpha &= \left\{\bar{V}^\alpha(t) + (h/2)\bar{F}_2^\alpha\right\} \bar{\partial}\bar{\partial}\bar{S}[z[t] + (h/2) f_2] \\
F_4^\alpha &= \left\{\bar{V}^\alpha(t) + h\bar{F}_3^\alpha\right\} \bar{\partial}\bar{\partial}\bar{S}[z[t] + h f_3] \\
V^\alpha(t+h) &= V^\alpha(t) + \frac{h}{6}\,(F_1^\alpha + 2F_2^\alpha + 2F_3^\alpha + F_4^\alpha)
\end{aligned}
$$

**To check the solutions**

$$\bar{\partial}_i \bar{S}\left[\bar{z}[e,t']\right] - V_{zi}^\alpha[e,t']\,\kappa^\alpha e^\alpha = 0.$$

# Algorithm of HMC on Lefschetz thimbles (cont'd)

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

### Constrained dynamical system

Equations of motion:

$$\dot{z}_i = w_i,$$
$$\dot{w}_i = -\bar{\partial}_i \bar{S}[\bar{z}] - i V_{zi}^{\alpha}\,\lambda^{\alpha} \qquad \lambda^{\alpha} \in \mathbb{R}\ (\alpha = 1, \cdots, n)$$

Constraints:

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

the set of normal vectors

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

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

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

A conserved Hamiltonian:

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

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

# Algorithm of HMC on Lefschetz thimbles (cont'd)

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

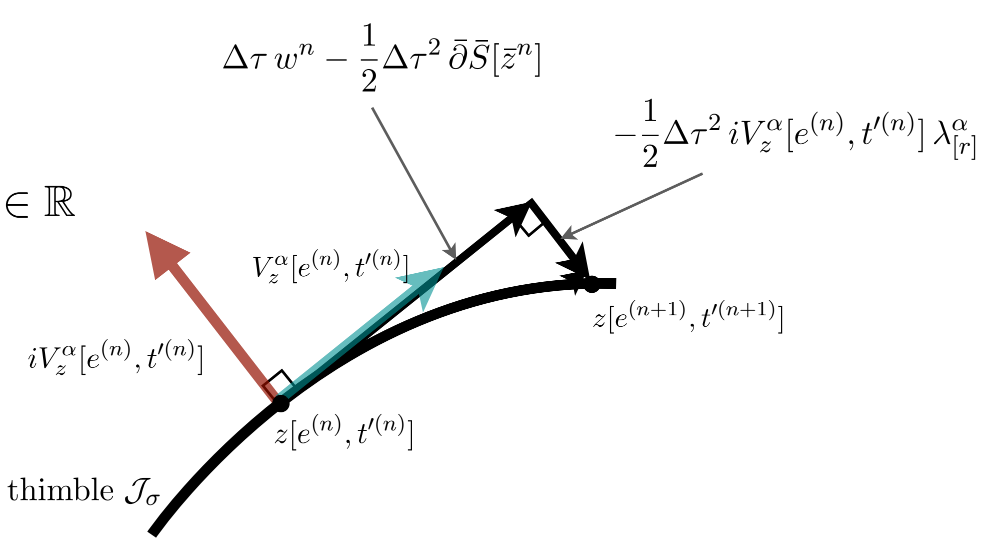
### Second-order constraint-preserving symmetric integrator

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

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

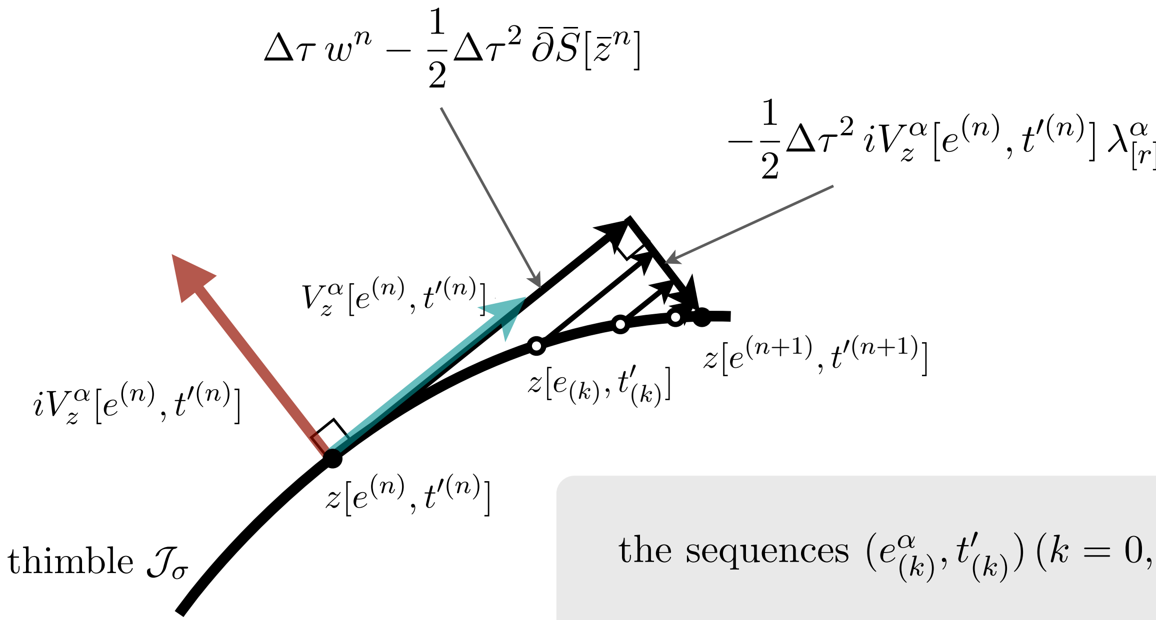
$\lambda^\alpha_{[r]}$ and $\lambda^\alpha_{[v]}$ are fixed by

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




**To solve the constraints ...**

# Solving the constraints




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

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

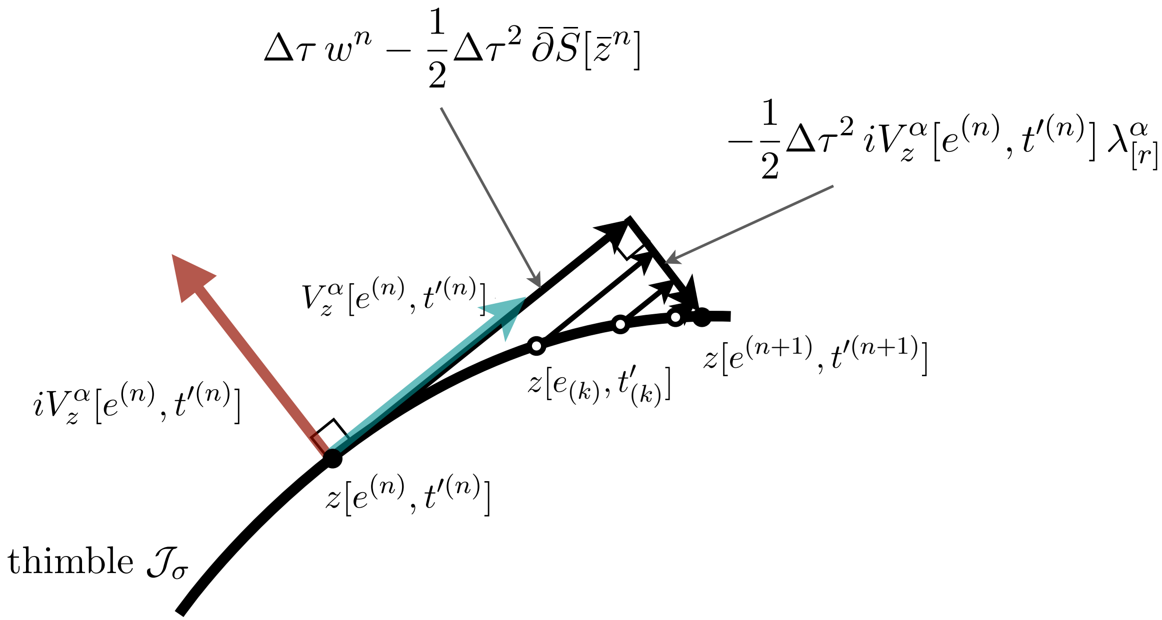
$$\Delta t'_{(k)} = t'_{(k+1)} - t'_{(k)},$$

$$\Delta e^\alpha{}_{(k)} + e^{\alpha(n)}\kappa^\alpha \Delta t'_{(k)} = \mathrm{Re}\Big[\{V_z^{-1}[e^{(n)}, t'^{(n)}]\}^\alpha_i \times \Big(z_i[e^{(n)}, t'^{(n)}] + \Delta\tau\, w_i^n - \frac{1}{2}\Delta\tau^2\, \bar\partial_i \bar S[\bar z^n] - z_i[e_{(k)}, t'_{(k)}]\Big)\Big]$$

$$\frac{1}{2}\Delta\tau^2\, \lambda^\alpha_{[r](k)} = \mathrm{Im}\Big[\{V_z^{-1}[e^{(n)}, t'^{(n)}]\}^\alpha_i \big(z_i[e^{(n)}, t'^{(n)}] - z_i[e_{(k)}, t'_{(k)}]\big)\Big]$$

$$\Big\| V_z^\alpha[e^{(n)}, t'^{(n)}]\big(\Delta e^\alpha{}_{(k)} + e^{\alpha(n)}\kappa^\alpha \Delta t'_{(k)}\big)\Big\|^2 \le n\,\epsilon'^2$$

# Solving the constraints




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

# Algorithm of HMC on Lefschetz thimbles (cont'd)

## a HMC update

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

1. Set the initial field configuration $z_i$:

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

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:

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

3. Repeat $n_{\rm step}$ times of the second order symmetric integration the step size $\Delta\tau = \tau_{\rm traj}/n_{\rm step}$.

4. Accept or reject by $\Delta H = H[w^{n_{\rm step}}, z^{n_{\rm step}}] - H[w^0, z^0]$.

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

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

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

# Algorithm of HMC on Lefschetz thimbles (cont'd)

## c) To measure observables by reweighting the residual sign factors

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

$$\langle O[z] \rangle_{\mathcal{J}_\sigma} = \frac{\langle {\rm e}^{i\phi_z} O[z] \rangle'_{\mathcal{J}_\sigma}}{\langle {\rm e}^{i\phi_z} \rangle'_{\mathcal{J}_\sigma}} \qquad {\rm e}^{i\phi_z} = \det U_z = \frac{\det V_z}{|\det V_z|}$$

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

**A possible sign problem !!**

**Need a careful and systematic study !!**

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

$$S = \sum_{x\in\mathbb{L}^4}\Big\{\big(\varphi^\dagger(x+\hat{0})\mathrm{e}^{+\mu} - \varphi^\dagger(x)\big)\big(\mathrm{e}^{-\mu}\varphi(x+\hat{0}) - \varphi(x)\big)$$

$$+\sum_{k=1}^{3}|\varphi(x+\hat{k}) - \varphi(x)|^2 + \frac{\kappa}{2}\varphi^\dagger(x)\varphi(x) + \frac{\lambda}{4}\big(\varphi^\dagger(x)\varphi(x)\big)^2\Big\}$$

$$= \sum_{x\in\mathbb{L}^4}\Big\{-\phi_a(x)\phi_b(x+\hat{0})\big[\delta_{ab}\cosh(\mu) - i\epsilon_{ab}\sinh(\mu)\big]$$

$$-\sum_{k=1}^{3}\phi_a(x)\phi_a(x+\hat{k}) + \frac{(8+\kappa)}{2}\phi_a(x)\phi_a(x) + \frac{\lambda}{4}\big(\phi_a(x)\phi_a(x)\big)^2\Big\}$$

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

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

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

$$S[z] = \sum_{x\in\mathbb{L}^4}\Big\{+\frac{1}{2}z_a(x)z_a(x) + \frac{\lambda_0}{4}\big(z_a(x)z_a(x)\big)^2 - K_0\sum_{k=1}^{3}z_a(x)z_a(x+\hat{k})$$

$$-K_0\, z_a(x)z_b(x+\hat{0})\big[\delta_{ab}\cosh(\mu) - i\epsilon_{ab}\sinh(\mu)\big]\Big\}.$$

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

L=4 (, ... 12)

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

cf. G.Aarts (Complex Langevin simulation)

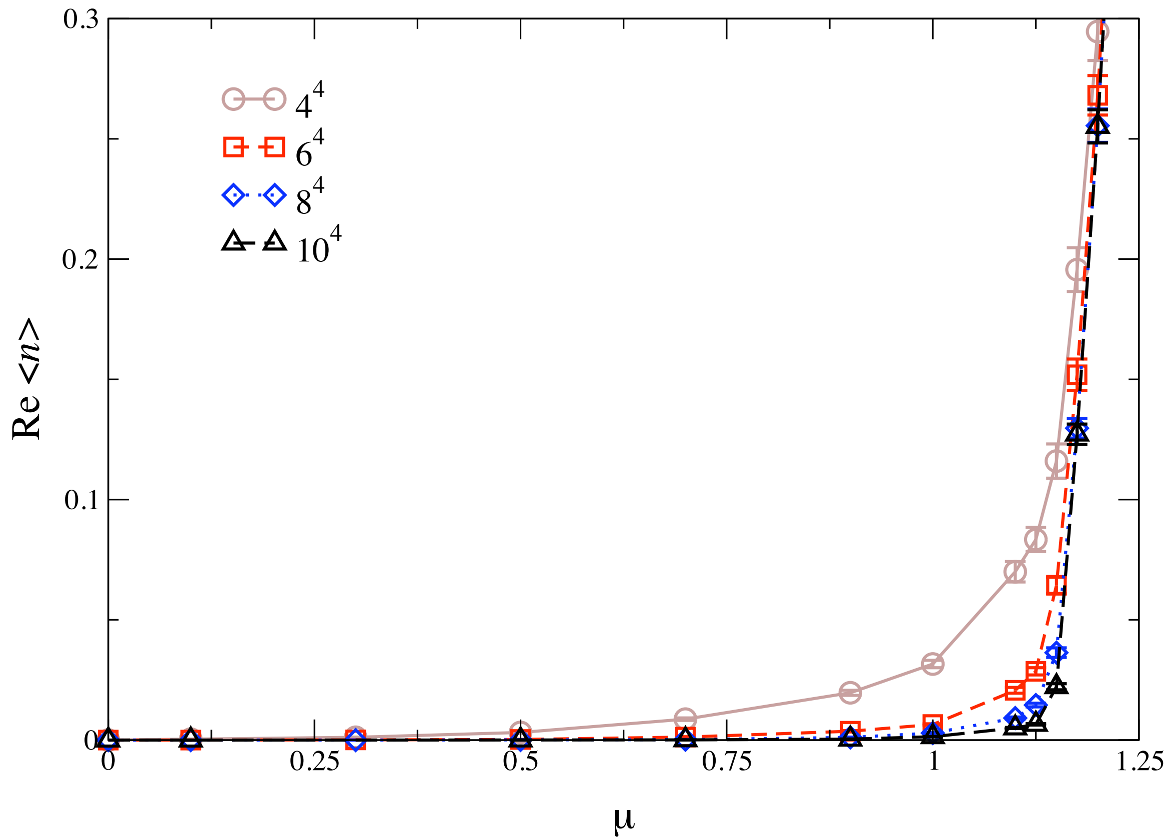
**Can stochastic quantization evade the sign problem?**
**-- the relativistic Bose gas at finite chemical potential**
G.Aarts, PRL 102:131601, 2009 arXiv:0810.2089

cf. G. Aarts (Complex Langevin simulation)

# Relativistic Bose gas

## complex Langevin

density $\langle n \rangle = (1/\Omega)\partial \ln Z/\partial\mu$

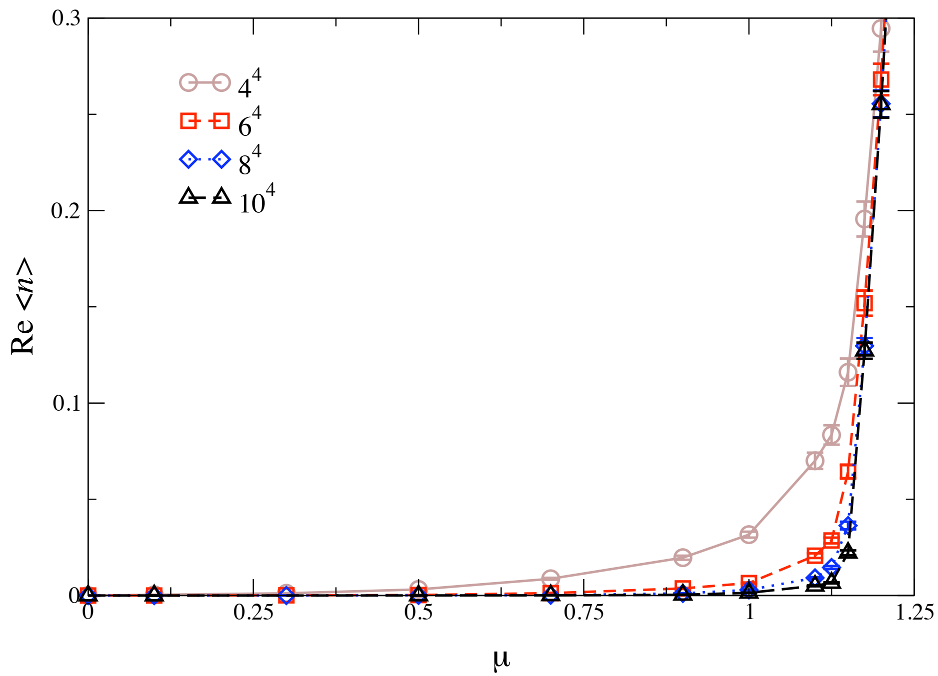



second order phase transition in thermodynamic limit cf. G. Aarts PRL 102(2009) 131601 (Complex Langevin simulation)

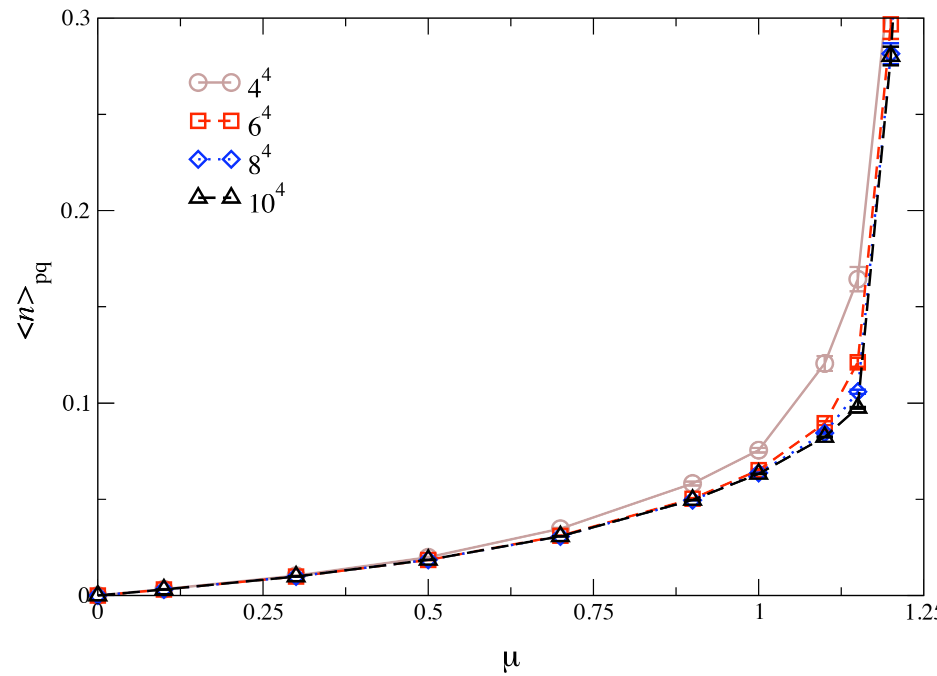
# Silver Blaze and the sign problem

## COMPLEX VS PHASE QUENCHED

density




complex

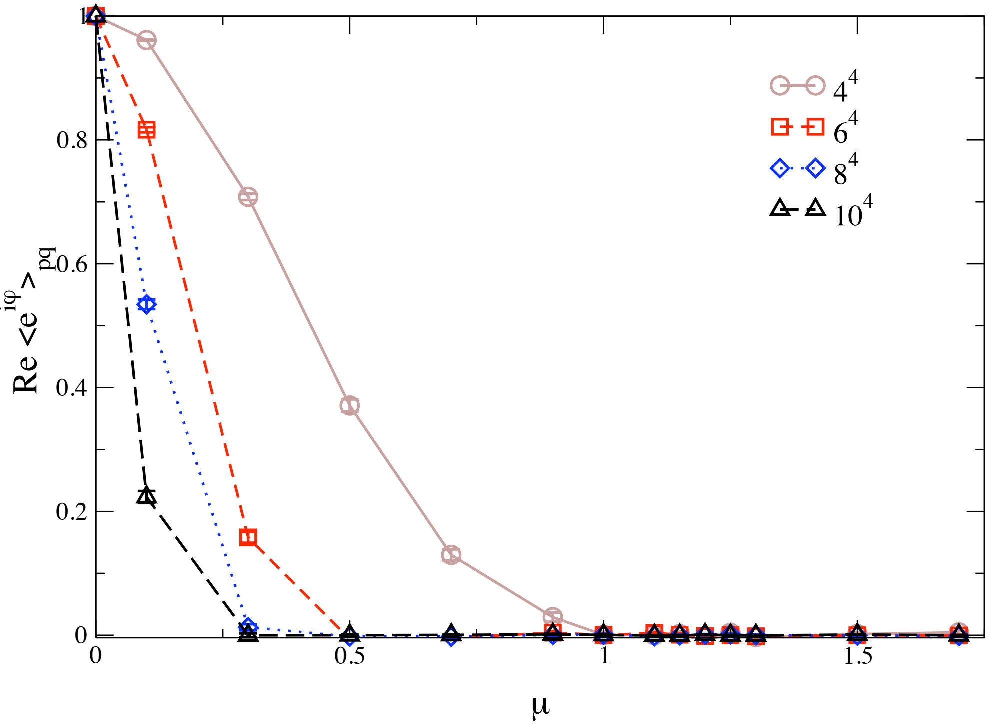



phase quenched

phase $e^{i\varphi} = e^{-S}/|e^{-S}|$ does precisely what is expected cf. G. Aarts (Complex Langevin simulation)

# HOW SEVERE IS THE SIGN PROBLEM?

AVERAGE PHASE FACTOR




average phase factor $\langle e^{i\varphi} \rangle_{\rm pq}$

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

## critical points with constant field $z_a(x)=z_a$

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

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

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

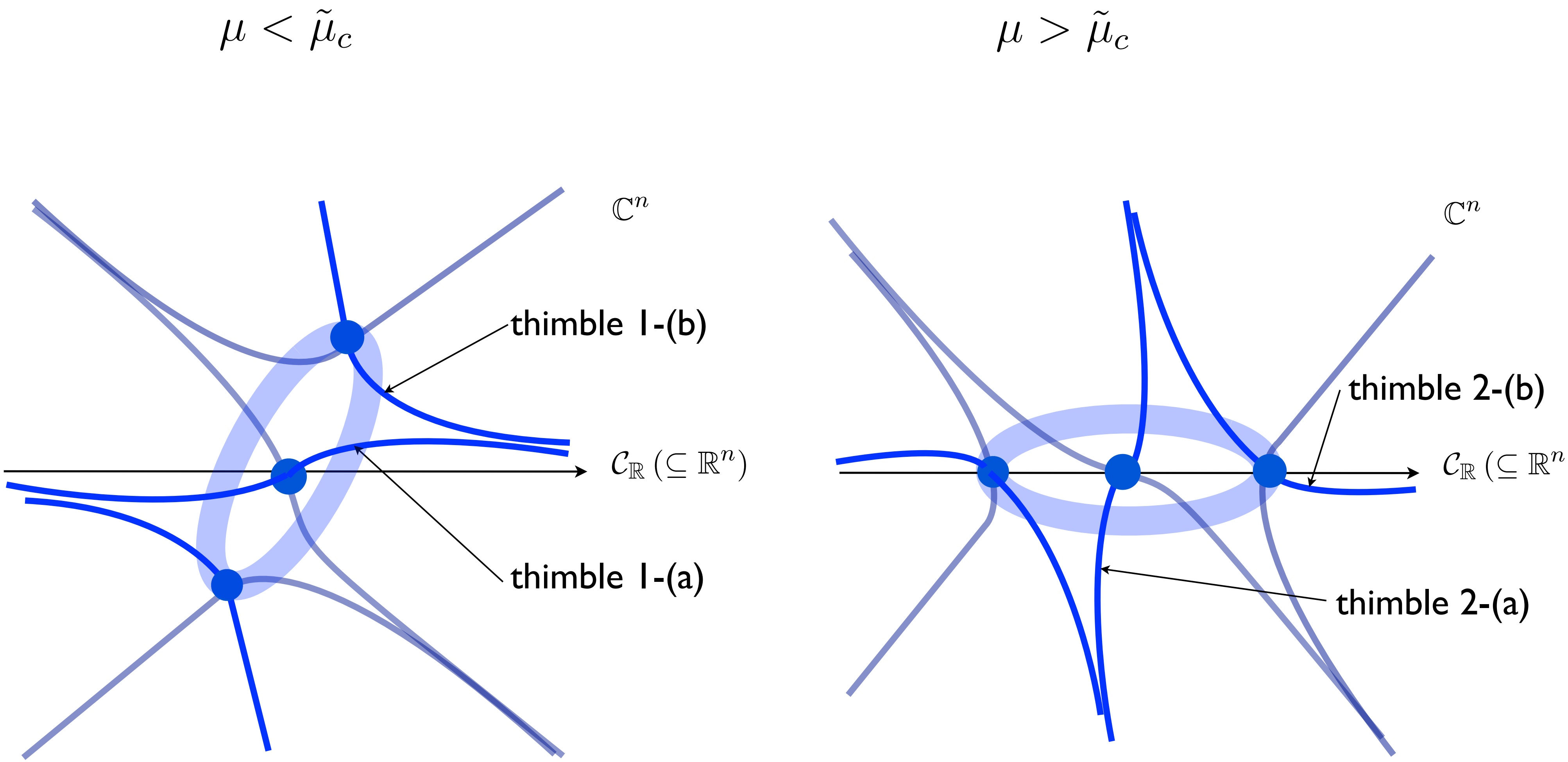
   (a) $z_1 = z_2 = 0$ ; $S[z] = 0$, → the thimble 1-(a)

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

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

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

   (b) $z_1 = \phi_0\cos\theta,\ z_2 = \phi_0\sin\theta$ ; $S[z] = -L^4\frac{\lambda_0}{4}\phi_0^4$, → the thimble 2-(b)
   where $\phi_0 = \sqrt{\frac{-\left(1-6K_0-2K_0\cosh(\mu)\right)}{\lambda_0}}$.



$\mu < \tilde{\mu}_c$
$\mu > \tilde{\mu}_c$
$\mathbb{C}^n$
thimble 1-(b)
$\mathcal{C}_{\mathbb{R}}\ (\subseteq \mathbb{R}^n)$
thimble 1-(a)
$\mathbb{C}^n$
thimble 2-(b)
$\mathcal{C}_{\mathbb{R}}\ (\subseteq \mathbb{R}^n)$
thimble 2-(a)

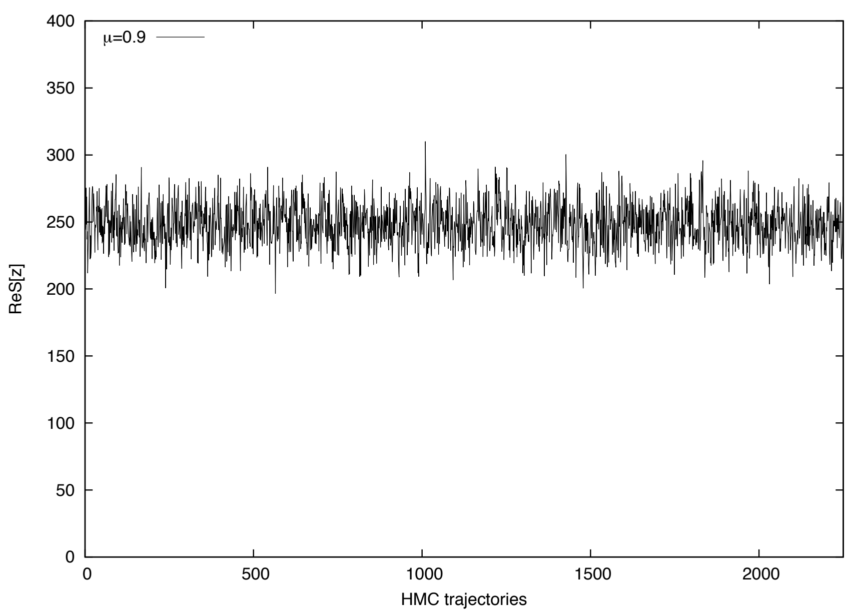
# Test in the $\lambda\varphi^4{}_\mu$ model (cont'd)

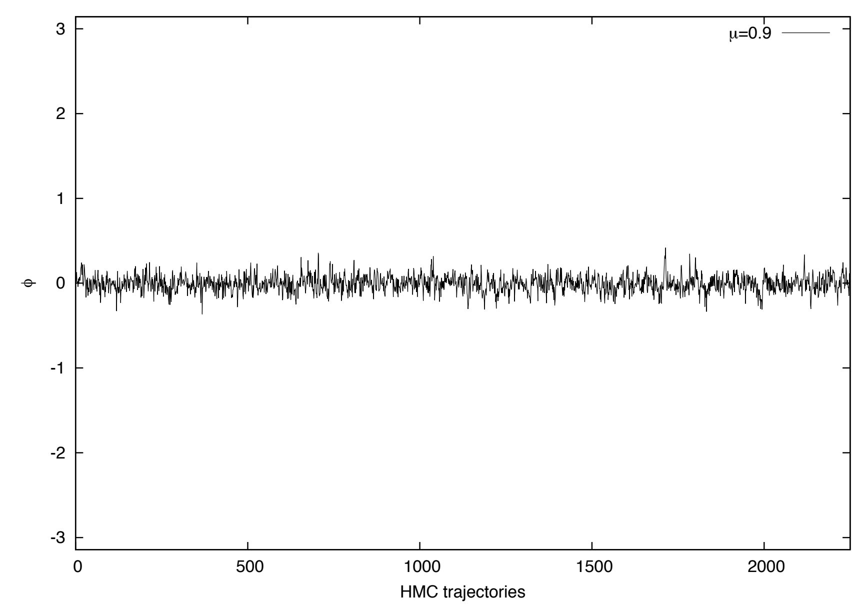
## HMC on the thimble 1-(a) $\mu < \tilde{\mu}_c$

simulation parameters :

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

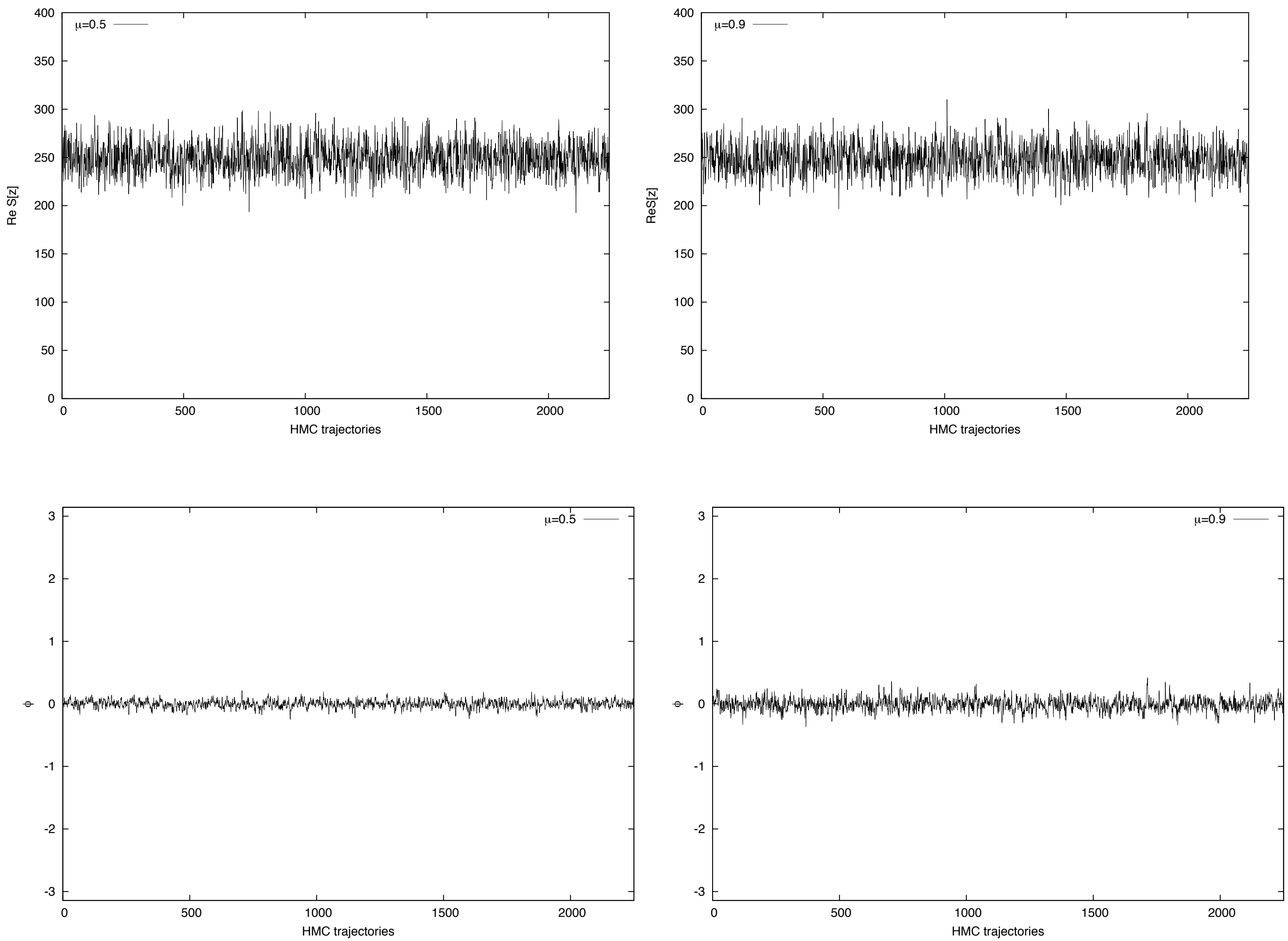
HMC histories (μ = 0.9)



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

## HMC on the thimble 1-(a)



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

## HMC on the thimble 1-(a)

residual phase averages:

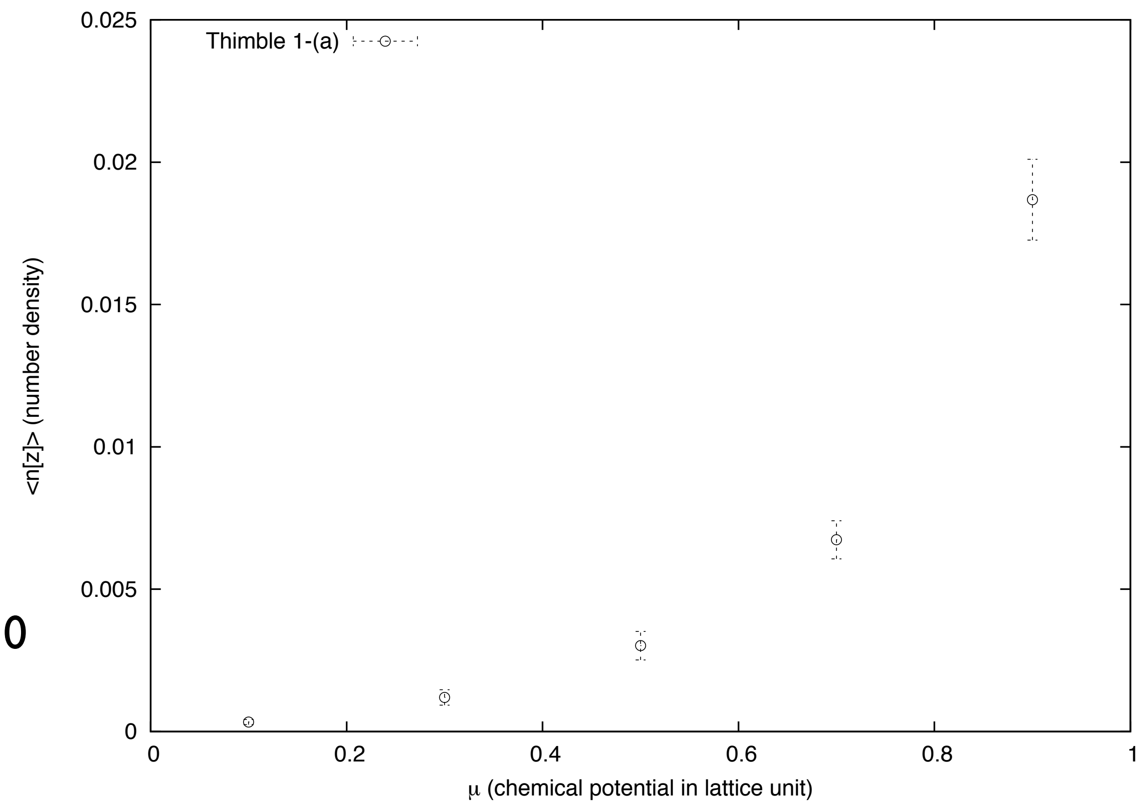
$$e^{i\phi_z} = \det U_z = \frac{\det V_z}{|\det V_z|}$$

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

generated 4,250 traj.
sampling 300 conf. with the separation of 10

number density :

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



# Test in the λφ⁴ μ model (cont'd)

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

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

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

**zero mode**

$$\kappa^0 = 0$$

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

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

**Critical fluctuation :** **lowest mode** $\kappa^1 = 2\lambda_0\phi_0^2$, $v_a(x)^1 = \delta_{a1}/\sqrt{V}$ **gets very light !** $(\mu \gtrsim \tilde{\mu}_c)$

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

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

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

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

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

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

$$\frac{d}{dt} z_a(t) = \bar{\partial}_{ax}\bar{S}[\bar{z}]\big|_{z_a(x;t)=z_a(t)} = \lambda_0\left(\bar{z}_b(t)\bar{z}_b(t) - \phi_0^2\right)\bar{z}_a(t)$$

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

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

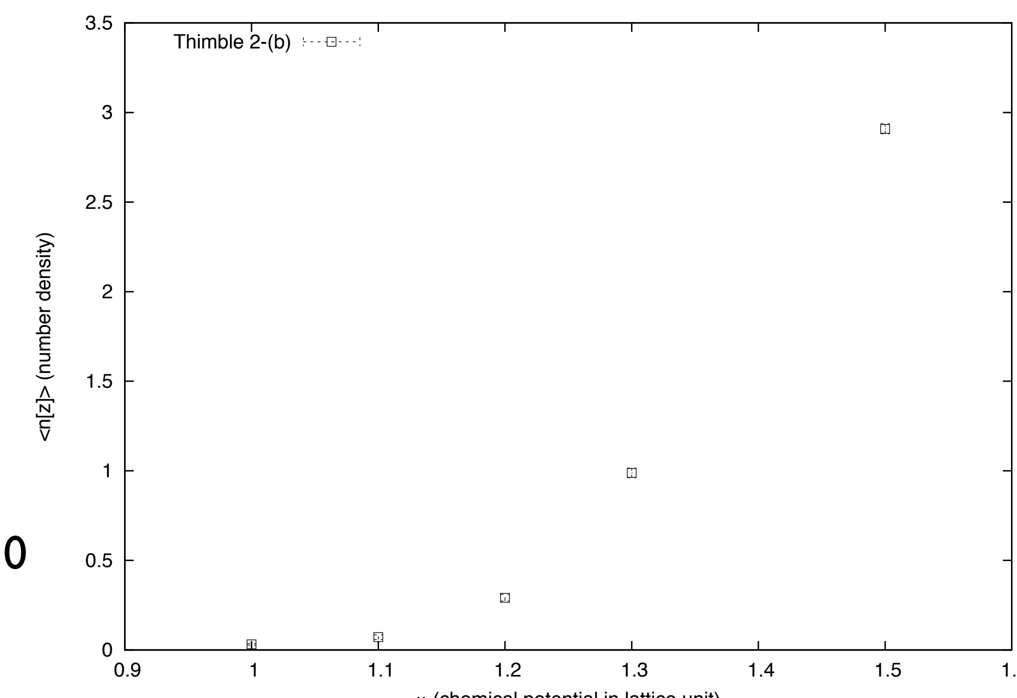
simulation parameters :

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

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) |

number density :

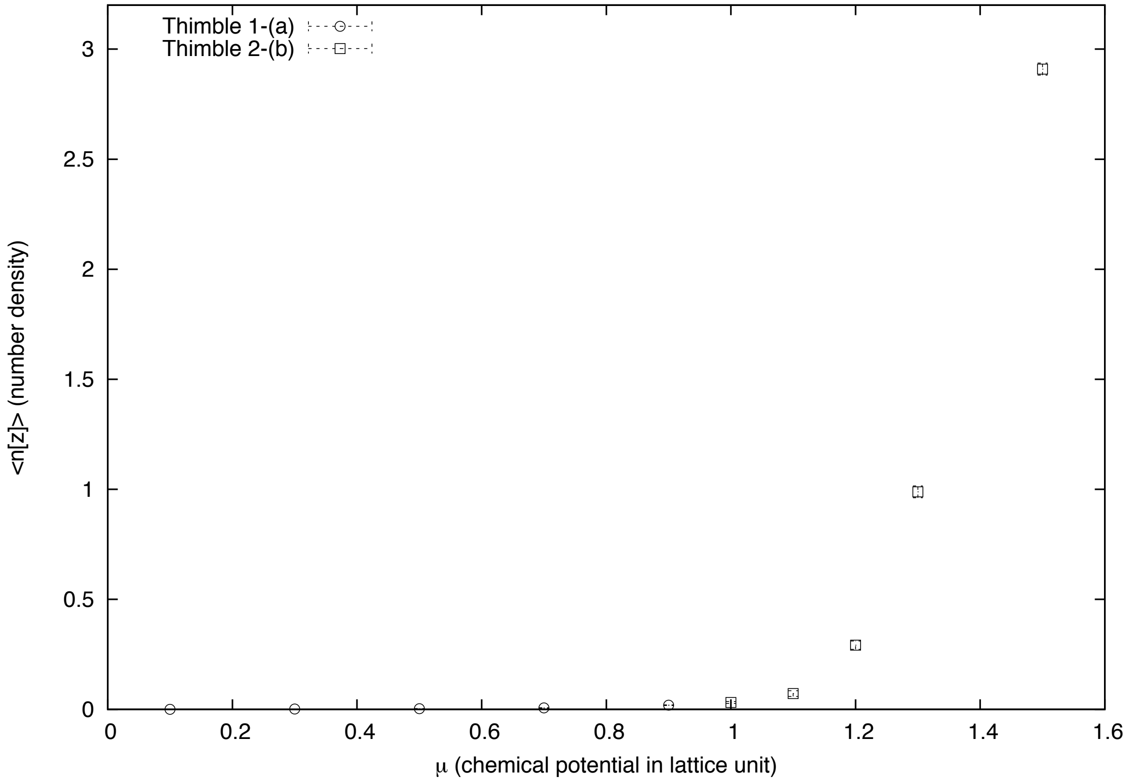



generated 11,250 traj.
sampling 1,000 conf. with the separation of 10

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

## HMC on the thimbles 1-(a) & 2-(b)

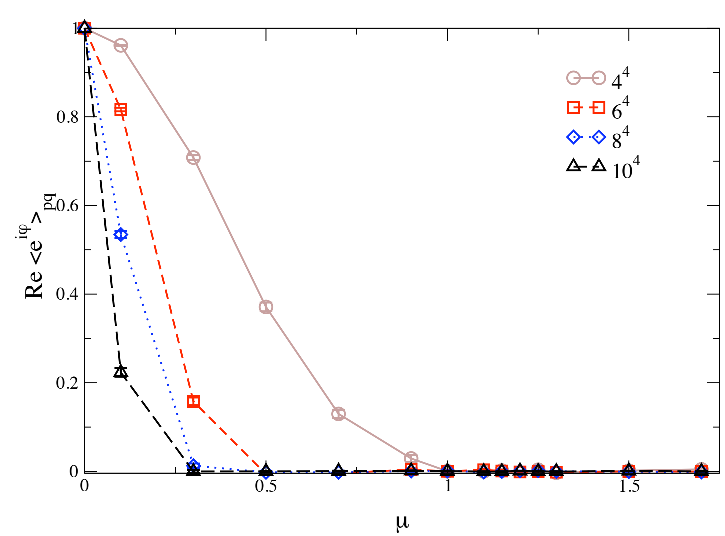
number density :




| $\mu$ | Re $\langle n[z]\rangle_{\mathcal{J}_{\rm vac}}$ (j.-k. error) | | Re $\langle e^{i\phi_z}\, n[z]\rangle'_{\mathcal{J}_{\rm vac}}$ | Re $\langle n[z]\rangle'_{\mathcal{J}_{\rm vac}}$ |
|---|---|---|---|---|
| 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 |

### How severe is the sign problem?

AVERAGE PHASE FACTOR



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

## Comparison to Complex Langevin simulations

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

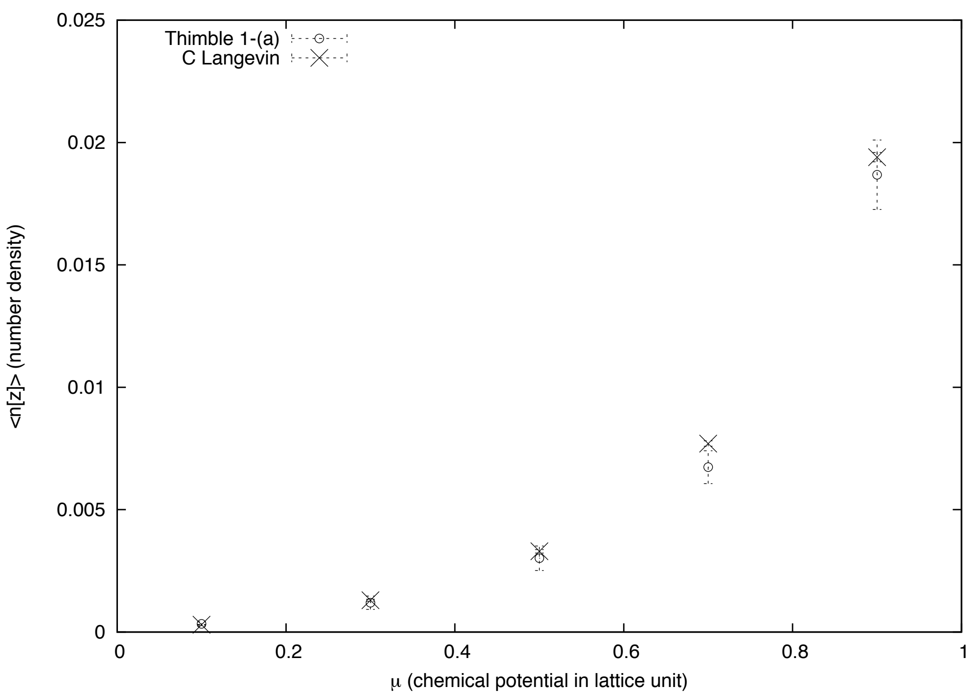
$$\langle \mathcal{O} \rangle = \lim_{t\to\infty} \frac{1}{t} \int_0^t dt' \, \mathcal{O}(z(t'))$$

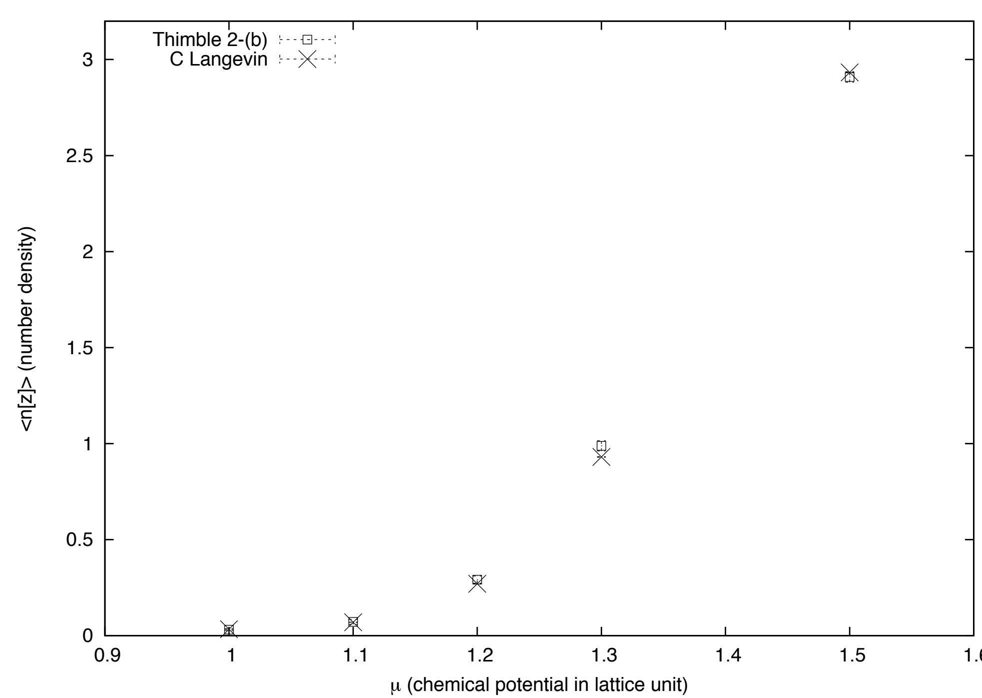
parameters of CL simulations:

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

sampling 10,000 configurations with the separation of 500

number density :



## 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 )
  - Need the careful study of <u>the systematic errors</u>
    - setup of the asymptotic regions
    - contributions of other thimbles, ex. thimble 2-(a), ...
  - Need the study of <u>the residual sign problem on larger lattices</u>
    - numerical cost per traj.
    - $O(V^2 \times n_{Lefs} \times n_{step})$ (tangent vectors), $O(V^3 \times n_{step})$ ($V^{-1}$, detV)
- Possible applications to $QCD_{\mu}$ cf. D. Sexty, arXiv:1307.7748