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

Jan. 20, 2014 @ KEK

Plan

1. **Introduction**
2. **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
3. **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 ?
4. **Test in the $\lambda\varphi^4{}_\mu$ model**
5. **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 P. Hasenfratz and F. Karsch*]

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

Example:

Yukawa-theory with Higgs, top and bottom quarks (as a part of lattice GWS model)

- exact chiral $SU(2)_L$ symmetry (thanks to G-W rel.) — *Luscher (1998)*
- reflection positivity (in spite of G-W rel.) — *Usui, Y.K. (2010)*
- complex effective action

$$\gamma_5 D + D\gamma_5 = 2aD\gamma_5 D$$

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 problem):
rewighting; histgram; dual variables;
Tayler expansion in μ; analytic continuation in μ (complex μ), etc.

One possible approach is to complexify the lattice models

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

- complexified Langevin dynamics

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

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

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

- Path-Integral contours deformed to Lefschetz thimbles

  F. Pham (1983); E. Witten, arXiv:1001.2933;
  AuroraScience Collaboration,
  Phys. Rev. D 86, 074506 (2012), arXiv:1205.3996

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

Lattice models on Lefschetz thimbles

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

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

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

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

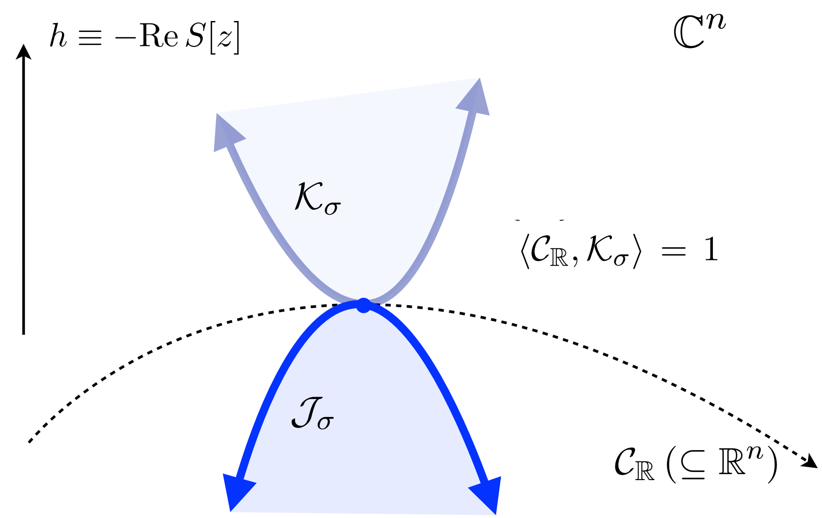
$$\mathcal{C}_{\mathbb{R}} = \sum_{\sigma \in \Sigma} n_\sigma \mathcal{J}_\sigma, \qquad n_\sigma = \langle \mathcal{C}_{\mathbb{R}}, \mathcal{K}_\sigma \rangle$$

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

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

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

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_σ in the limit t goes to $-\infty$



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

Lattice models on Lefschetz thimbles

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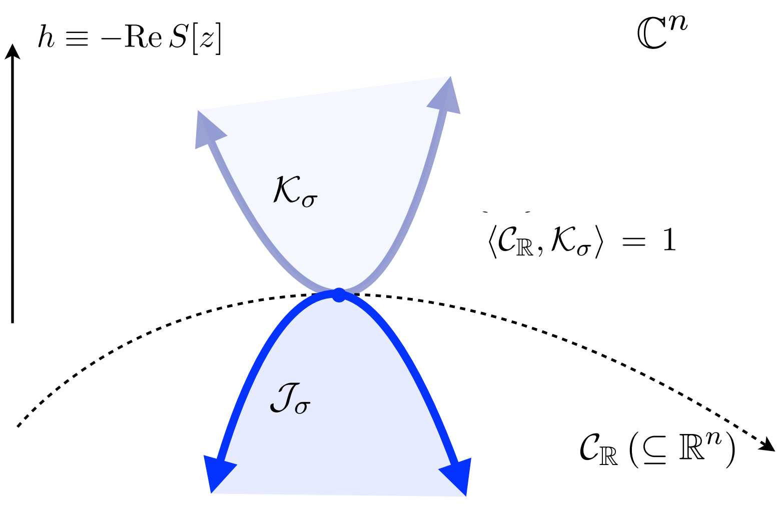
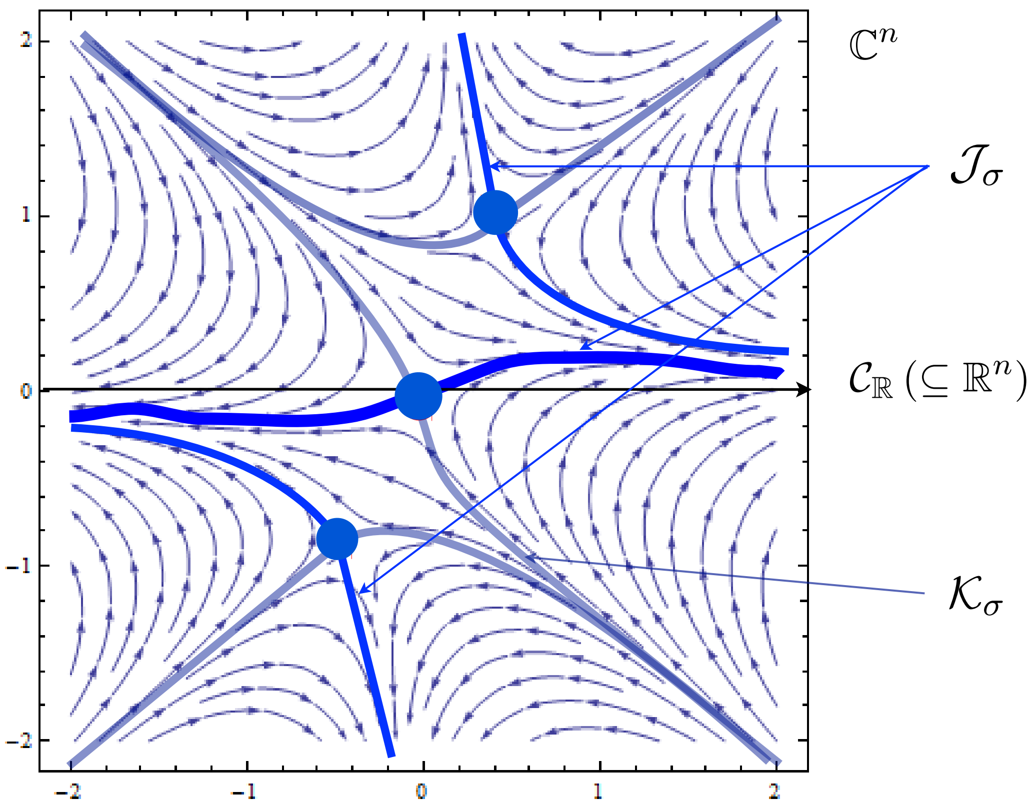
$$\frac{d}{dt} h = -\frac{1}{2} \left\{ \frac{\partial S[z]}{\partial z} \cdot \frac{d}{dt} z(t) + \frac{\partial \bar{S}[\bar{z}]}{\partial \bar{z}} \cdot \frac{d}{dt} \bar{z}(t) \right\} = -\left| \frac{\partial S[z]}{\partial z} \right|^2 \leq 0$$

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

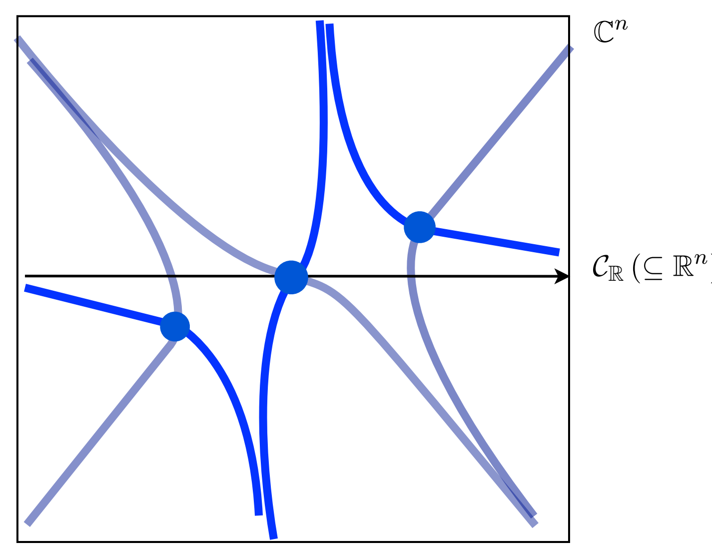


a simple example (n=1)

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



arg(κ)~0



arg(κ)~π

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

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

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

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

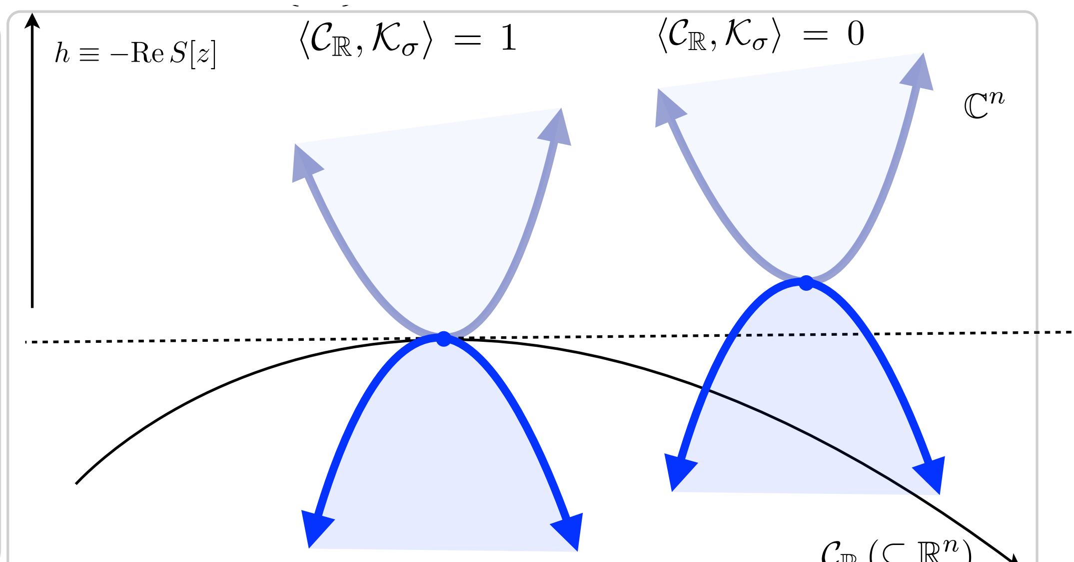
$\{z_\sigma\}$ satisfying $-\mathrm{Re}S[z_\sigma] > \max\{-\mathrm{Re}S[x]\}\ (x\in\mathcal{C}_\mathbb{R})$

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

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

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

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



Observables

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

It is not straightforward to compute the sum, in general

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

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

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

in the saddle point approximation

Since 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, and
It may give rise to **an extra phase factor** !
>> **residual sign problem**

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)

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

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

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

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

Geometric properties of Lefschetz thimbles

a) Tangent spaces of Lefschetz thimbles

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

<u>at a generic point z on $\mathcal{J}_\sigma$</u>

$$\frac{d}{dt}V_{zi}^\alpha(t)=\bar\partial_i\bar\partial_j\bar S[\bar z]\;\bar V_{zj}^\alpha(t)\qquad(\alpha=1,\cdots,n)$$

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

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

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

<u>In the vicinity of critical point z_σ</u>

linearized flow equation and its solution:

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

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

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

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

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

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

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

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

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

E is a real upper triangle matrix

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

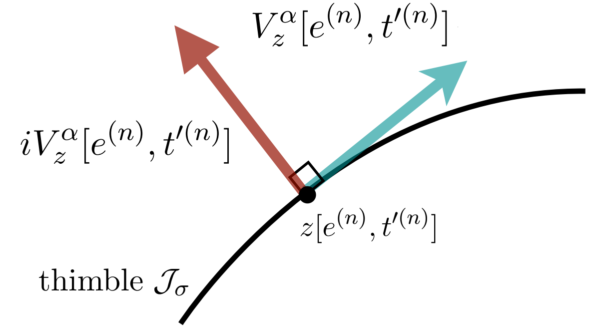
$$=\mathrm{Im}\{V_z^\alpha\partial^2S[z]V_z^\beta(t)+\bar V_z^\alpha\bar\partial^2\bar S[\bar z]\bar V_z^\beta(t)\}=0$$

b) Normal directions of thimbles

the set of normal vectors

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

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



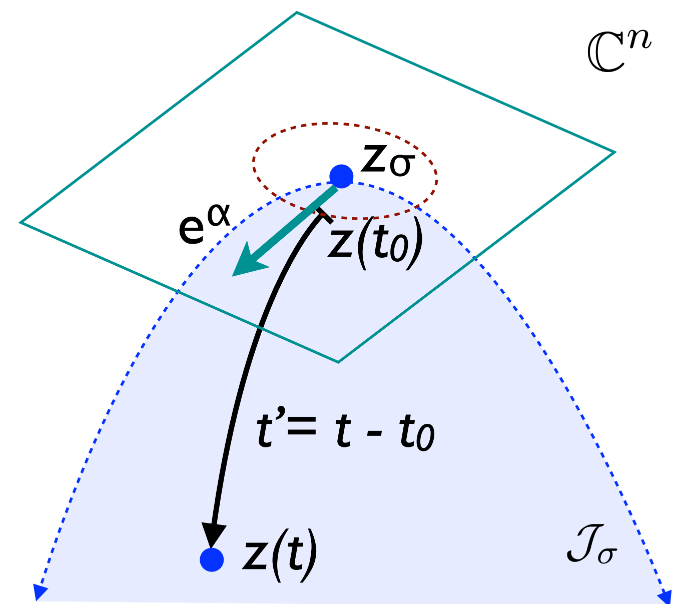
c) Parametrization of points z on thimbles

Asymptotic solutions of Flow equations

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

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

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



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

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

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

Algorithm of HMC on Lefschetz thimbles

the saddle-point structures !

a) To generate a thimble

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

solve the flow eqs. for **both z[e,t'] & V_z^{α}[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

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

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

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

$\{\langle \mathrm{e}^{i\phi_z} \rangle'_{\mathcal{J}_\sigma}\} (\sigma \in \Sigma)$ **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:

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

Constraints:

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

A conserved Hamiltonian:

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

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

b) To formulate/solve Molecular Dynamics on the thimble

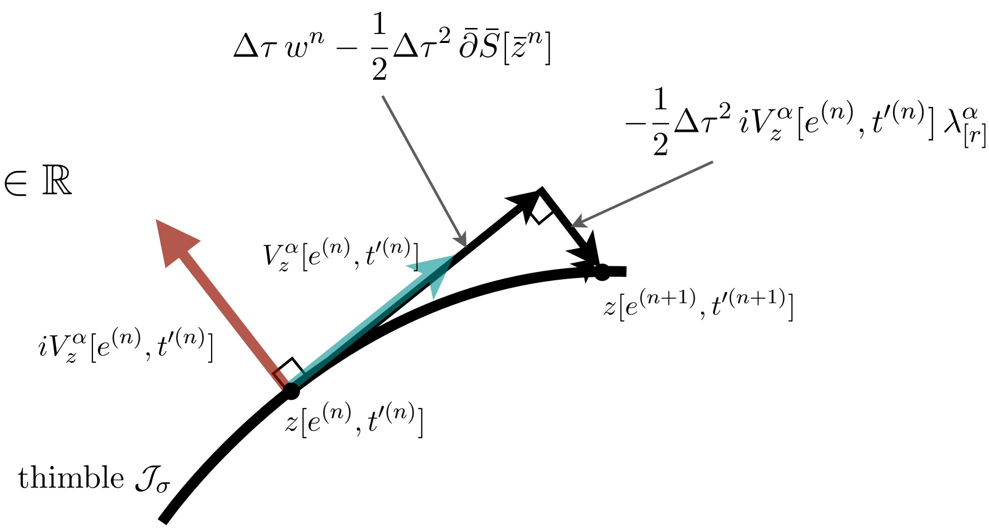
Second-order constraint-preserving symmetric integrator

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

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

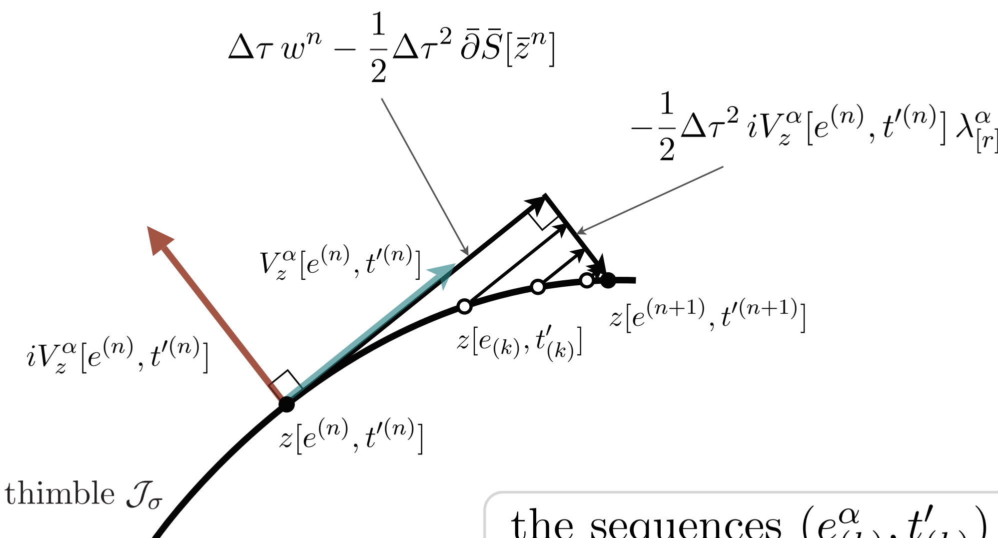
$\lambda_{[r]}^\alpha$ and $\lambda_{[v]}^\alpha$ are fixed by

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



the constraints to be solved

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



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

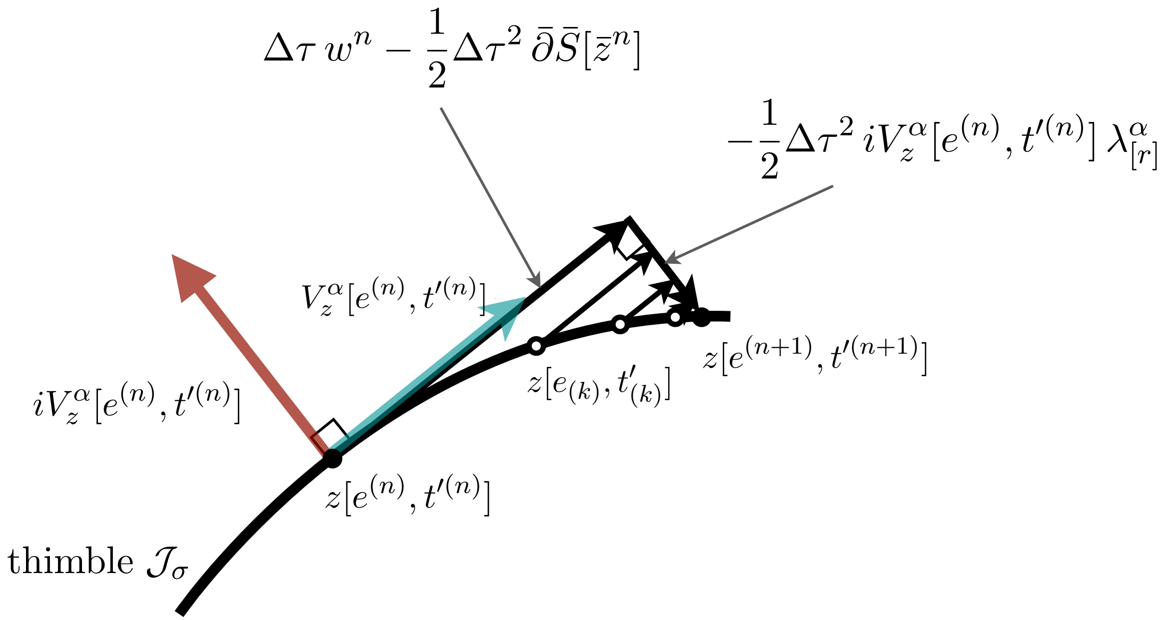
$$\Delta e^\alpha_{(k)} = e^\alpha_{(k+1)} - e^\alpha_{(k)}, \qquad \sum_{\alpha=1} \Delta e^\alpha_{(k)} e^{\alpha(n)} = 0,$$

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

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

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

the constraints to be solved



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

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 (ξ_i, η_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 $V_z^{-1}[e,t']$.

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

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

$$S = \sum_{x\in\mathbb{L}^4}\Big\{\big(\varphi^\dagger(x+\hat{0})e^{+\mu}-\varphi^\dagger(x)\big)\big(e^{-\mu}\varphi(x+\hat{0})-\varphi(x)\big) + \sum_{k=1}^{3}|\varphi(x+\hat{k})-\varphi(x)|^2+\frac{\kappa}{2}\varphi^\dagger(x)\varphi(x)+\frac{\lambda}{4}\big(\varphi^\dagger(x)\varphi(x)\big)^2\Big\}$$

$$= \sum_{x\in\mathbb{L}^4}\Big\{-\phi_a(x)\phi_b(x+\hat{0})\big[\delta_{ab}\cosh(\mu)-i\epsilon_{ab}\sinh(\mu)\big] - \sum_{k=1}^{3}\phi_a(x)\phi_a(x+\hat{k})+\frac{(8+\kappa)}{2}\phi_a(x)\phi_a(x)+\frac{\lambda}{4}\big(\phi_a(x)\phi_a(x)\big)^2\Big\}$$

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

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

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

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

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

L=4 (, ... 12)

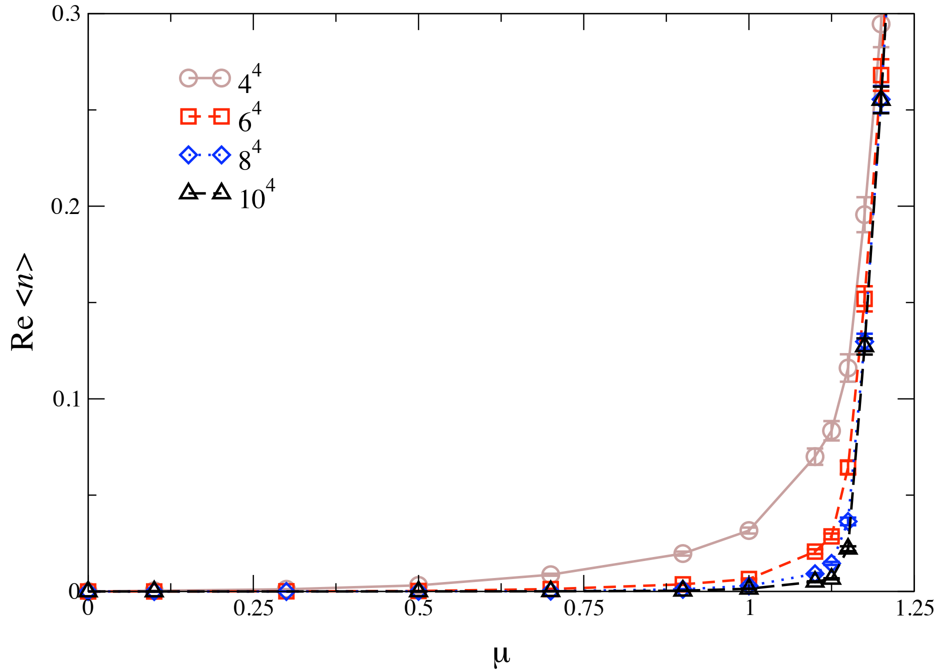
K=1.0, λ=1.0, μ=0.0~1.8

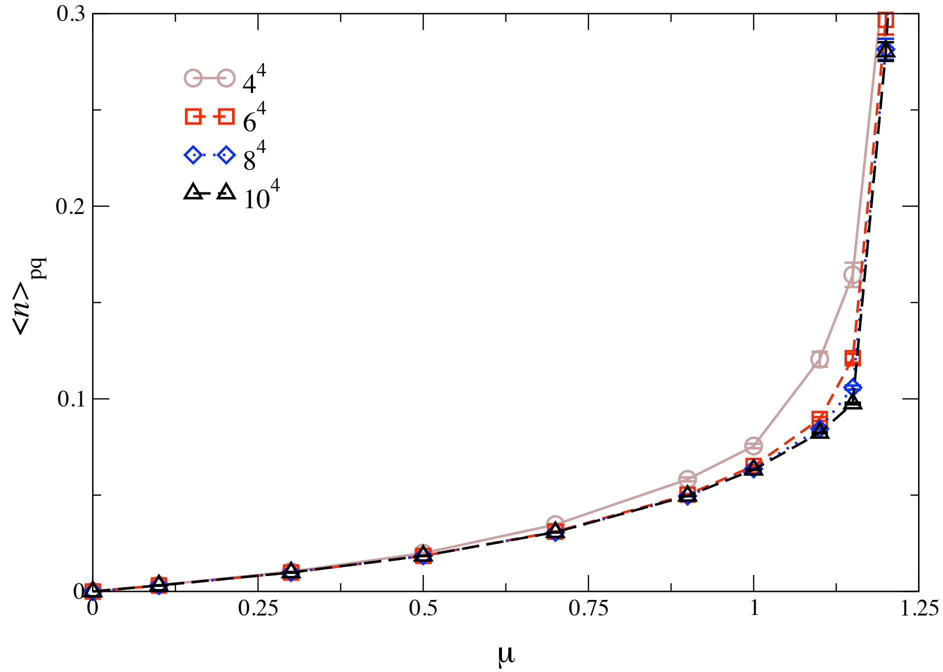
cf. G. Aarts PRL 102(2009) 131601 (Complex Langevin simulation)

SILVER BLAZE AND THE SIGN PROBLEM

COMPLEX VS PHASE QUENCHED

density



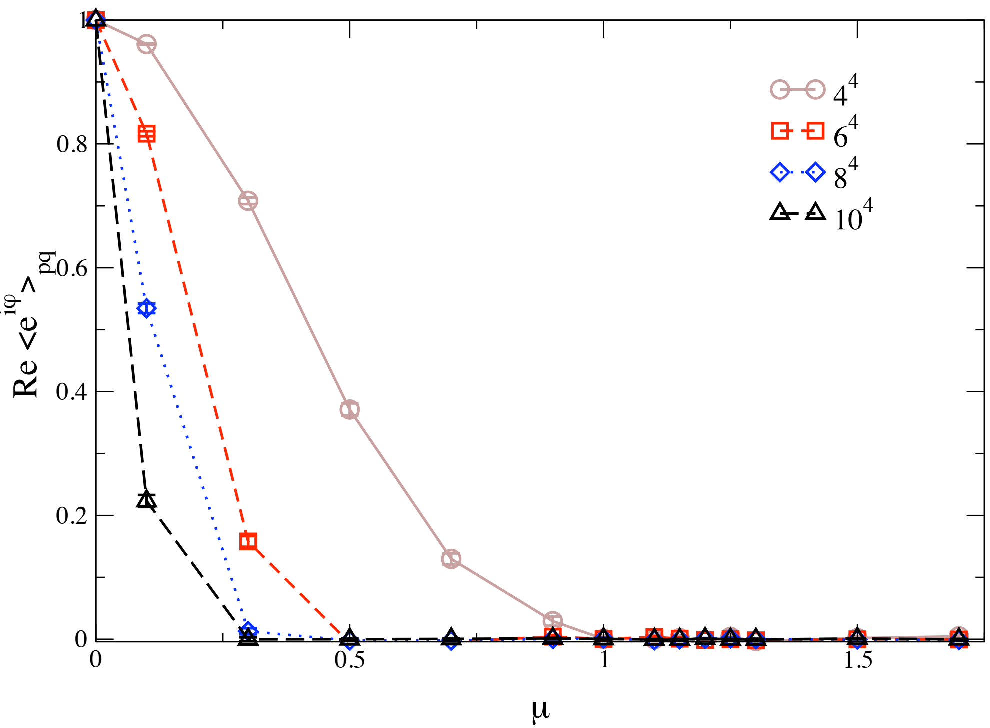


complex　　　　phase quenched

phase $e^{i\varphi} = e^{-S}/|e^{-S}|$ does precisely what is expected cf. G. Aarts PRL 102(2009) 131601 (Complex Langevin simulation)

HOW SEVERE IS THE SIGN PROBLEM?

AVERAGE PHASE FACTOR



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

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 $\mu \leq \tilde{\mu}_c$,

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

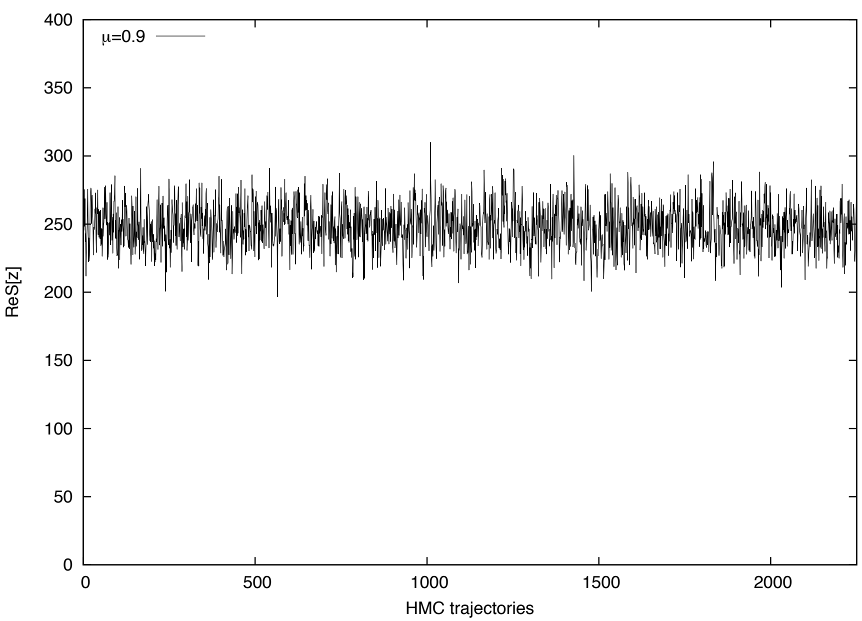
   (b) $z_1 = \phi_0\cos\theta,\ z_2 = \phi_0\sin\theta\ ;\ S[z] = -L^4\frac{\lambda_0}{4}\phi_0^4,$ → the thimble 2-(b)
   where $\phi_0 = \sqrt{\frac{-\left(1-6K_0-2K_0\cosh(\mu)\right)}{\lambda_0}}$.

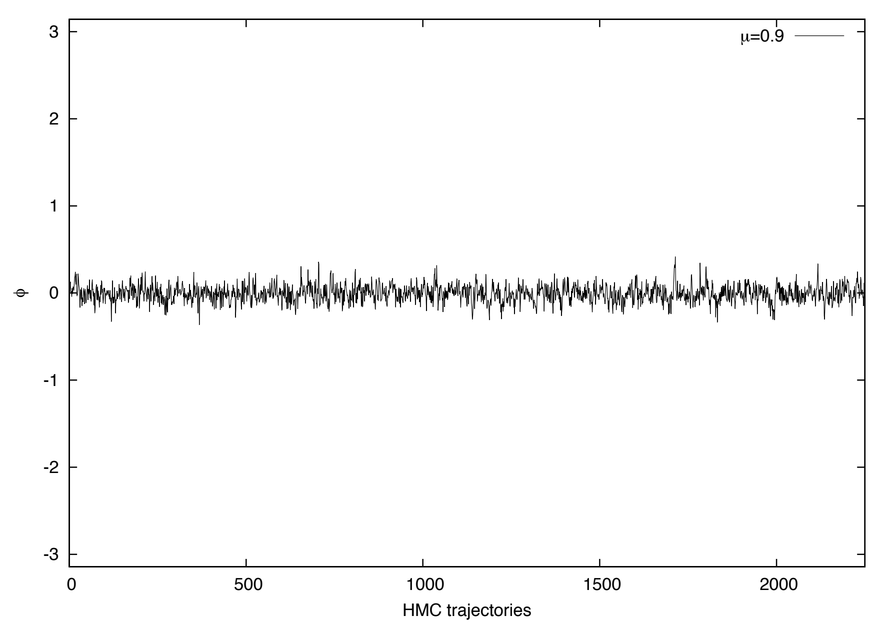
HMC on the thimble 1-(a) $\mu < \tilde{\mu}_c$

simulation parameters :

	Parameters	Resulting conditions
Thimble (Solving flow eqs.)	$t_0 = -5.0$ $n_{\rm lefs} = 100$ $h = t'/n_{\rm lefs} \simeq 0.05$	$\lvert {\rm Re}\big(S[z(t_0)] - S[z_{\rm vac}]\big)\rvert \lesssim 1.0$ $\lvert {\rm Im} S[z]\rvert \lesssim 1.0 \times 10^{-4}$ $\lVert \bar{\partial}\bar{S} - V^\alpha \kappa^\alpha e^\alpha \rVert^2 / 2V \leq 1.0 \times 10^{-4}$
Molecular Dynamics (Solving constraint)	$\tau_{\rm traj} = 1.0$ $n_{\rm step} = 20$ $\Delta\tau = 0.05$ $\epsilon' = 1.0 \times 10^{-3}$	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		$\tau_{\rm int} \simeq 2$ for ${\rm Re} S[z]$ $\tau_{\rm int} \simeq 3$ for ϕ_z

HMC histories (μ = 0.9)

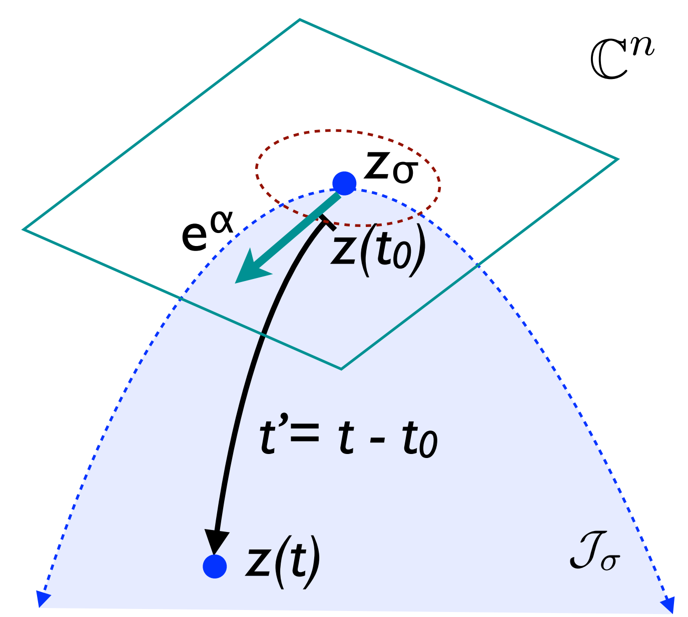




c) Parametrization of points z on thimbles

Asymptotic solutions of Flow equations

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



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

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

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

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

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

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

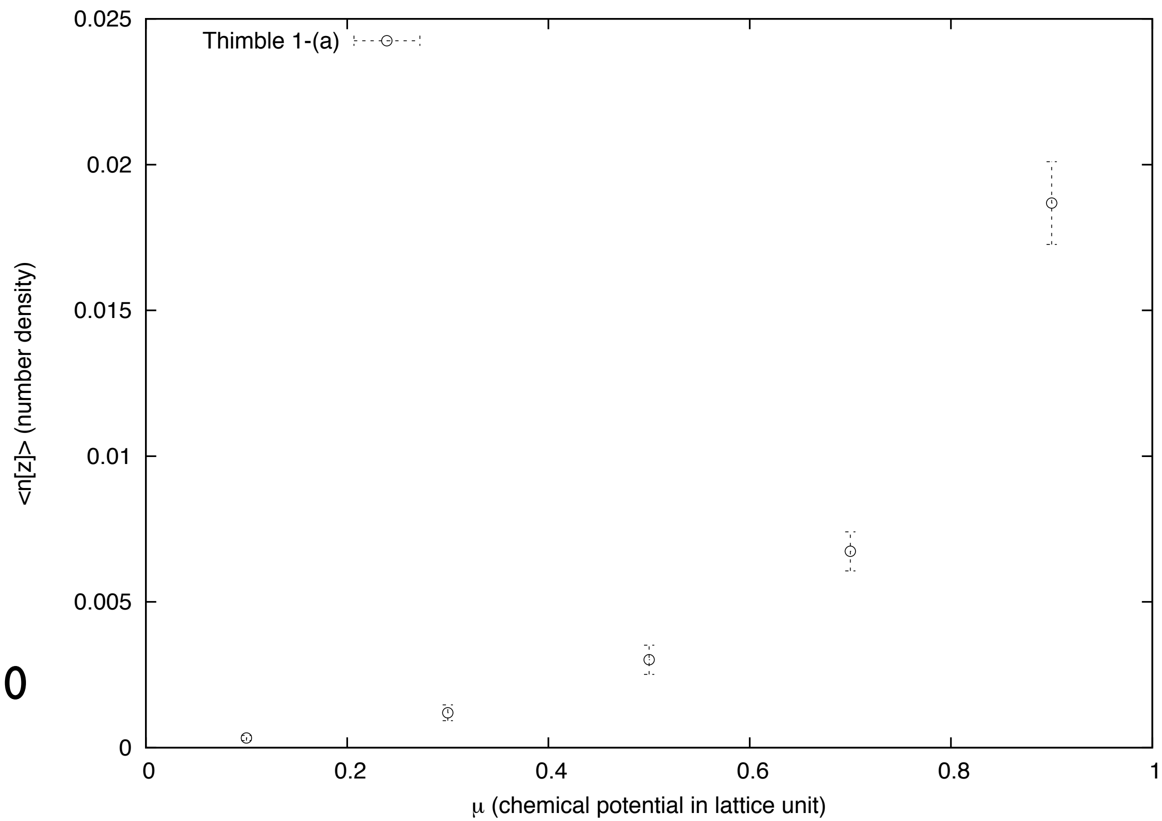
residual phase averages:

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

number density :

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

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



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

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

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

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

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

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

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

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

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

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

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

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

simulation parameters :

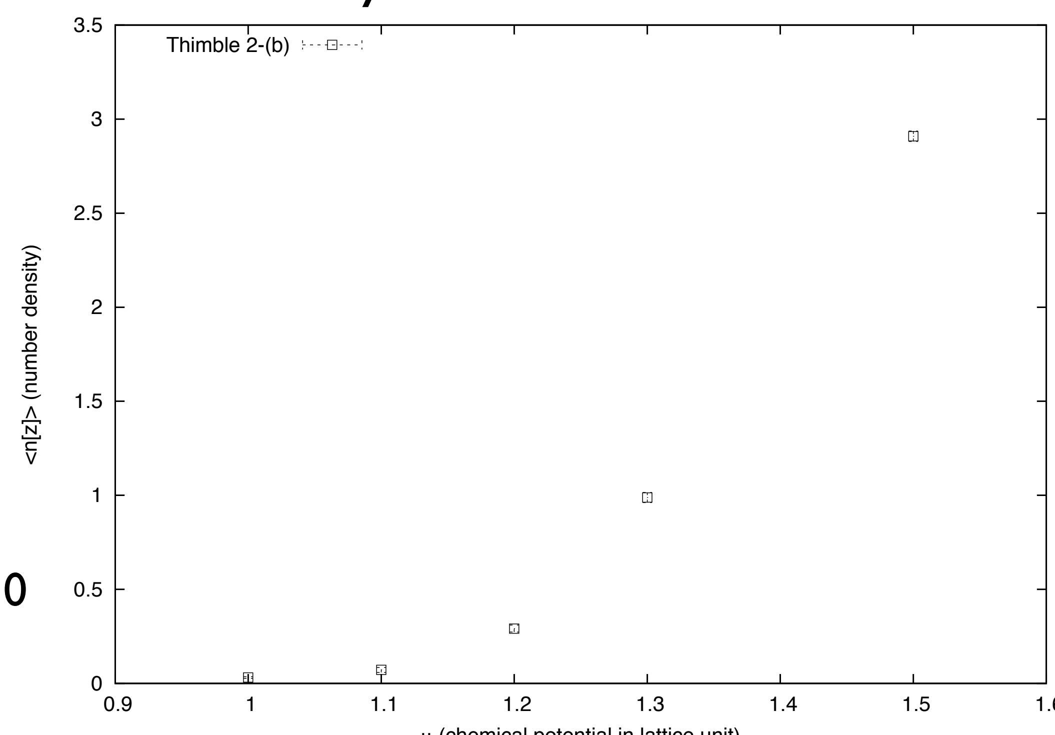
	Parameters	Resulting conditions
Thimble	$t_0 = -3.0$ $n_{\mathrm{lefs}} = 100$ $h = t'/n_{\mathrm{lefs}} \simeq 0.03$	$\lvert\mathrm{Re}\big(S[z(t_0)] - S[z_{\mathrm{vac}}]\big)\rvert \lesssim 2.0 \times 10^1$ $\lvert\mathrm{Im}(S[z] - S[z_{\mathrm{vac}}])\rvert \lesssim 5.0 \times 10^{-2}$ $\lVert\bar{\partial}\bar{S}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

residual phase averages:

μ	$\langle \mathrm{e}^{i\phi_z} \rangle'_{\mathcal{J}_{\mathrm{vac}}}$
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)

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

number density :



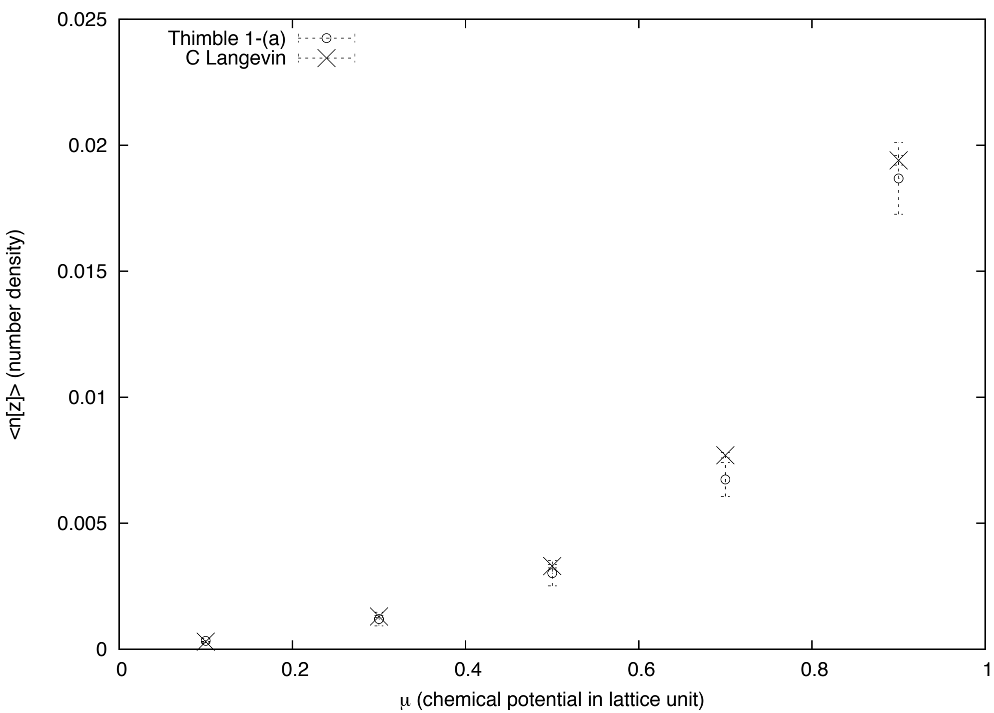
Comparison to Complex Langevin simulations

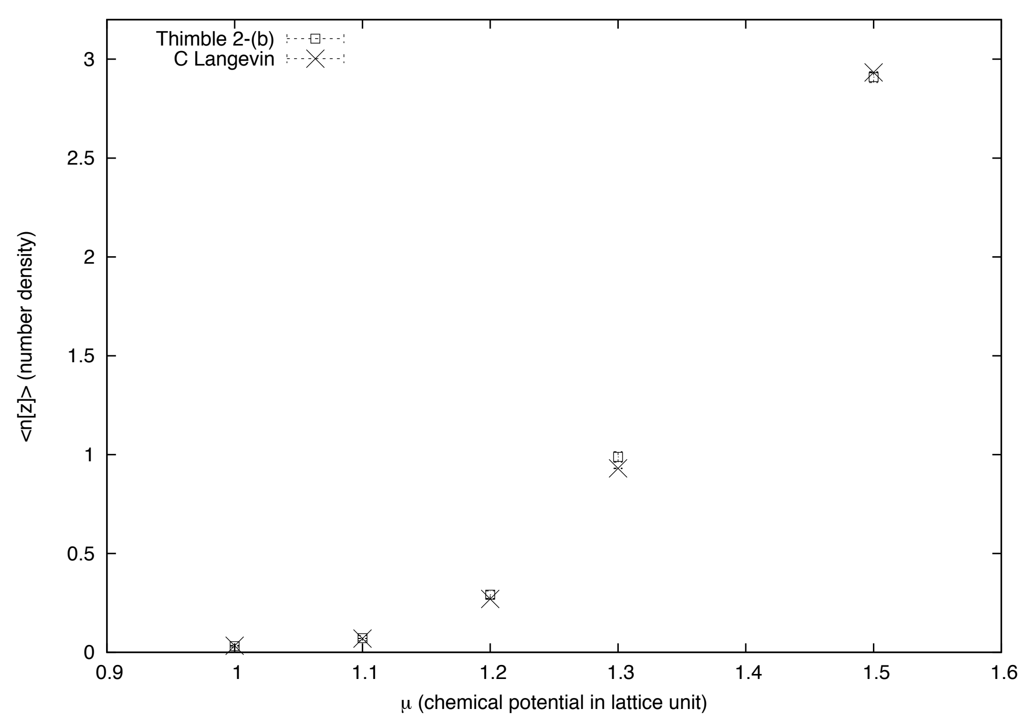
$$\frac{dz(t)}{dt} = -\frac{\partial S[z]}{\partial z} + \eta(t); \quad < \eta(t)\eta(t') >= 2\delta(t-t')$$

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

parameters of CL simulations:
  step size ε=5.0 x 10^{-5} , 5,000,000 time steps
  sampling 10,000 configurations with the separation of 500

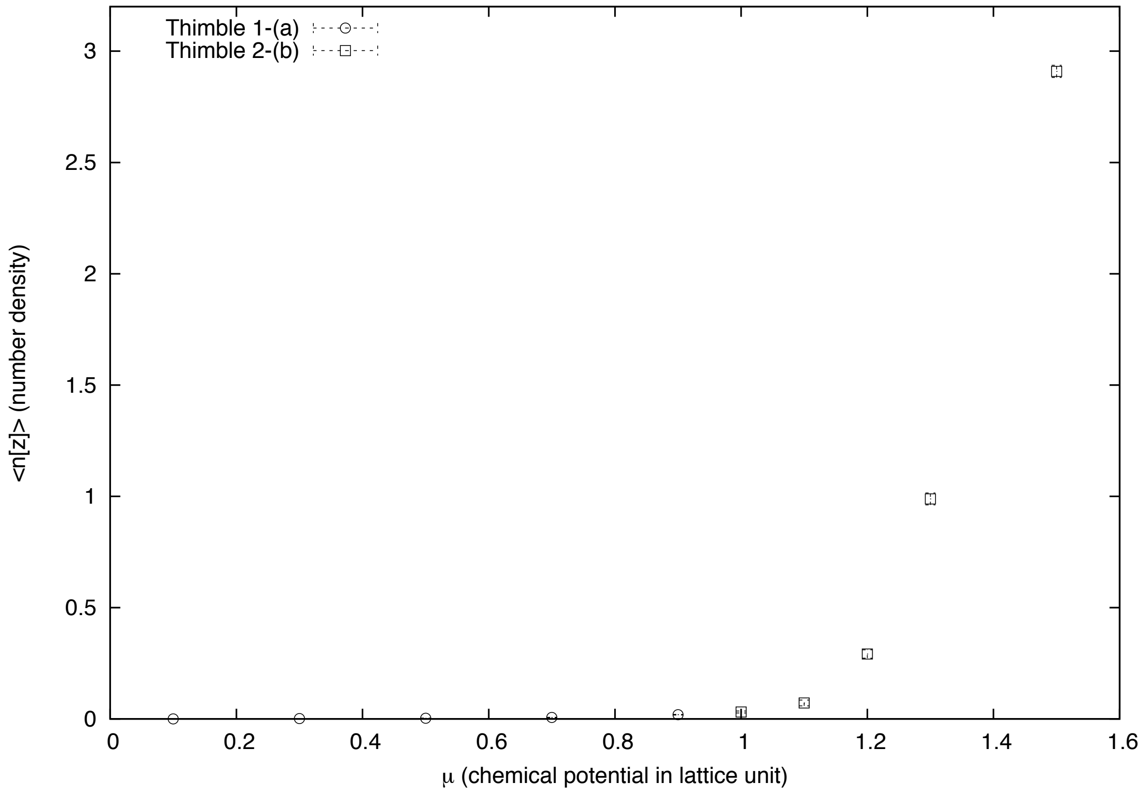
number density :





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

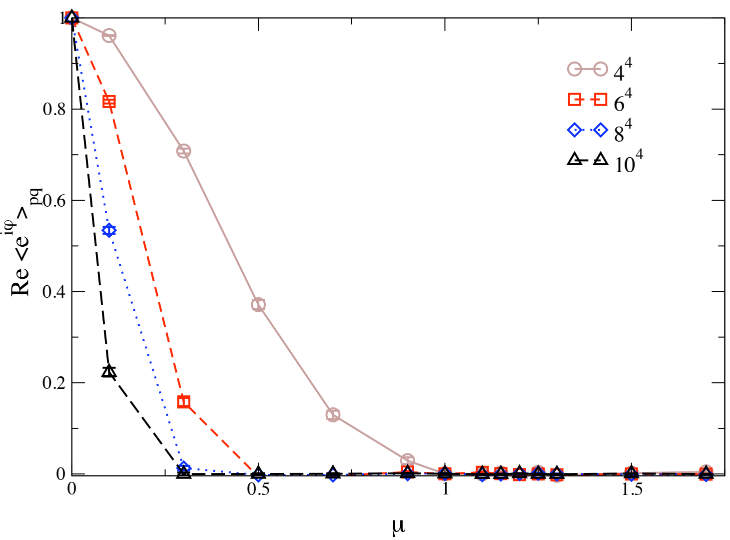
number density :



μ	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



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 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.
    - $O(V^2 \times n_{Lefs} \times n_{step})$ (tangent vectors), $O(V^3 \times n_{step})$ (V^{-1}, detV)
- Possible applications to QCD_μ cf. D. Sexty, arXiv:1307.7748