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

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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 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)*]

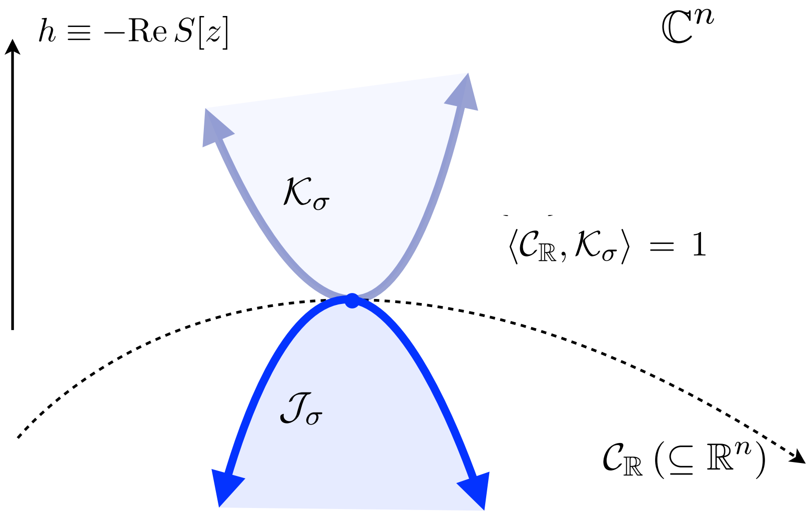
$$\mathcal{C}_{\mathbb{R}} = \sum_{\sigma \in \Sigma} n_\sigma \mathcal{J}_\sigma, \qquad n_\sigma = \langle \mathcal{C}_{\mathbb{R}}, \mathcal{K}_\sigma \rangle$$

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

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

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 -∞



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

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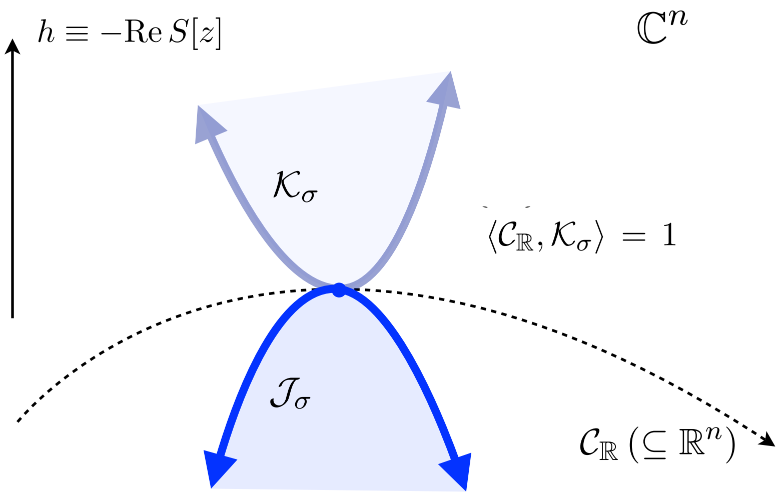
$$\frac{d}{dt} h = -\frac{1}{2} \left\{ \frac{\partial S[z]}{\partial z} \cdot \frac{d}{dt} z(t) + \frac{\partial \bar{S}[\bar{z}]}{\partial \bar{z}} \cdot \frac{d}{dt} \bar{z}(t) \right\} = - \left| \frac{\partial S[z]}{\partial z} \right|^2 \leq 0$$

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



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

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

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

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

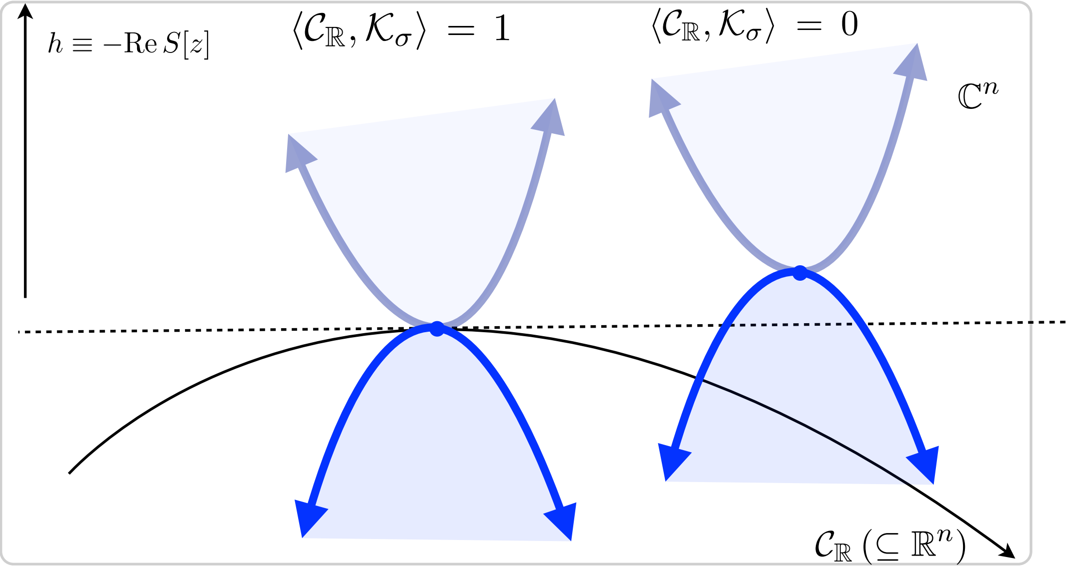
$\{z_\sigma\}$ satisfying $-\mathrm{Re}S[z_\sigma] > \max\{-\mathrm{Re}S[x]\}\ (x \in \mathcal{C}_\mathbb{R})$

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

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

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

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



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

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It is not straightforward to compute the sum, in general

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

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

in the saddle point approximation

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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

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

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

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

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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

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

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

Geometric properties of Lefschetz thimbles

a) Tangent spaces of Lefschetz thimbles

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

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

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

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

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

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

In the vicinity of critical point z$_\sigma$

linearized flow equation and its solution:

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

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

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

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

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

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

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

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

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

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

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

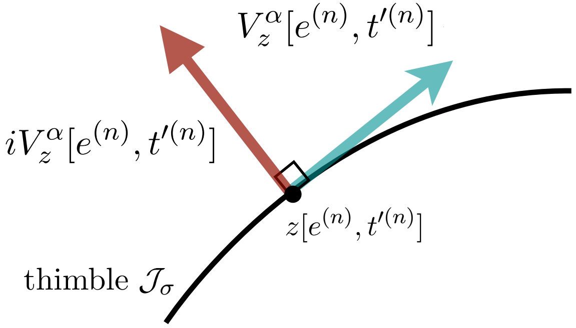
E is a real upper triangle matrix

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

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

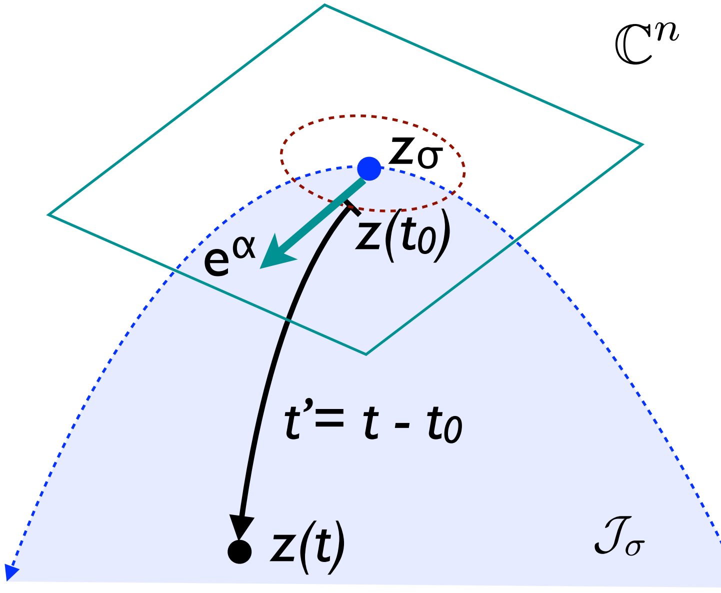
the **direction** of the flow : $e^\alpha \ (\alpha = 1, \cdots, n; \|e\|^2 = n)$

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

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

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

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



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

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

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

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

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

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

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numerically very demanding !

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

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

Constraints:

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

A conserved Hamiltonian:

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

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

b) To formulate/solve Molecular Dynamics on the thimble

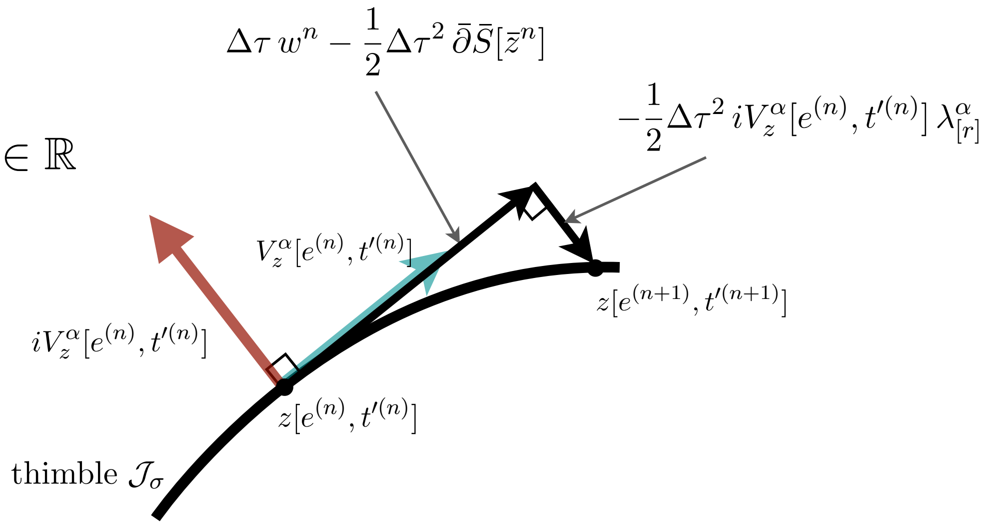
Second-order constraint-preserving symmetric integrator

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

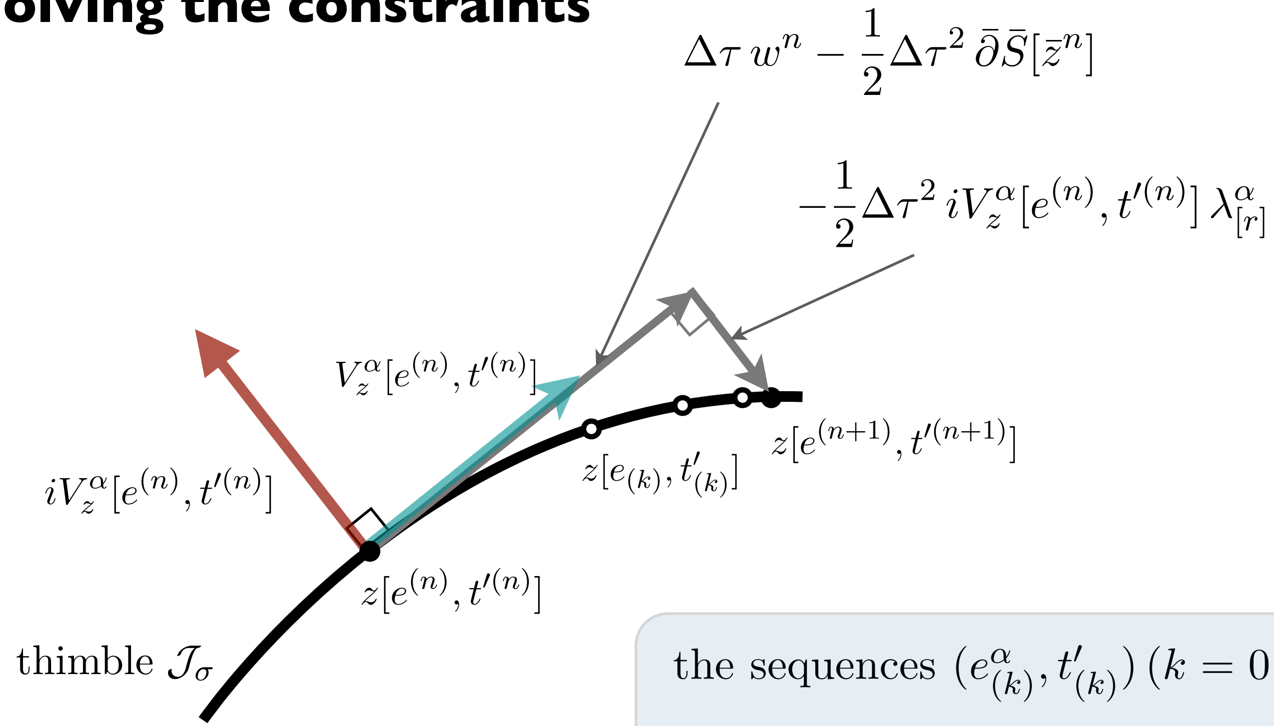
$$
\begin{aligned}
w^{n+1/2} &= w^n \quad - \frac{1}{2}\Delta\tau\, \bar\partial \bar S[\bar z^n] \quad - \frac{1}{2}\Delta\tau\, i V_z^\alpha[e^{(n)}, t'^{(n)}]\, \lambda^\alpha_{[r]},\\
z^{n+1} &= z^n \quad + \Delta\tau\, w^{n+1/2},\\
w^{n+1} &= w^{n+1/2} - \frac{1}{2}\Delta\tau\, \bar\partial \bar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

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

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



Solving the constraints



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

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

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

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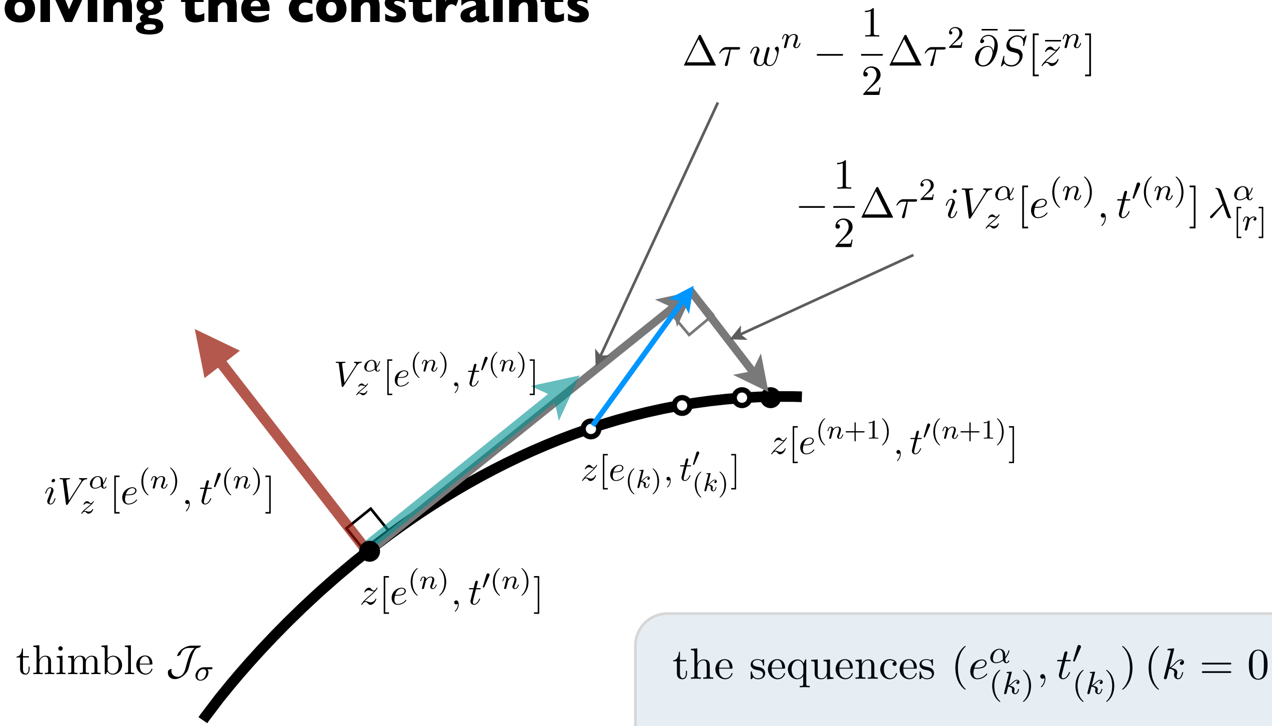

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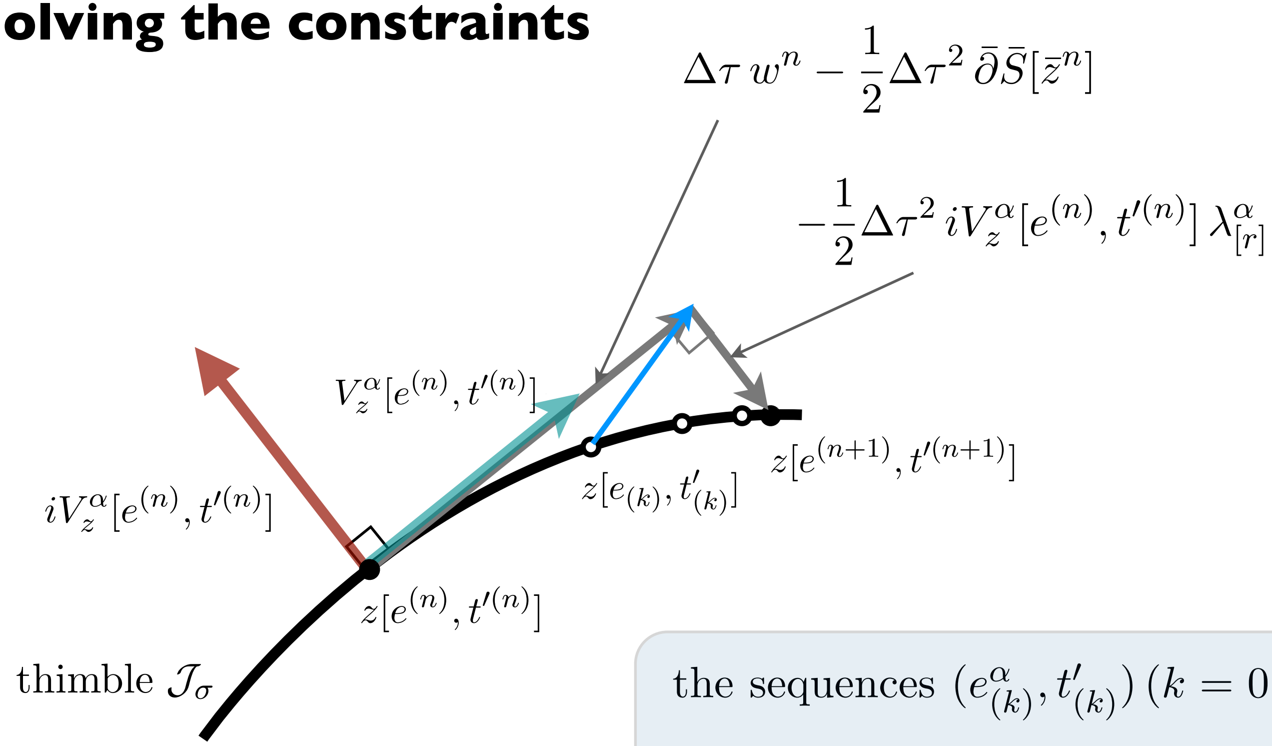

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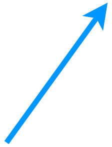
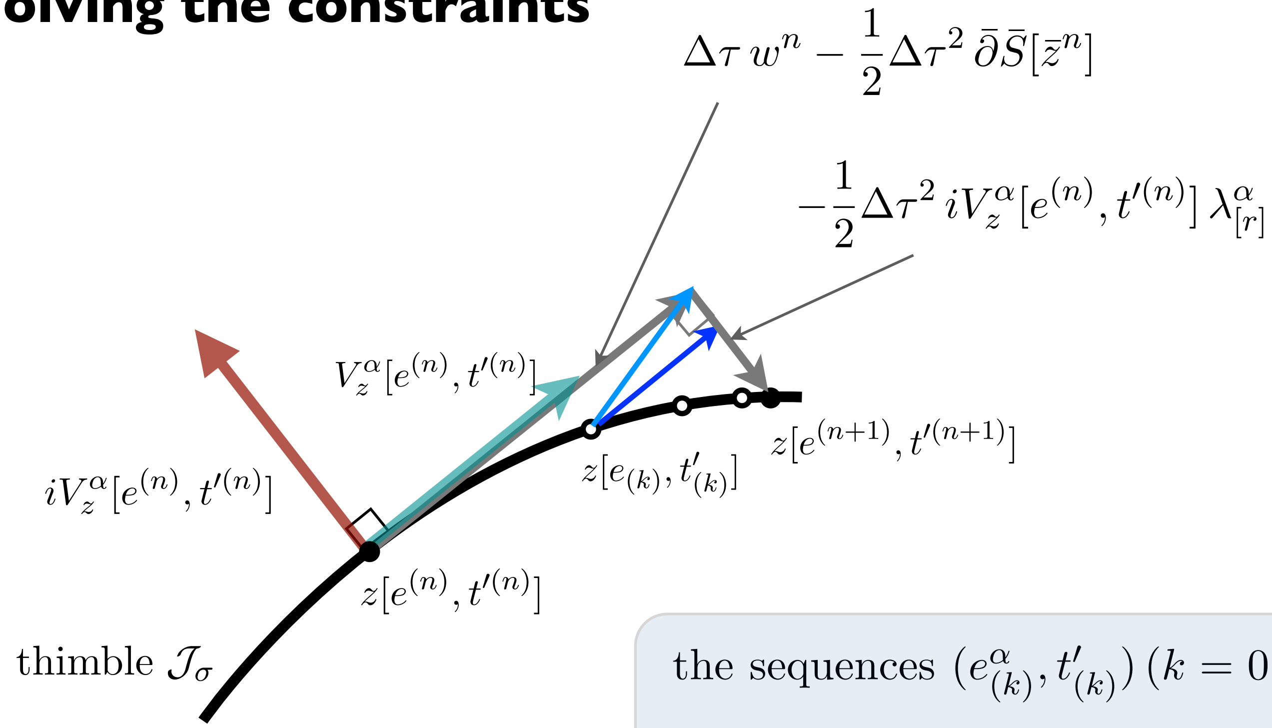


$$\Delta z_{(k)}[e^{(n)}, t'^{(n)}] \equiv z_i[e^{(n)}, t'^{(n)}] + \Delta\tau\, w_i^n - \frac{1}{2}\Delta\tau^2\, \bar\partial_i \bar S[\bar z^n] - z_i[e_{(k)}, t'_{(k)}]$$

Solving the constraints



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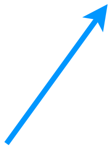
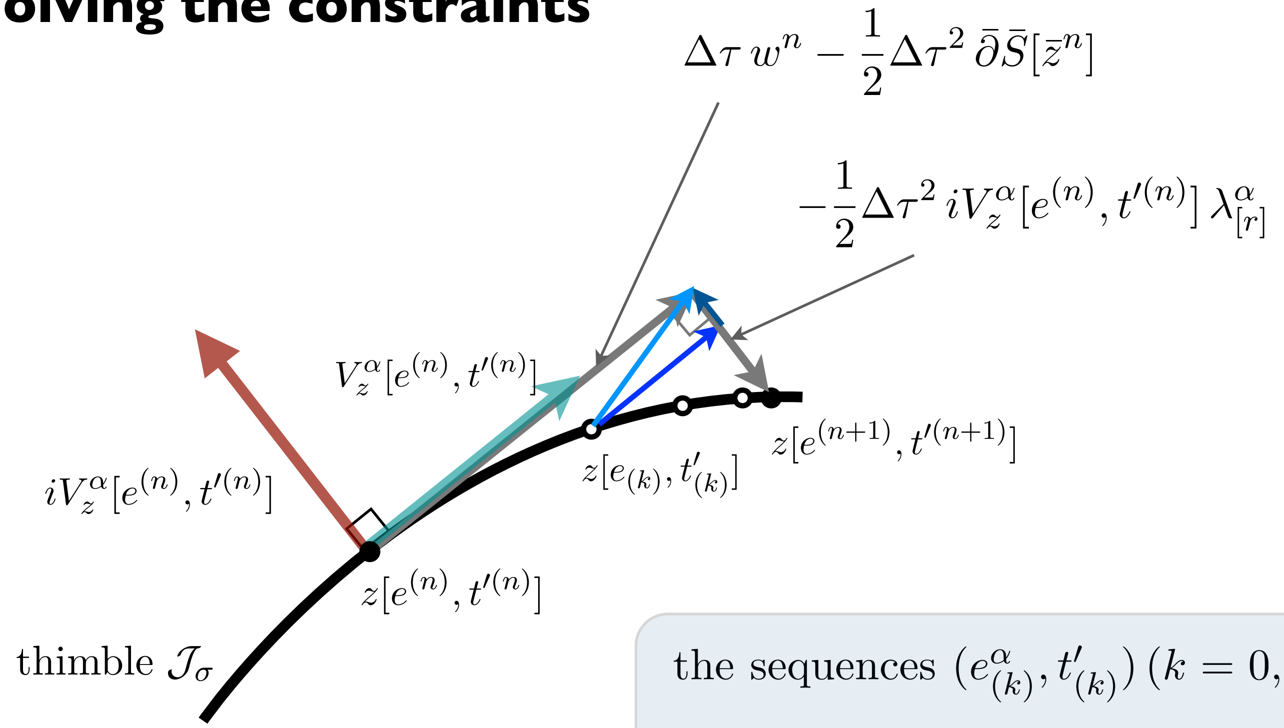


$$\Delta z_{(k)}[e^{(n)}, t'^{(n)}] \equiv z_i[e^{(n)}, t'^{(n)}] + \Delta\tau\, w^n_i - \frac{1}{2}\Delta\tau^2\, \bar\partial_i \bar S[\bar z^n] - z_i[e_{(k)}, t'_{(k)}]$$

Solving the constraints



$\Delta\tau\, w^n - \frac{1}{2}\Delta\tau^2\, \bar\partial \bar S[\bar z^n]$

$-\frac{1}{2}\Delta\tau^2\, iV_z^\alpha[e^{(n)}, t'^{(n)}]\, \lambda^\alpha_{[r]}$

$V_z^\alpha[e^{(n)}, t'^{(n)}]$

$iV_z^\alpha[e^{(n)}, t'^{(n)}]$

$z[e_{(k)}, t'_{(k)}]$

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

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

thimble $\mathcal{J}_\sigma$

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

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

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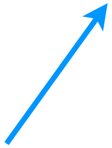
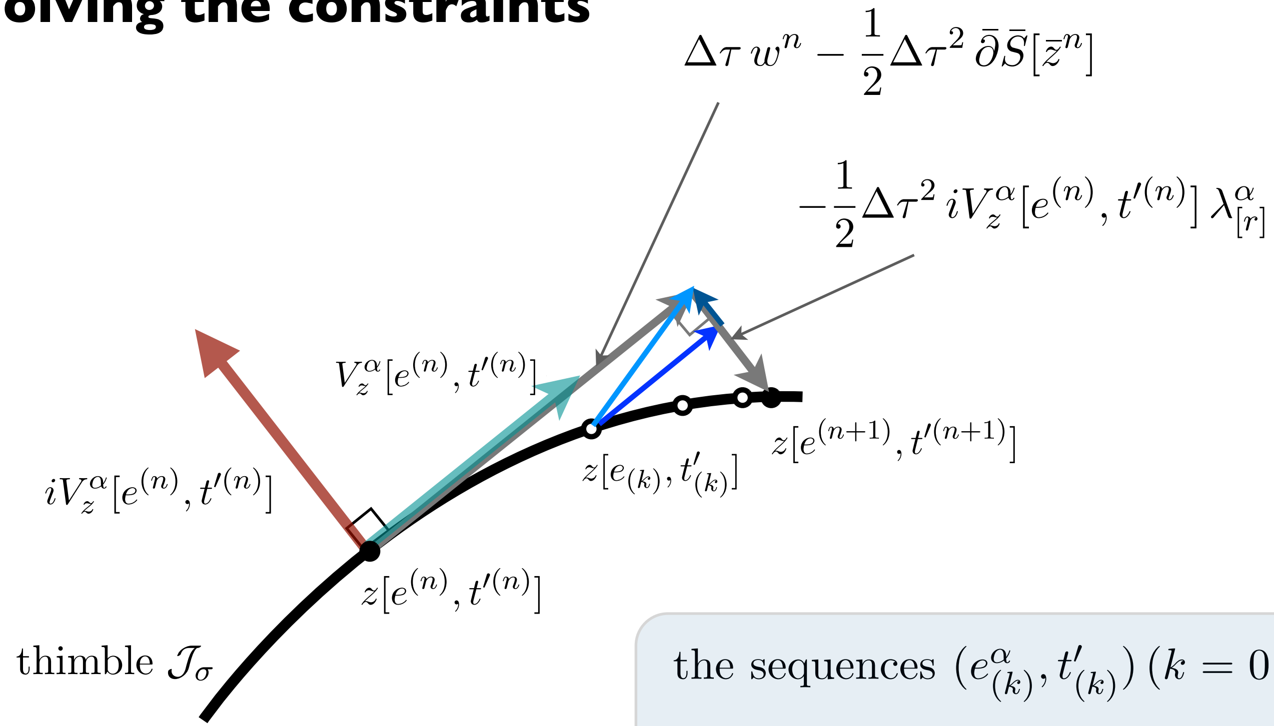


$$\Delta z_{(k)}[e^{(n)}, t'^{(n)}] \equiv z_i[e^{(n)}, t'^{(n)}] + \Delta\tau\, w_i^n - \frac{1}{2}\Delta\tau^2\, \bar\partial_i \bar S[\bar z^n] - z_i[e_{(k)}, t'_{(k)}]$$

Solving the constraints



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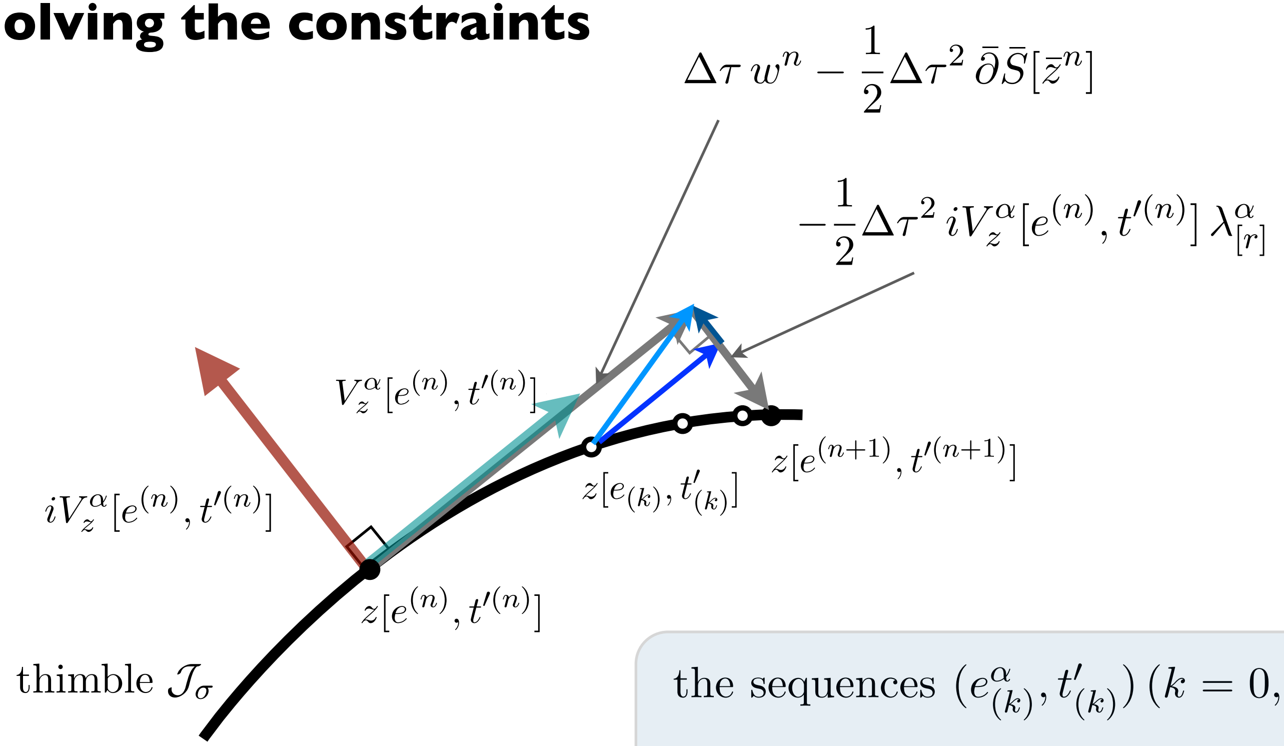
Solving the constraints



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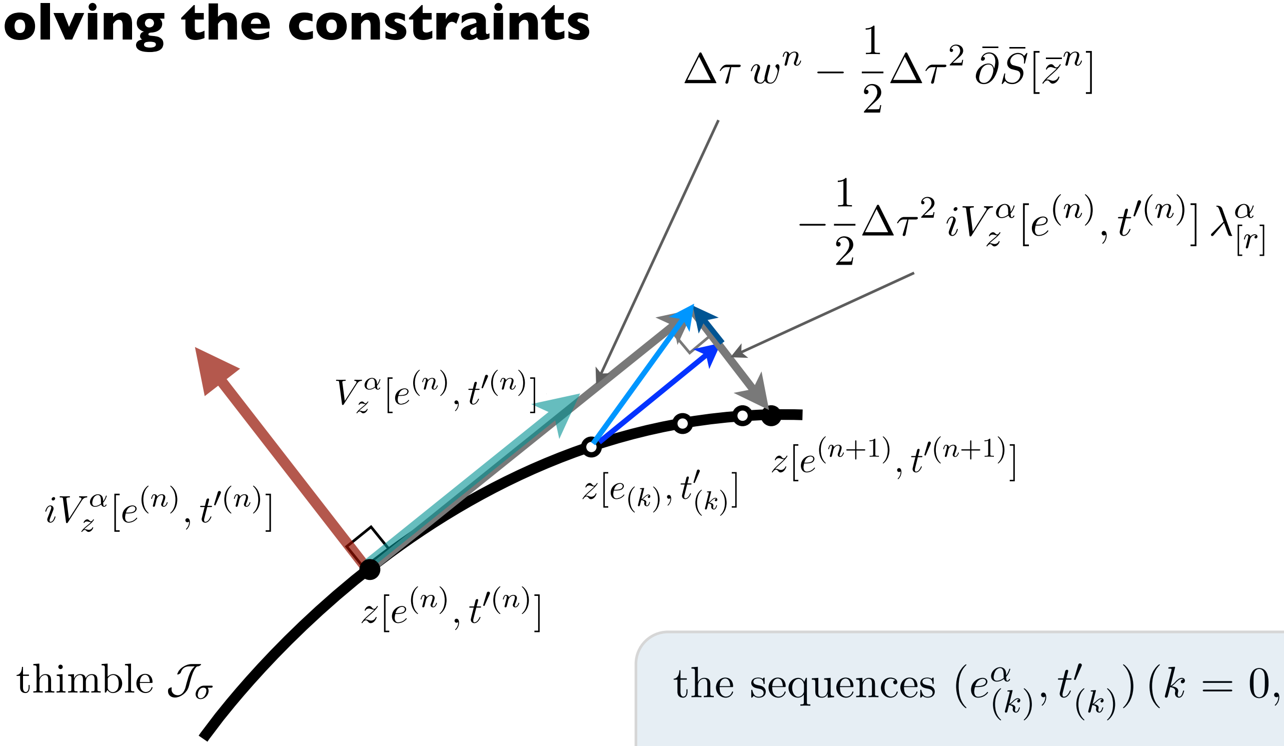
↖ $$\Delta z_{(k)}[e^{(n)}, t'^{(n)}]_{\perp} = iV^\alpha_z[e^{(n)}, t'^{(n)}]\Big(\frac{1}{2}\Delta\tau^2\, \lambda^\alpha_{[r](k)}\Big)$$

Solving the constraints



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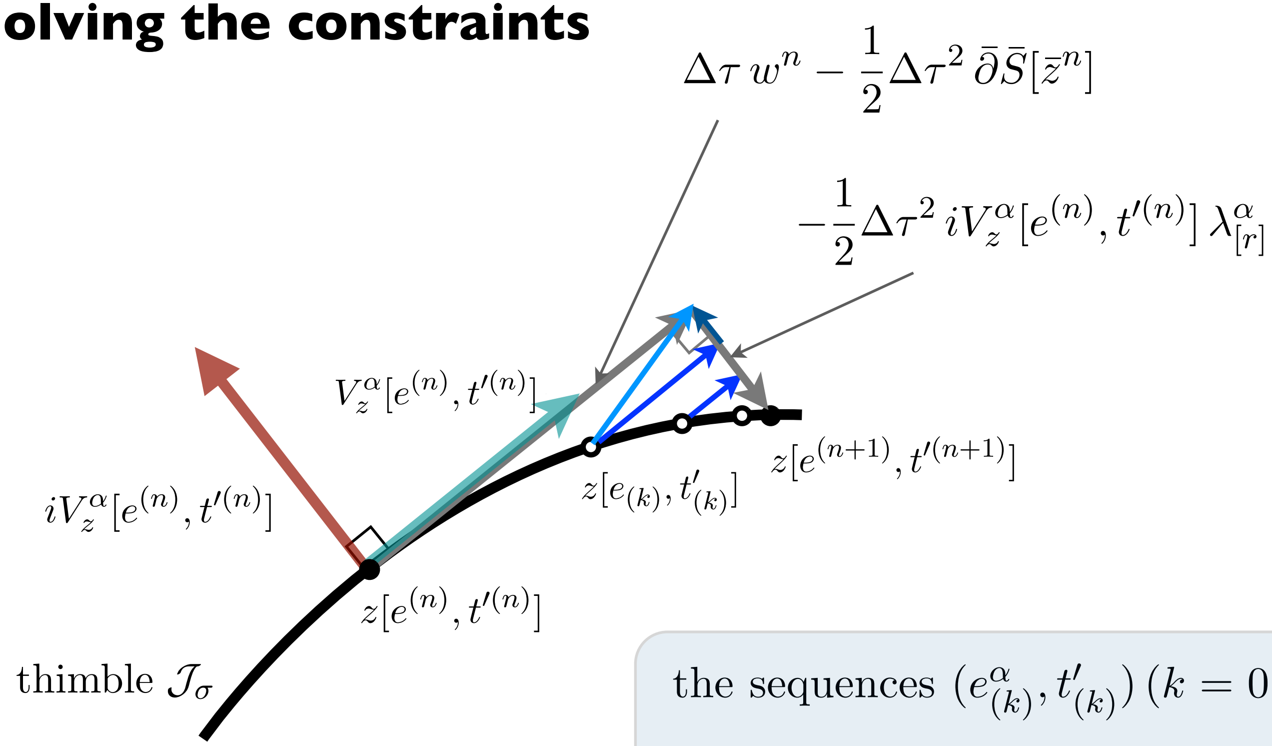
$$\Big\| V^\alpha_z[e^{(n)}, t'^{(n)}]\big(\Delta e^\alpha{}_{(k)} + e^{\alpha(n)}\kappa^\alpha \Delta t'_{(k)}\big)\Big\|^2 \le n\,\epsilon'^2$$

Solving the constraints



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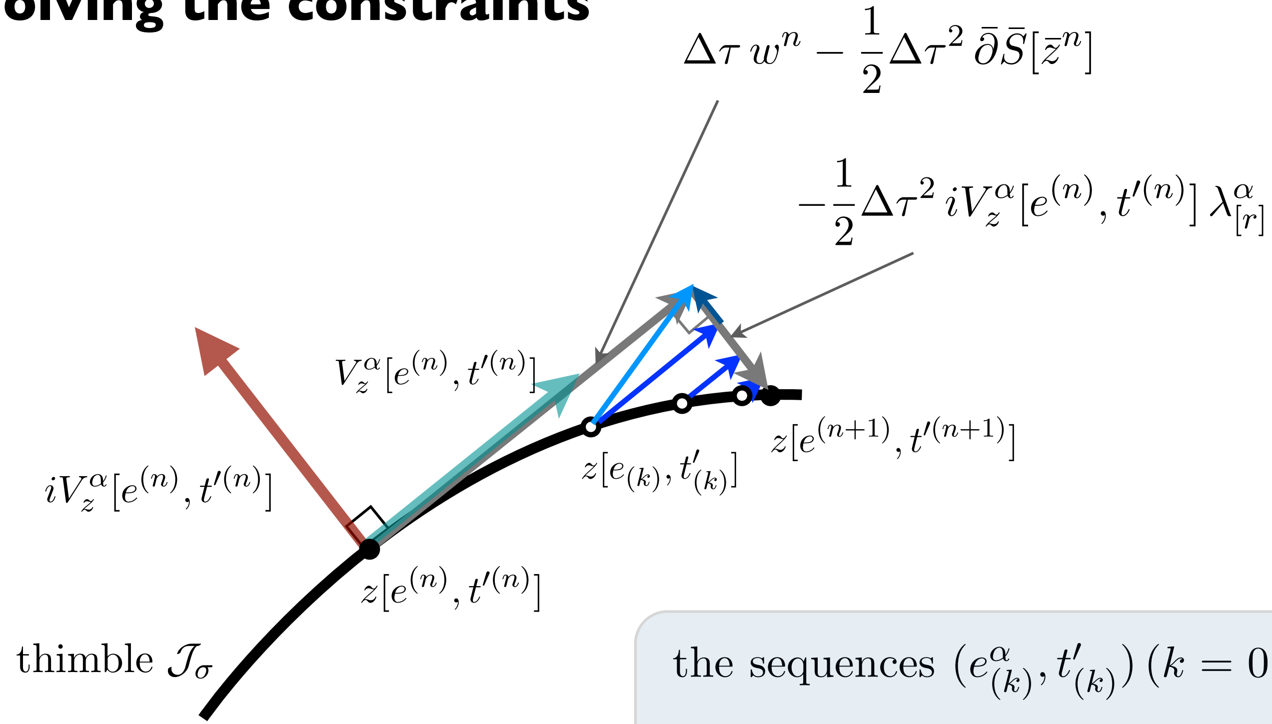
Solving the constraints



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

the constraints to be solved

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

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

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

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

where

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

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

stopping cond. :

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

$$\frac{1}{2}\Delta\tau\,\lambda^\alpha_{[v]} = \mathrm{Im}\Big[\{V_z^{-1}[e^{(n+1)},t'^{(n+1)}]\}^\alpha_i \big(w_i^{n+1/2} - \frac{1}{2}\Delta\tau\,\bar\partial_i\bar S[\bar z^{n+1}]\big)\Big]$$

a HMC update

A hybrid Monte Carlo update then consists of the following steps for a given trajectory length τ_{traj} and a number of steps n_{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_{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 $\eta^{\alpha}(\alpha = 1, \cdots, n)$, 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

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

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

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

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

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

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

K=1.0, λ=1.0, μ=0.0~1.8

L=4 (, ... 12)

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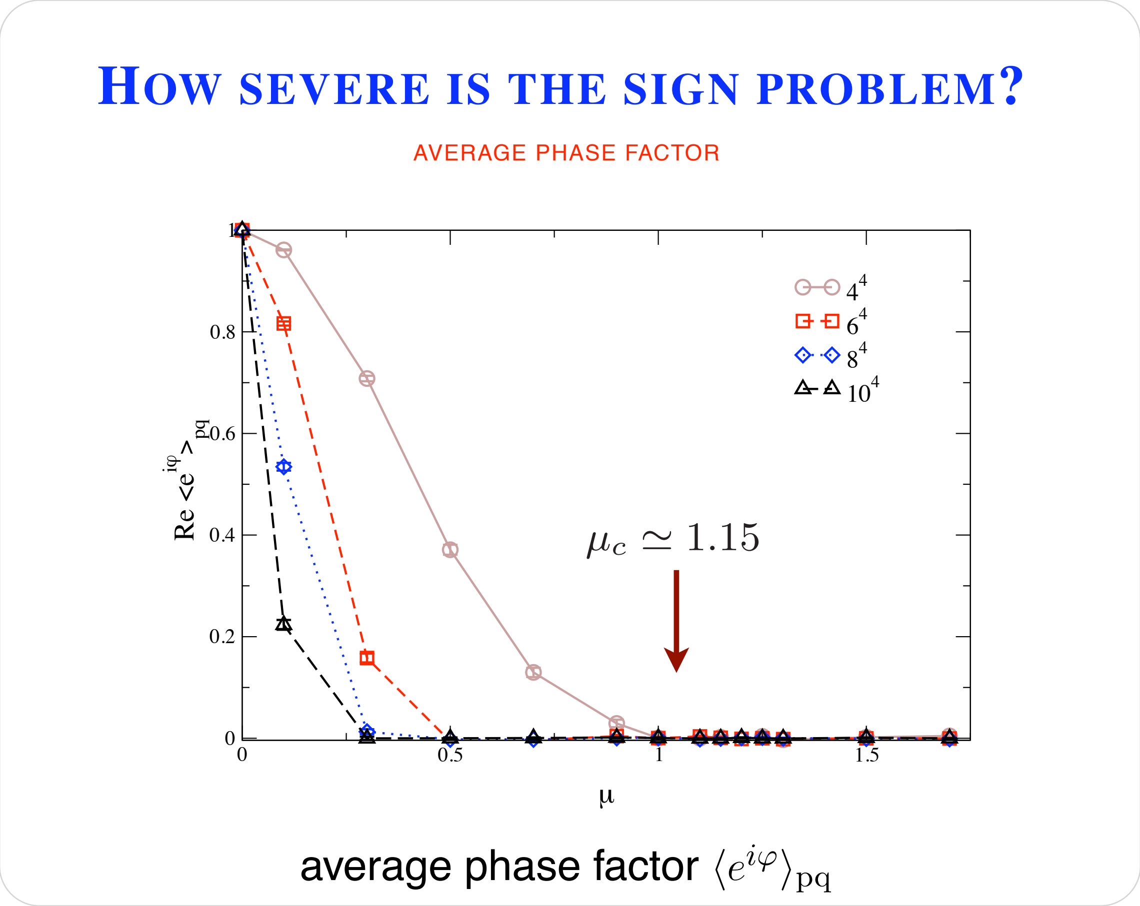
$$-K_0 \, z_a(x) z_b(x + \hat{0}) \big[\delta_{ab} \cos$$

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



How severe is the sign problem?

AVERAGE PHASE FACTOR

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

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

Kyoto, January 2010 – p.28

K=1.0, λ=1.0, μ=0.0~1.8

L=4 (, ... 12)

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

μ_c ~0.962 for K=1.0, λ=1.0

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) $z_1 = z_2 = 0\ ;\quad S[z]=0,$ ← the thimble 2-(a)
   - (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)

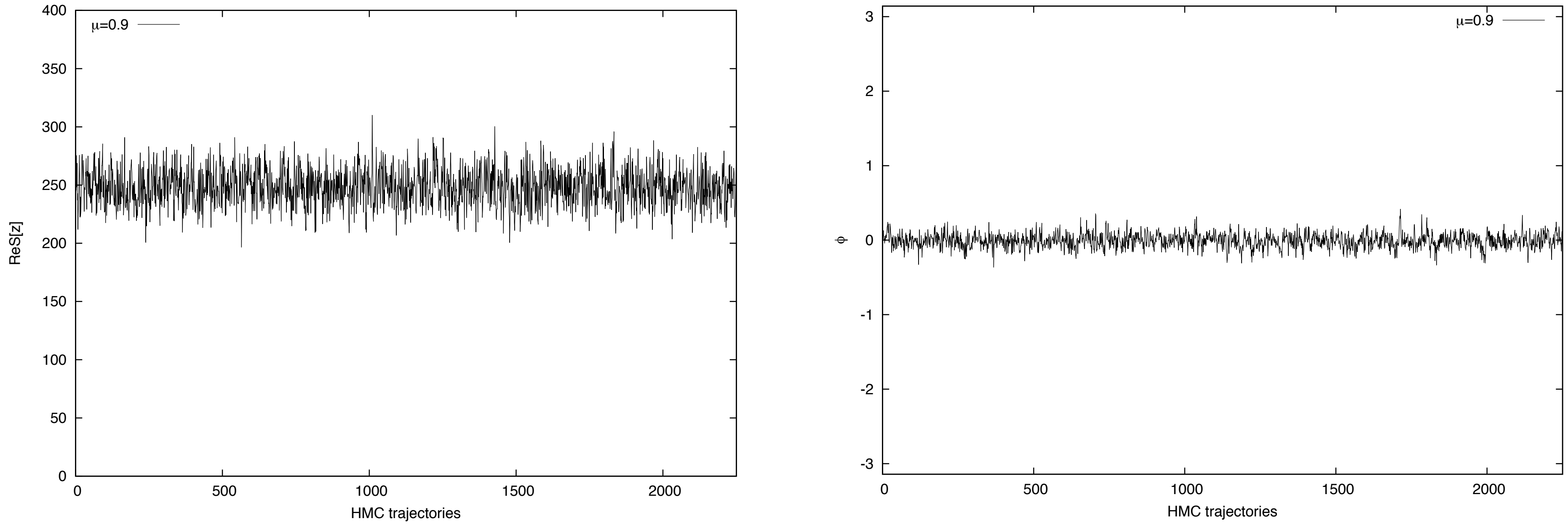
     where $\phi_0 = \sqrt{\frac{-\left(1-6K_0-2K_0\cosh(\mu)\right)}{\lambda_0}}.$

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

simulation parameters :

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



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

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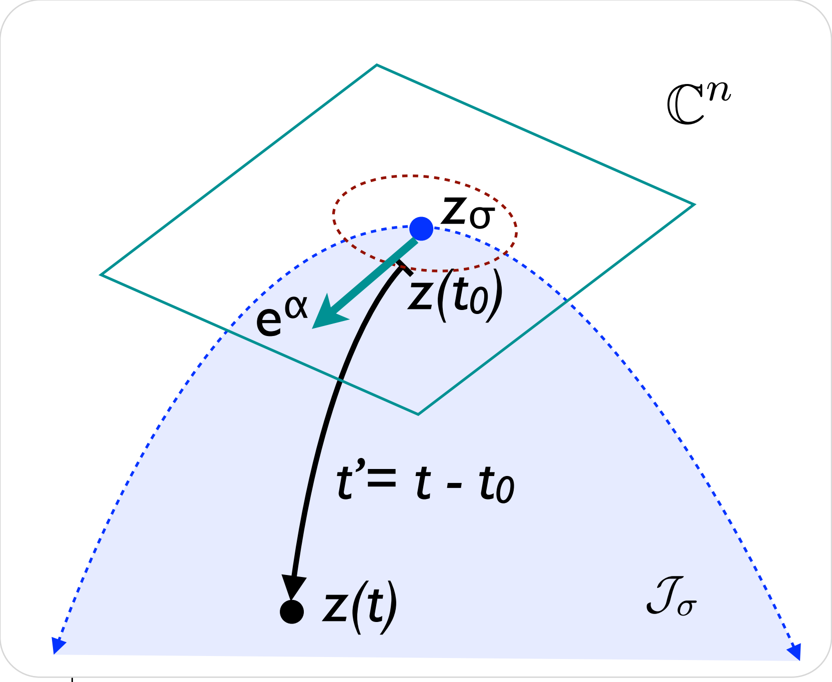

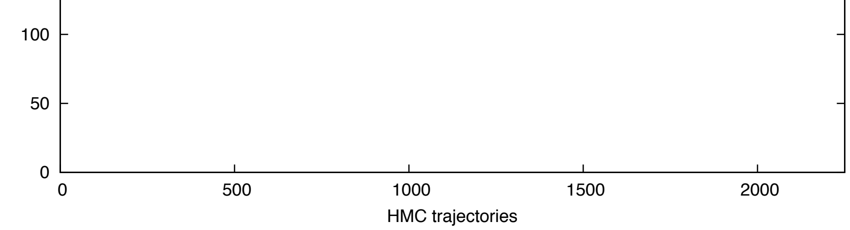

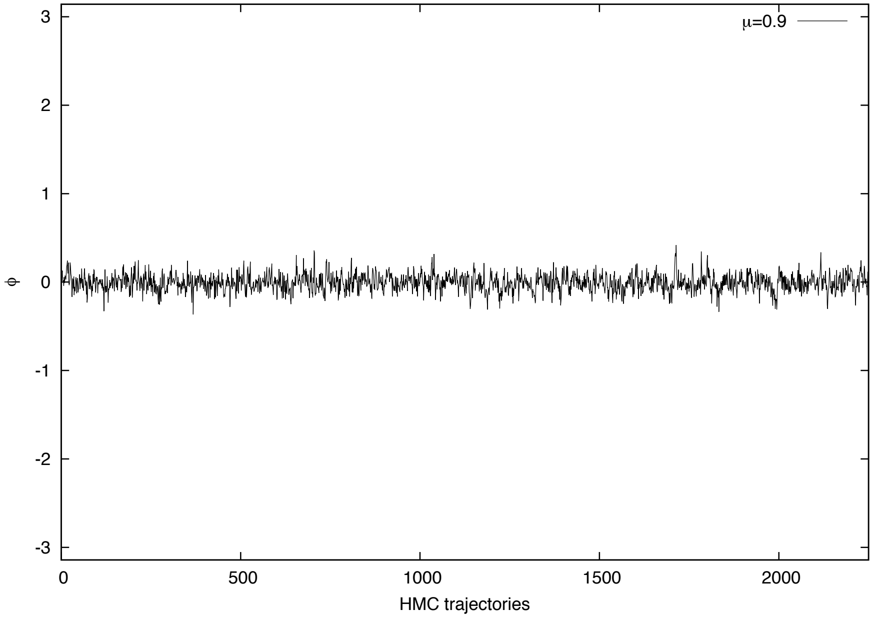

HMC on the thimble 1-(a) $\mu < \tilde{\mu}_c$

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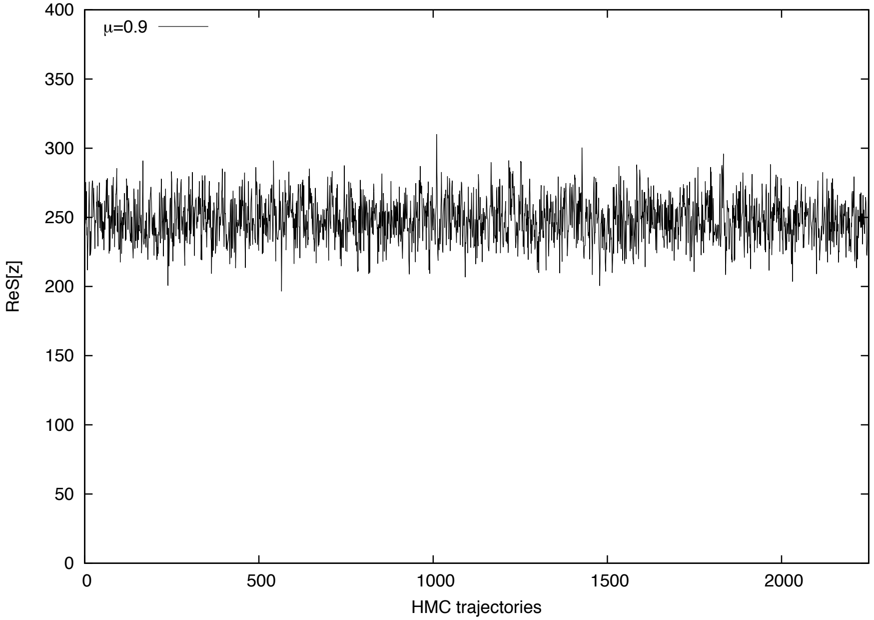

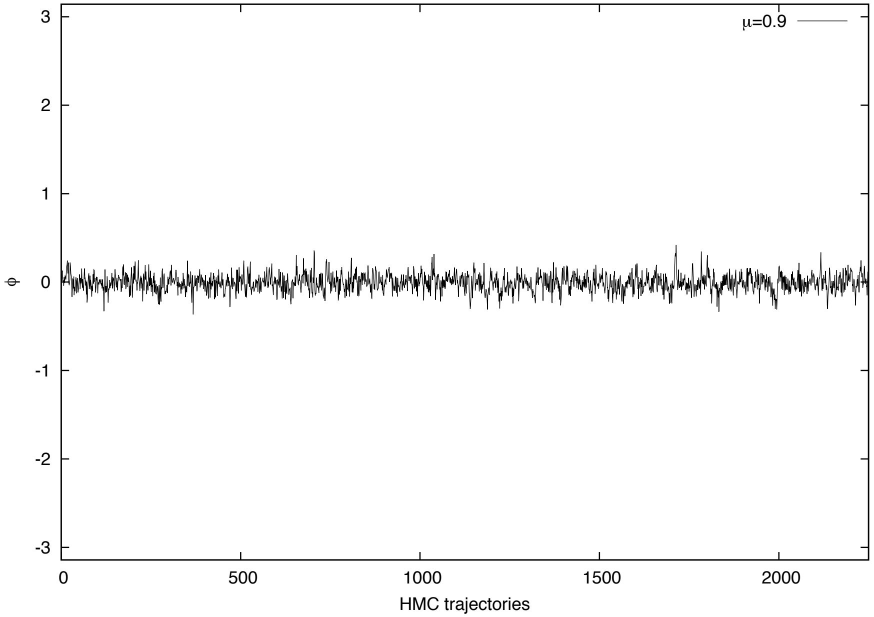

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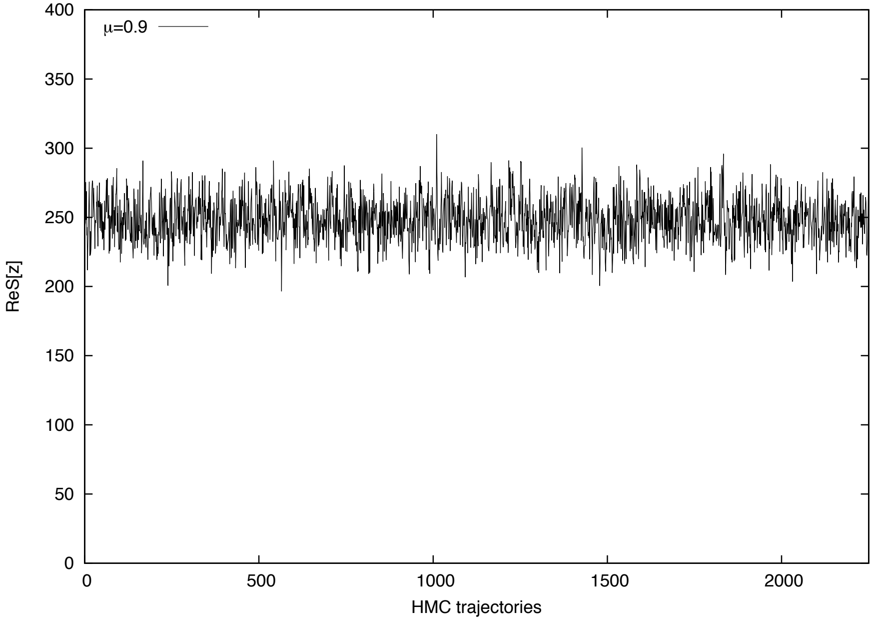
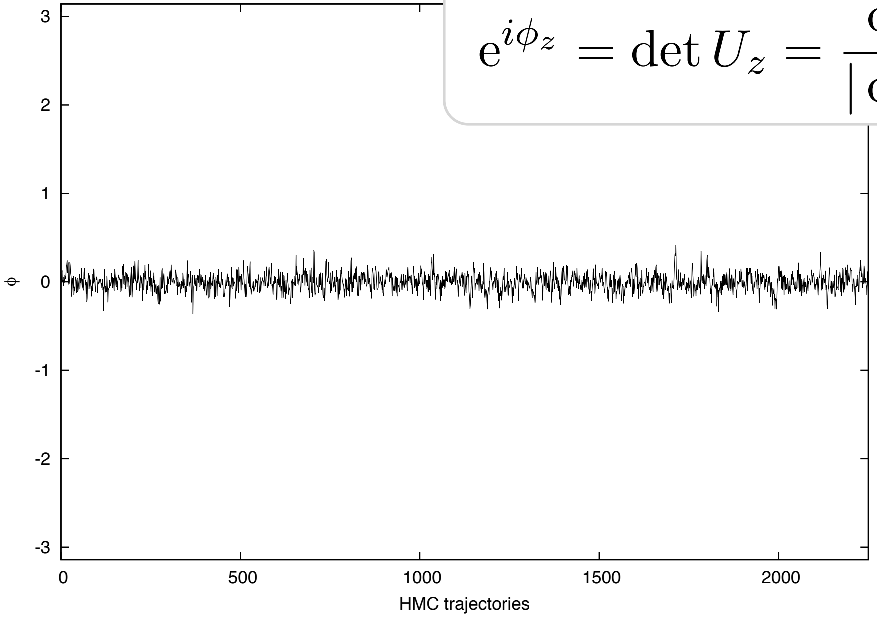




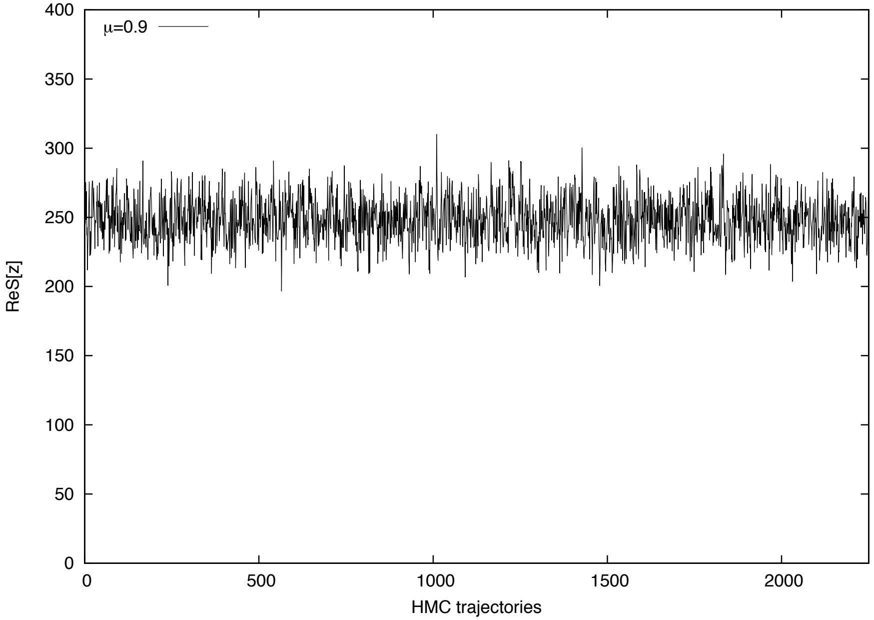
$$e^{i\phi_z} = \det U_z = \frac{\det V_z}{|\det V_z|}$$

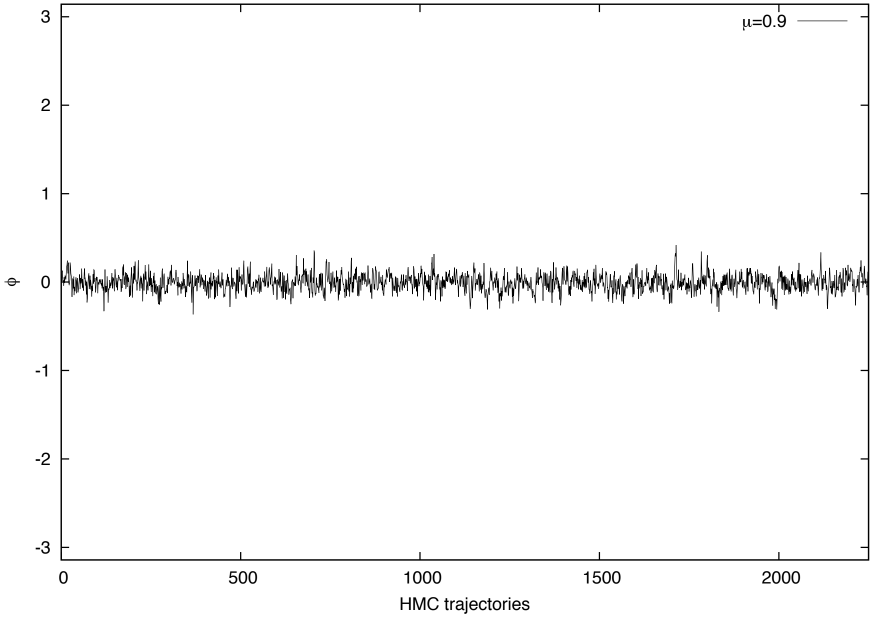
HMC on the thimble 1-(a) $\mu < \tilde{\mu}_c$

simulation parameters :

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

HMC histories (μ = 0.9)





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

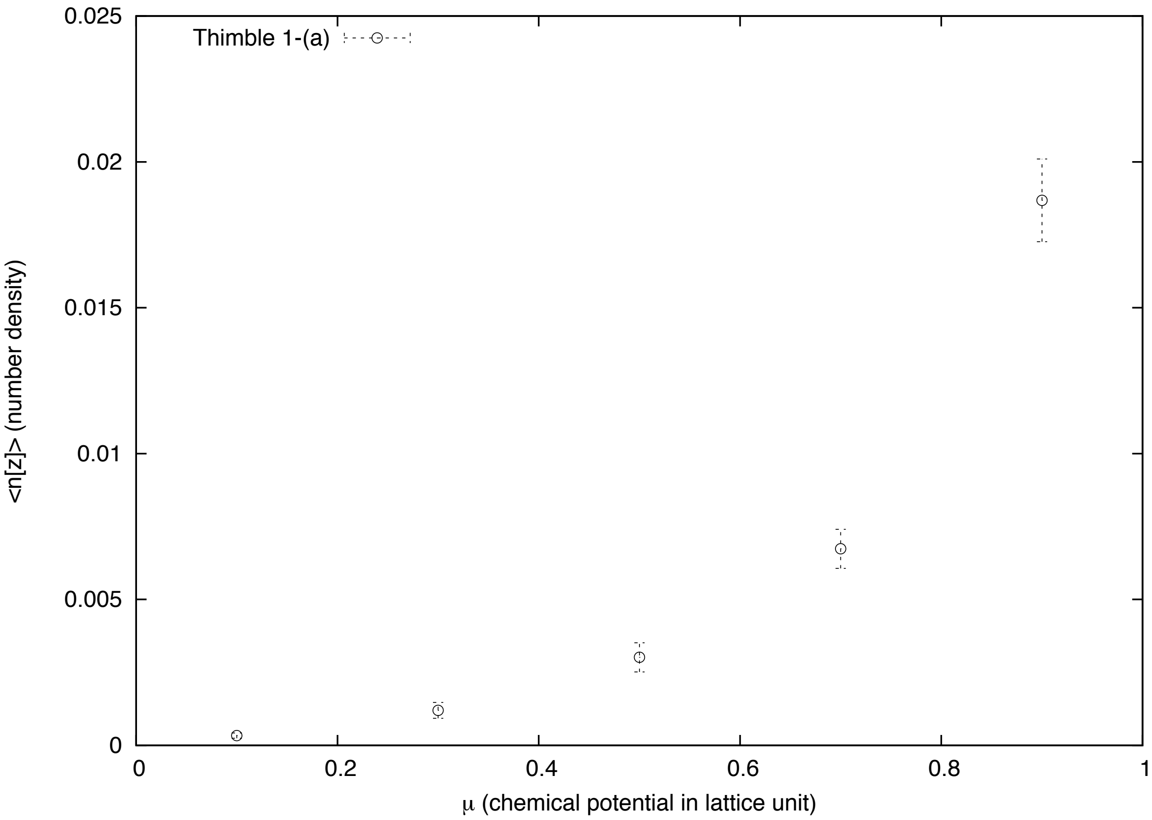
generated 4,250 traj.
sampling 300 conf. with the separation of 10

residual phase :

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

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

number density :



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

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

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

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

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

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

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

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

$$\frac{d}{dt} z_a(t) = \bar{\partial}_{ax} \bar{S}[\bar{z}]\big|_{z_a(x;t)=z_a(t)}$$

$$= \lambda_0 \big(\bar{z}_b(t) \bar{z}_b(t) - \phi_0^2\big) \, \bar{z}_a(t)$$

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

simulation parameters :

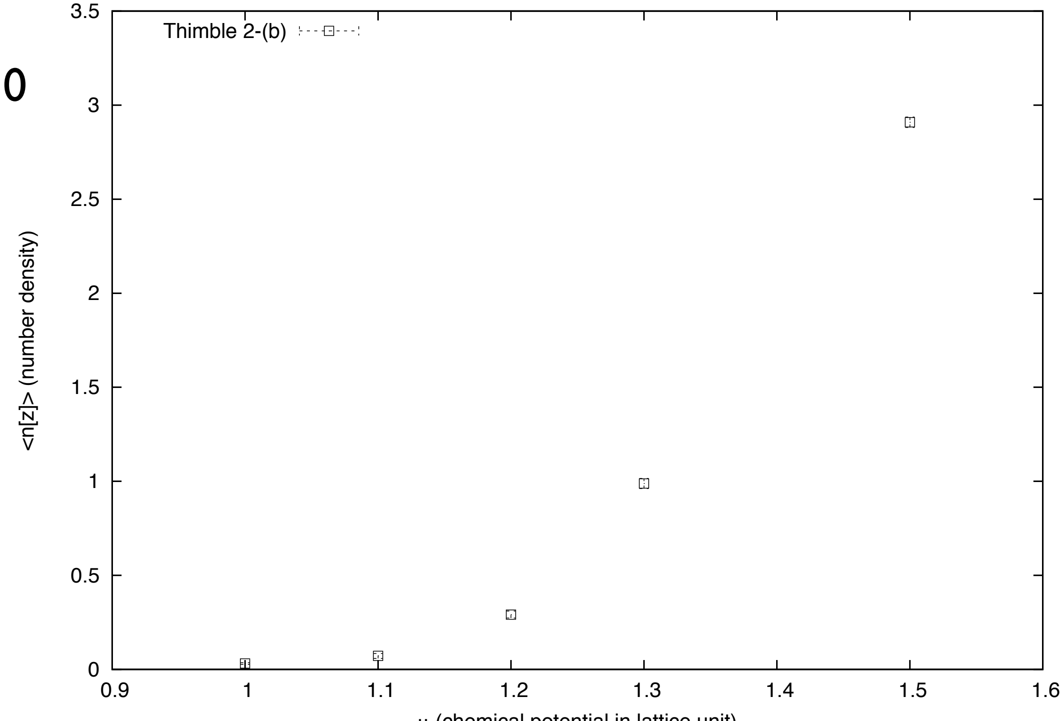
	Parameters	Resulting conditions
Thimble	$t_0 = -3.0$ $n_{\text{lefs}} = 100$ $h = t'/n_{\text{lefs}} \simeq 0.03$	$\lvert\mathrm{Re}\big(S[z(t_0)] - S[z_{\text{vac}}]\big)\rvert \lesssim 2.0 \times 10^1$ $\lvert\mathrm{Im}(S[z] - S[z_{\text{vac}}])\rvert \lesssim 5.0 \times 10^{-2}$ $\lVert\bar{\partial}\bar{S}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

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

number density :

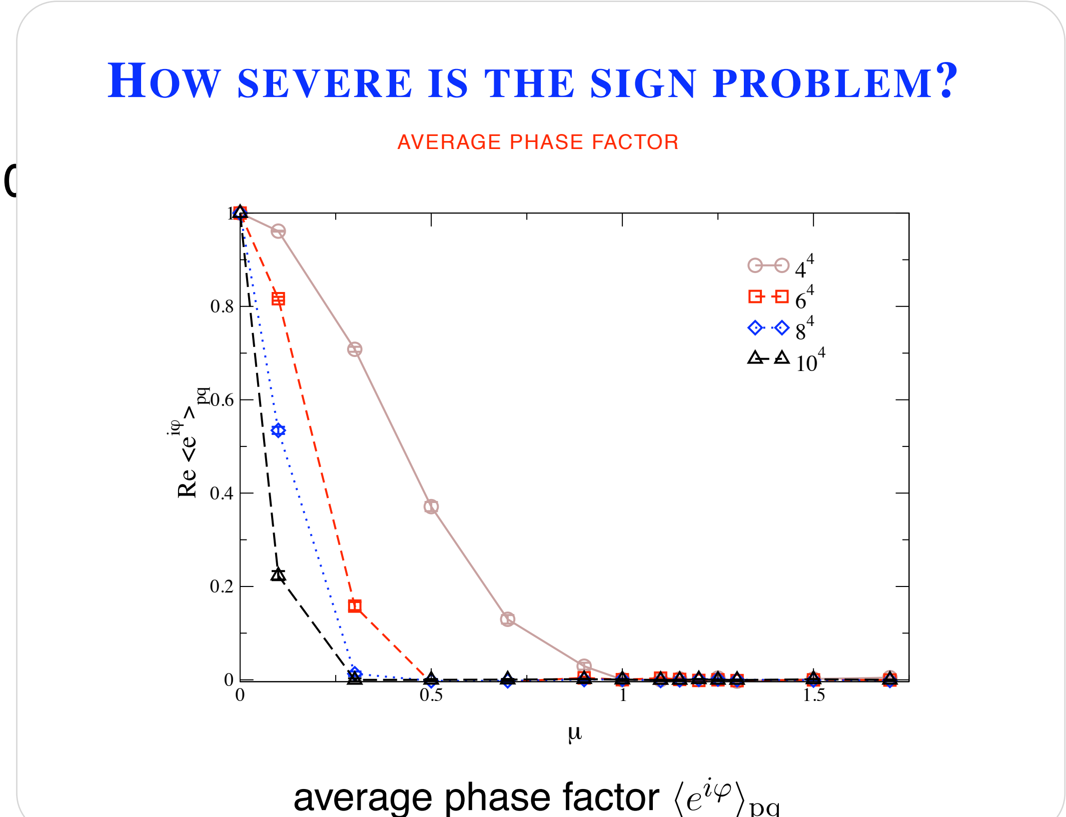


HMC on the thimble 2-(b) $\mu > \tilde{\mu}_c$

simulation parameters :

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

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



HOW SEVERE IS THE SIGN PROBLEM?

AVERAGE PHASE FACTOR

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

residual phase averages:

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

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

simulation parameters :

	Parameters	Resulting conditions
Thimble	$t_0 = -3.0$ $n_{\rm lefs} = 100$ $h = t'/n_{\rm lefs} \simeq 0.03$	$\lvert{\rm Re}\big(S[z(t_0)] - S[z_{\rm vac}]\big)\rvert \lesssim 2.0 \times 10^1$ $\lvert{\rm Im}(S[z] - S[z_{\rm vac}])\rvert \lesssim 5.0 \times 10^{-2}$ $\lVert\bar{\partial}\bar{S} - V^\alpha \kappa^\alpha e^\alpha\rVert^2/2V \le 3.0 \times 10^{-2}$
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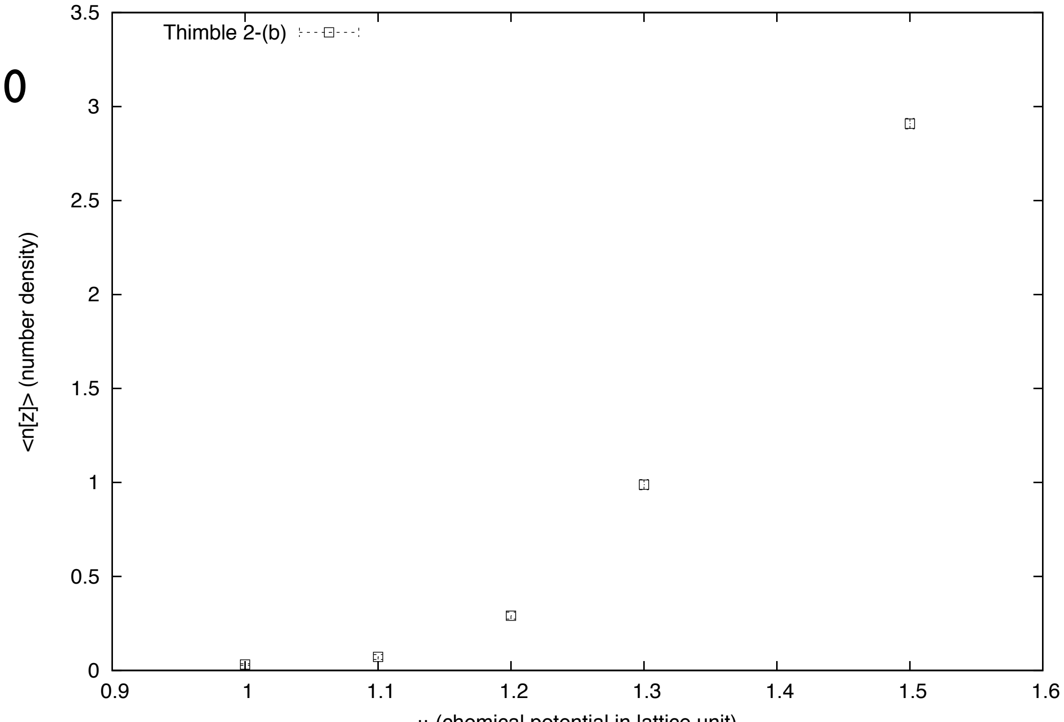
number density :



Comparison to Complex Langevin simulations

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

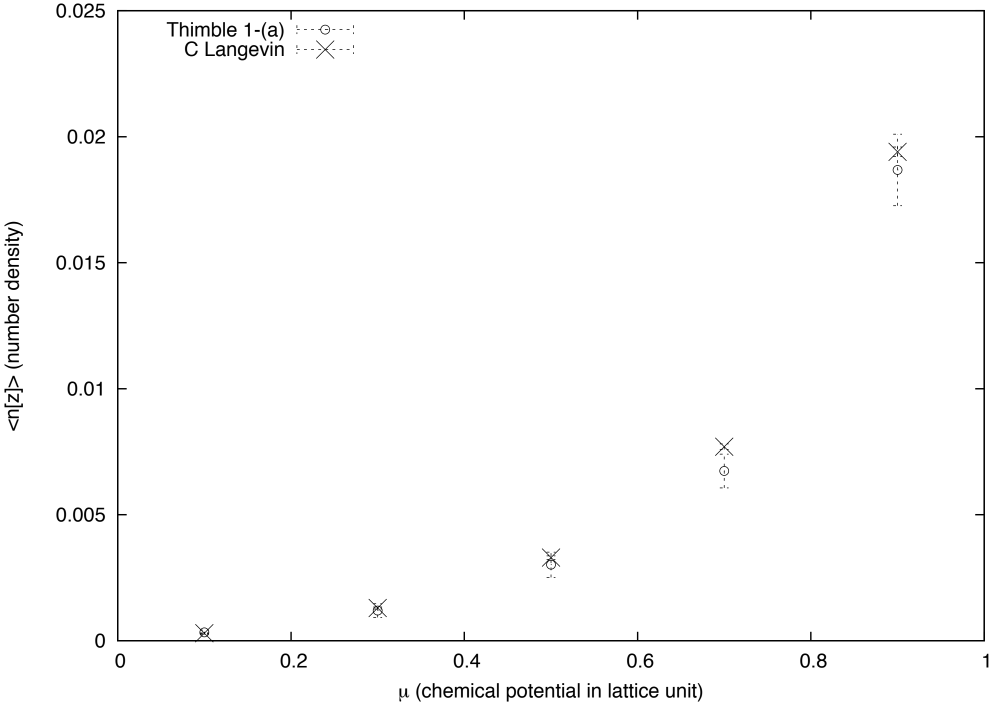
$$\langle \mathcal{O} \rangle = \lim_{t\to\infty} \frac{1}{t} \int_0^t dt'\, \mathcal{O}(z(t'))$$

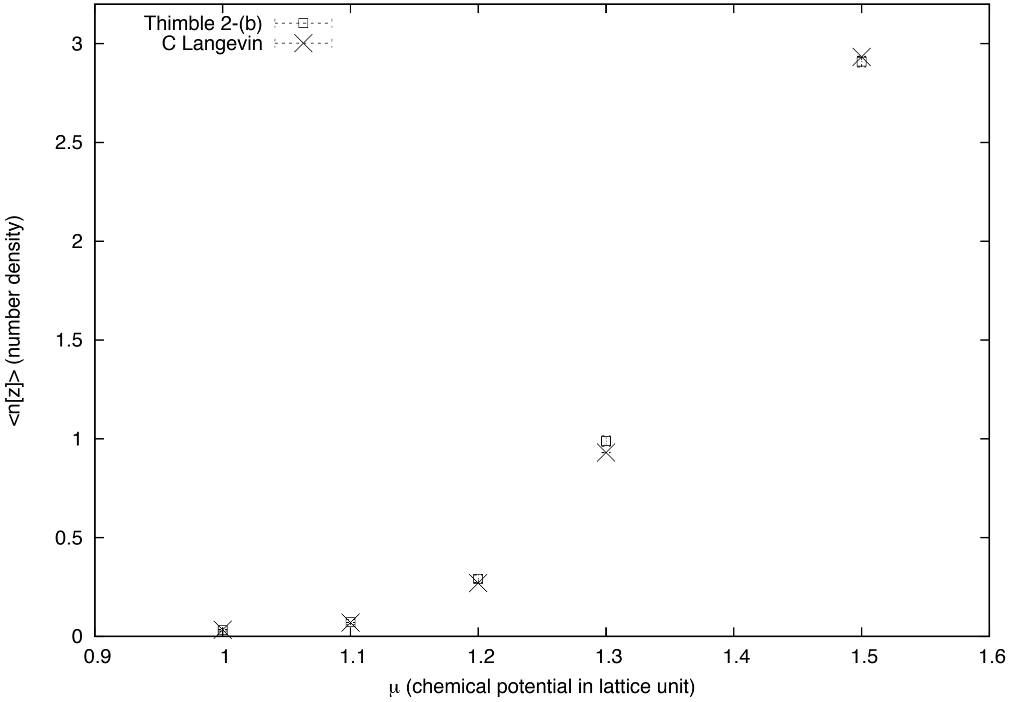
parameters of CL simulations:

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

sampling 10,000 configurations with the separation of 500

number density :





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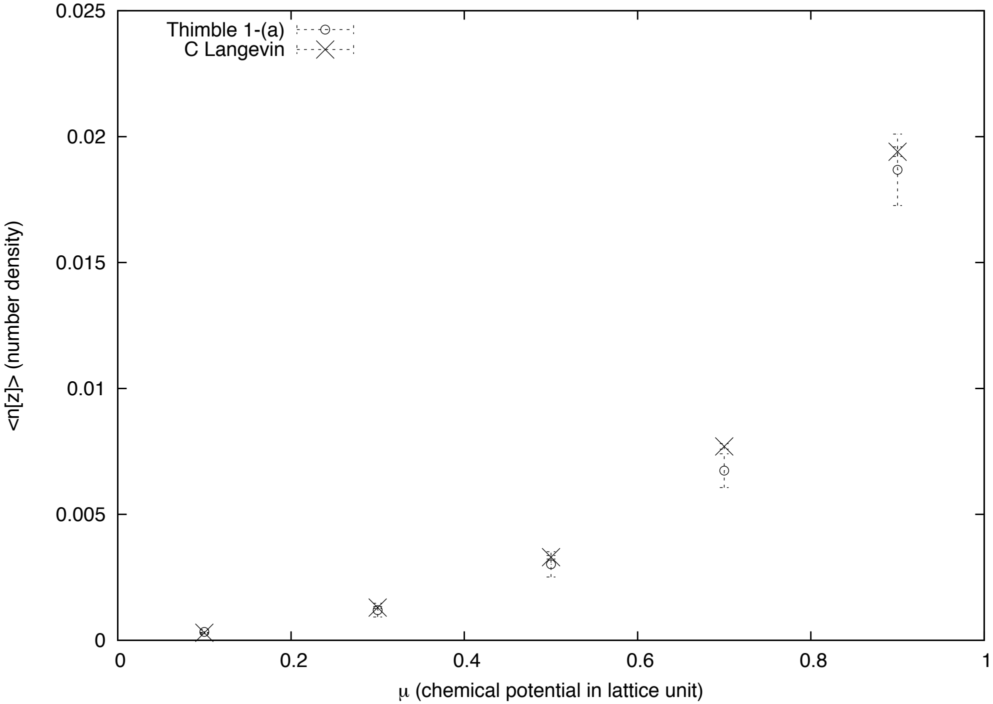
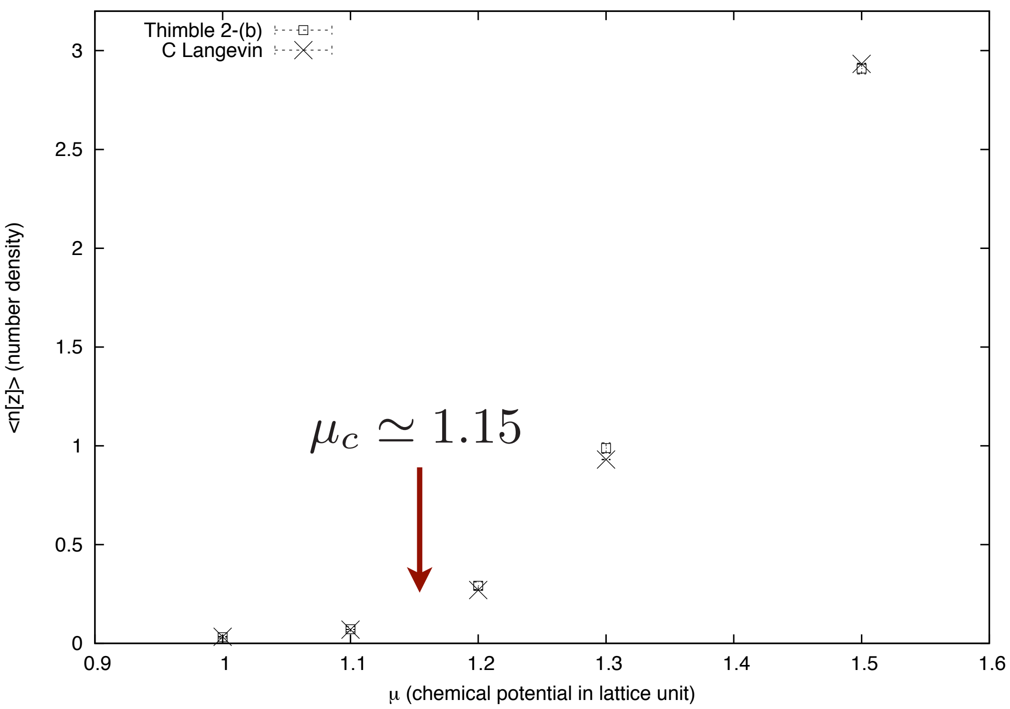
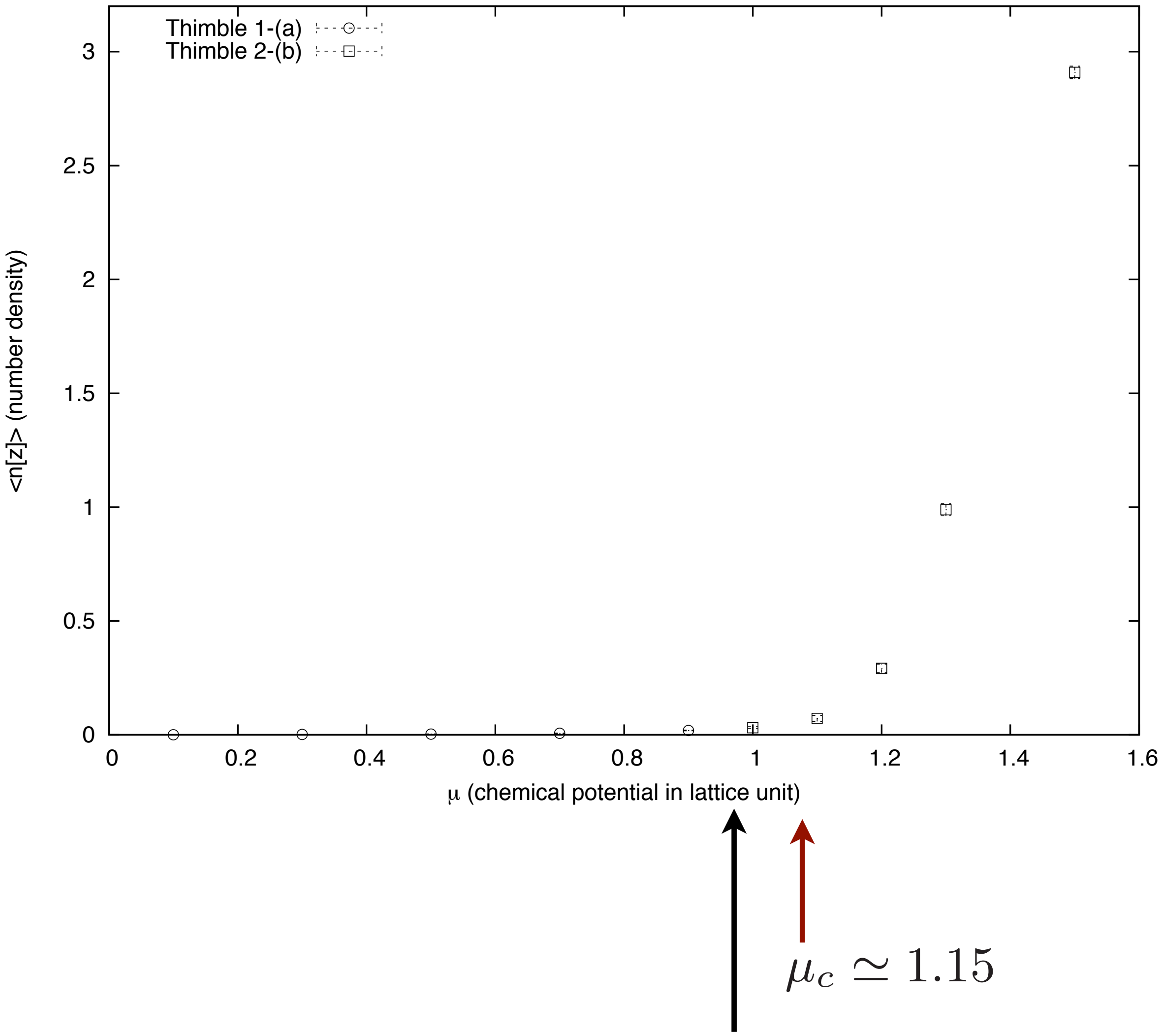




HMC on the thimbles 1-(a) & 2-(b)

number density :



$\mu_c \simeq 1.15$

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

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

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 <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. : literally, scales as $O(V^3 \times n_{step})$

  solving flow eqs. (all tangent vectors) : $O(V^2 \times n_{Lefs})$

  computing V^{-1}, detV (residual sign factors) : $O(V^3)$
- Dynamical fermions :

  possible applications to QCD $_{\mu}$ cf. D. Sexty, arXiv:1307.7748

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

μ_c ~0.962 for K=1.0, λ=1.0

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) $z_1 = z_2 = 0\ ;\quad S[z] = 0,$ ← the thimble 2-(a)
   (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 $\phi_0 = \sqrt{\frac{-\left(1-6K_0-2K_0\cosh(\mu)\right)}{\lambda_0}}.$

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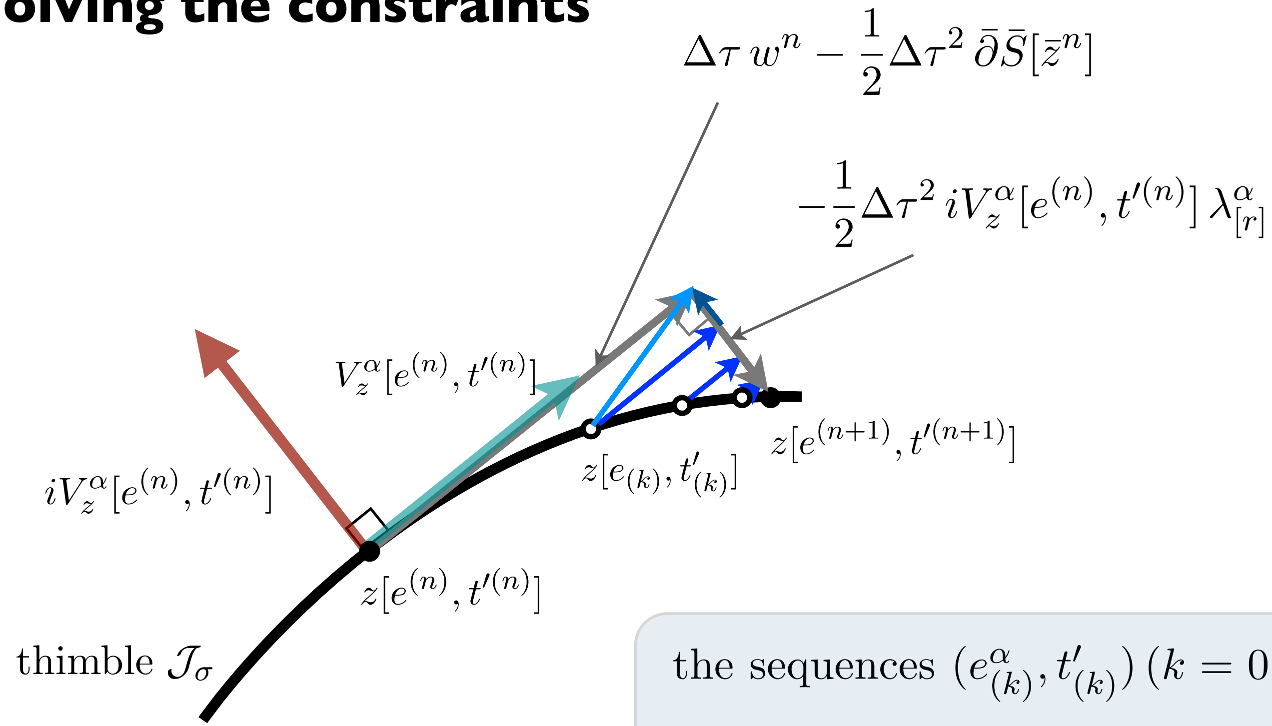
  - solving flow eqs. (~~all~~ tangent vectors) : $O(\cancel{V}^2 \times n_{Lefs})$ x CG x V^2(?)
  - computing $\cancel{V}^{-1}$, detV (residual sign factors) : $O(V^3)$
- Dynamical fermions : psuedo fermions can be implemented
  - possible applications to QCD $_\mu$ cf. D. Sexty, arXiv:1307.7748

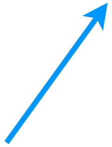
Solving the constraints



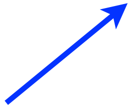
the sequences $(e^\alpha_{(k)}, t'_{(k)})$ $(k = 0, 1, \cdots)$ with $(e^\alpha_{(0)}, t'_{(0)}) = (e^{\alpha(n)}, t'^{(n)})$

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

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



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



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

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

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