Decimation map in 2D for accelerating HMC

Nobuyuki Matsumoto

RIKEN BNL Research Center
(→ BU from Sep)

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Based on collaboration with
P. Boyle, R. Brower, T. Izubuchi, L. Jin, C. Jung, A. Tomiya

in preparation

RIKEN's Programs for Junior Scientists
(SPDR)

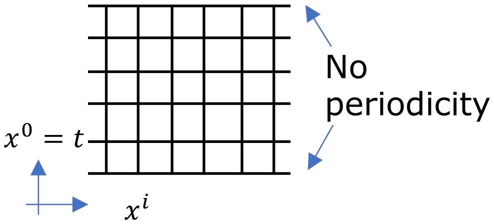
Introduction (1/2)

Goal Overcome critical slowing down & topological freezing and perform efficient simulations on fine lattices.

- Partial solution may be *open boundary condition*

  Lüscher-Schaefer 11

  But many statistical techniques assume translational invariance thus we want to keep the periodic boundary if possible.



Introduction (2/2)

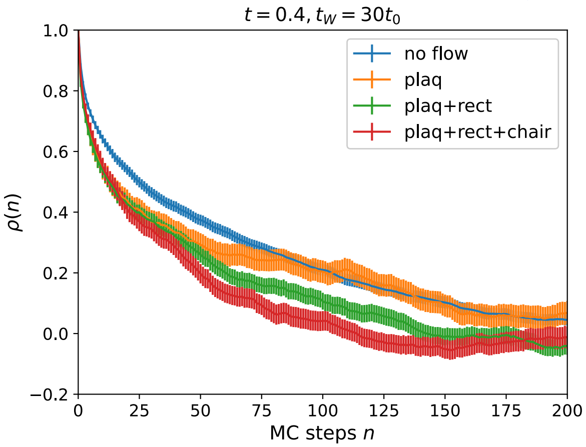
Short timeline

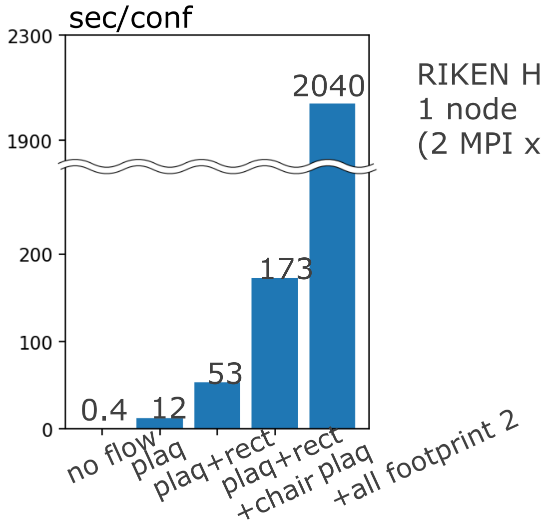
- Proposal of *trivializing map* **Lüscher 09** (Name borrowed from **Nicolai 80**)
- LO approximation w/ CP^{N-1} **Engel-Schaefer 11**

  "The reduction in the forces, ..., is compensated by the computational overhead"

- Wilson flow and its generalizations [4D SU(3) pure gauge]

  Jin LATTICE 2021 poster **Boyle-Izubuchi-Jin-Jung-NM-Lehner-Tomiya LATTICE2022 [2212.11387]**





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1 node
(2 MPI x 40 OpenMP)

Tunneling rate can increase, but still overwhelmed by overhead.

➡ Step back and reconsider strategy using 2D U(1)

- Significant developments in normalizing flow/generative models

  Albergo-Kanwar-Shanahan 19
  Bacchio-Kessel-Schaefer-Vaitl 22

  See *Plenary of G. Kanwar this morning (Mon)*

This work (1/1)

NM+ in prep

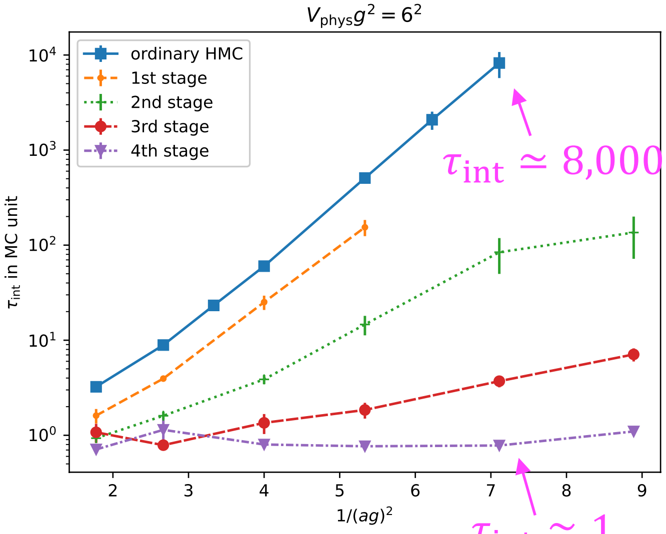
- Develop a variant of trivializing map: *"decimation map"*

Trivialization decomposed into several stages.
Each stage corresponds to integrating out local DOF

- Apply to 2D U(1) pure gauge with the guided MC (a generalization of HMC)

Horowitz 91

$\tau_{\mathrm{int}}(Q)$ in MC unit

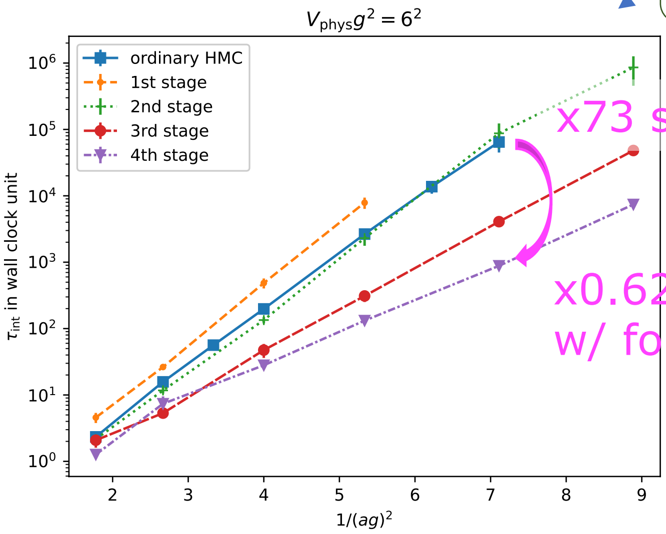


$\tau_{\mathrm{int}} \simeq 8{,}000$

$\tau_{\mathrm{int}} \simeq 1$

$\tau_{\mathrm{int}}(Q)$ in wall-clock time

Updated from ECT* ML workshop 06/28/2023



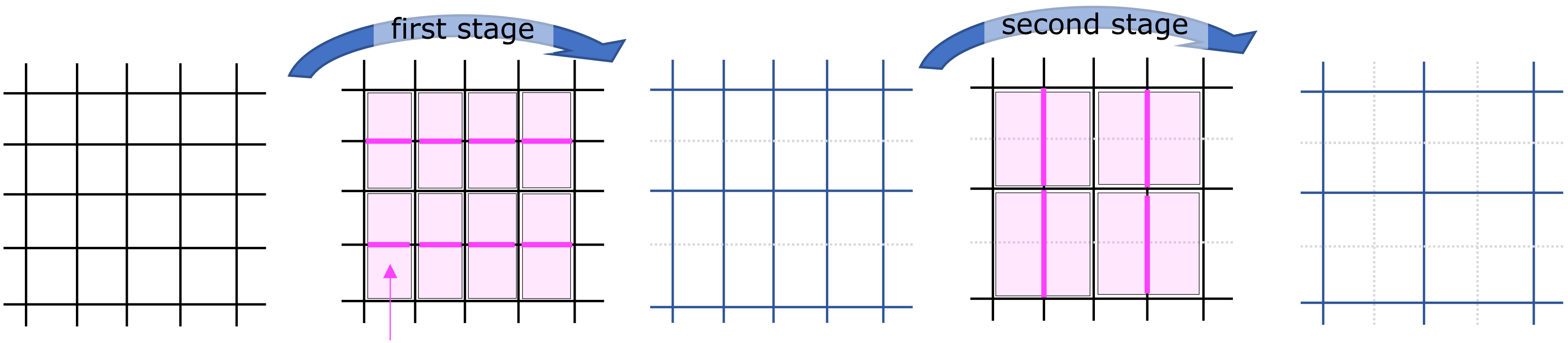
x73 speed up

x0.62 in exponent
w/ four stages

- Algorithm is exact, scalings known and controlled.

Decimation map (1/2)

- Trivialization w/ several stages



In each block, trivializing map as a gradient flow:

$$\dot{U}_t U_t^{-1} = -\partial K_t \quad \left(K_t\text{: flow kernel} \right)$$

and repeat…

cf. Lüscher 09

- K_t can be ontained from solving the linear equation: $\mathcal{L}_t K_t = -S^{(\text{loc})}$. $\left(\mathcal{L}_t \equiv -\partial^2 - t\,\partial S^{(\text{loc})} \cdot \partial \right)$

  We directly solve this with CGNE; only once as pre-calculation.

- Dividing the system into $\mathcal{T}$ and $\mathcal{R}$,

  to be trivialized remainder

local trivialization
(change of variables)

$$\begin{tikzcd} Z = \int (d\mathcal{T})(d\mathcal{R})\, e^{-S(\mathcal{T},\mathcal{R})} \arrow[r, phantom, "="] \arrow[d, "\text{integrate}"'] & \int (d\mathcal{T})(d\mathcal{R})\, e^{-S_{\text{eff}}(\cancel{\mathcal{T}},\mathcal{R})} \arrow[d, "\text{integrate}"] \\ \int (d\mathcal{R})\, e^{-S_{\text{eff}}(\mathcal{R})} \arrow[r, phantom, "\overset{!}{=}"] & \int (d\mathcal{R})\, e^{-S_{\text{eff}}(\mathcal{R})} \end{tikzcd}$$

must be the same!

Decimation map (2/2)

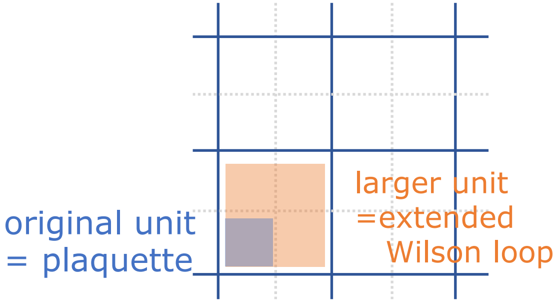
NM+ in prep

- This map leaves the physics in large units exactly unchanged.

  ∴ can be regarded as a coarse-graining map

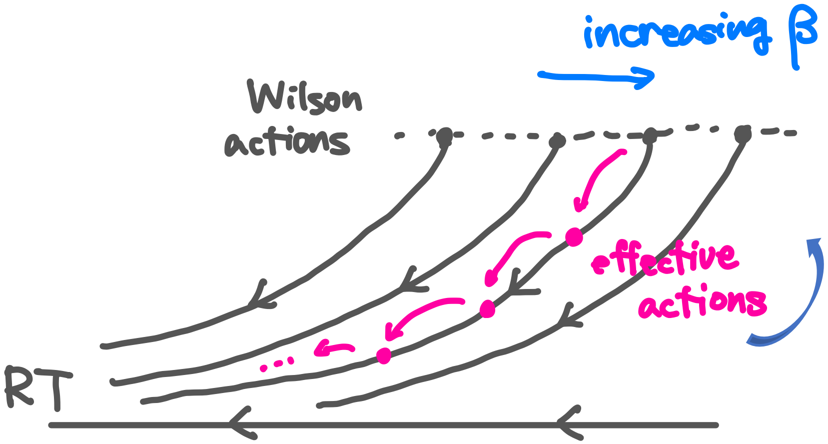
cf. Wilson-Kogut 74, Kadanoff 75, Migdal 76

see also *U. Wenger Mon, R. Abbott Mon*



original unit = plaquette

larger unit =extended Wilson loop



Integrate in the decimated links
when calculating observables.

Updates in coarse-grained lattice.

- Acceleration expected because of
  - Increase of the trivialized region
  - Coarser action for the large-unit variables

2D $U(1)$ (1/1)

Wilson action

$$S(U) \equiv -\beta \sum_x \cos\kappa_x$$

$\kappa_x \equiv \frac{1}{i}\log\left(U_{x,0}U_{x+0,1}U^{\dagger}_{x+1,0}U^{\dagger}_{x,1}\right)$: plaquette angle

$-\pi \leq \kappa_x < \pi$

$\beta = \frac{1}{(ag)^2}$

Solvable system, exact formulas from Fourier expansion.

see also *D. Hoying Tue*

Characteristic features

- Topological charge: $Q = \frac{-1}{2\pi}\sum_x \kappa_x \in \mathbb{Z}$ Simplest lattice gauge field theory with topology
- correlation length zero (ultralocal)

  deal with topological freezing rather than entire critical slowing down.
- topological susceptibility: $\chi_Q \sim \frac{g^2}{(2\pi)^2}$. $\therefore$ typical instanton size $\sim (2\pi)^2/g^2$.

Update algorithm (1/1)

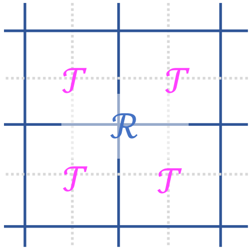
Guided-Hamiltonian Monte Carlo (a variant of HMC):
Horowitz 91 **Duane et al. 87**

- Replace the action in H by an approximate effective action (calculated in CG).
- Detailed balance still holds $\because$ Liouville theorem and reversibility

Pros

- Simplifies the calculation of force
- Transparent separation of UV/IR

$\mathcal{T}$ $\mathcal{R}$



Cons

- Acceptance rate needs to be controlled additionally by the flow step size ϵ: $\delta H \propto \epsilon^n$

($n = 2$ below)

- no gauge fixing
- periodic boundary
- Flow equation solved with the midpoint integrator ($\therefore$ net discretization error = $O(\epsilon^2)$ as mentioned)
- Bijective ensured by keeping ϵ in a bound. **cf. Lüscher 09**

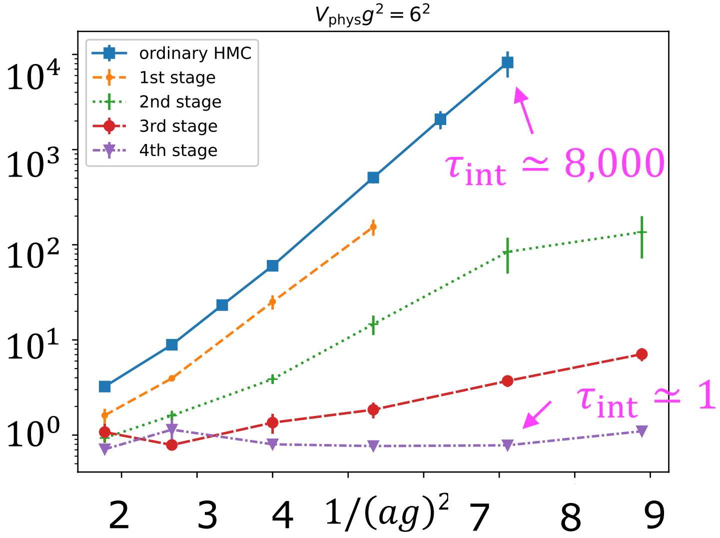
Cost scaling towards the continuum limit (1/1)

NM+ in prep

Physical volume fixed to $6\times 6/g^2$, ϵ scaled to keep acceptance rate ~0.9

~typical instanton size

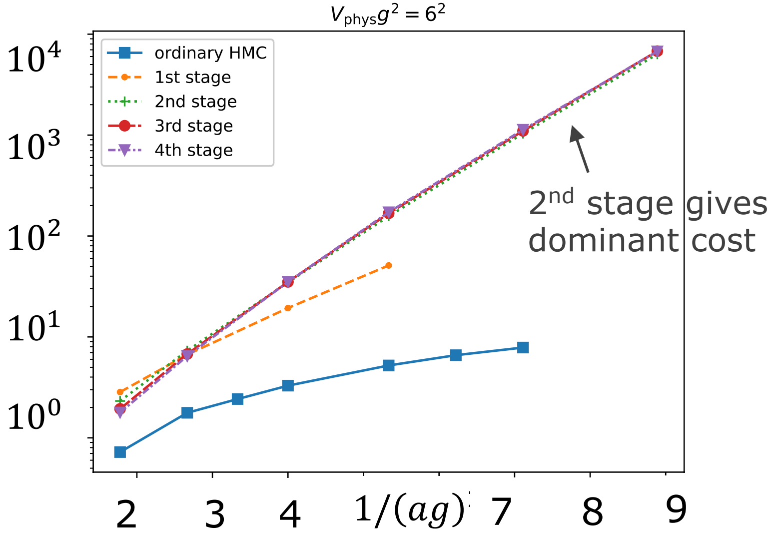
$\tau_{\rm int}(Q)$ in MC unit



$\tau_{\rm int} \simeq 8{,}000$

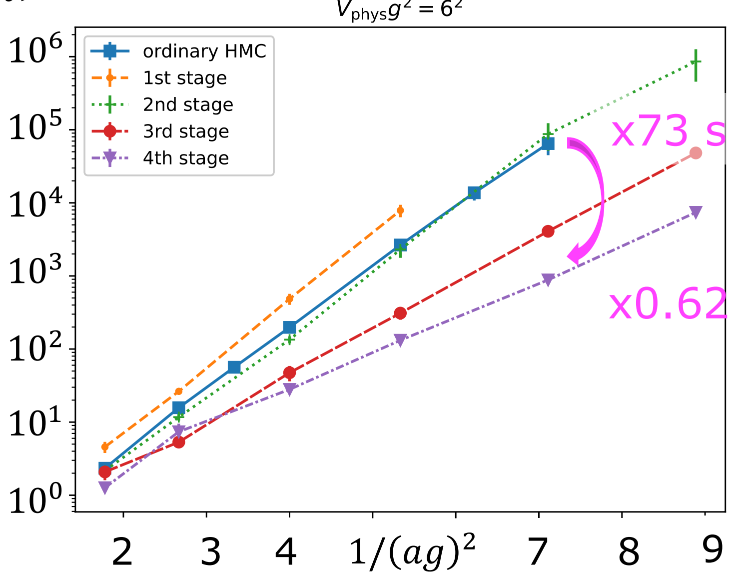
$\tau_{\rm int} \simeq 1$

Execution time/conf (no parallelization)



2nd stage gives dominant cost

$\tau_{\rm int}(Q)$ in wall-clock time



x73 speed up

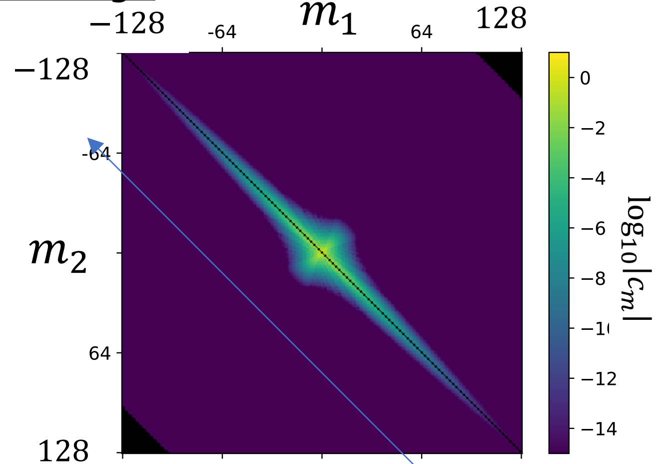
&

x0.62 in the exponent w/ four stages

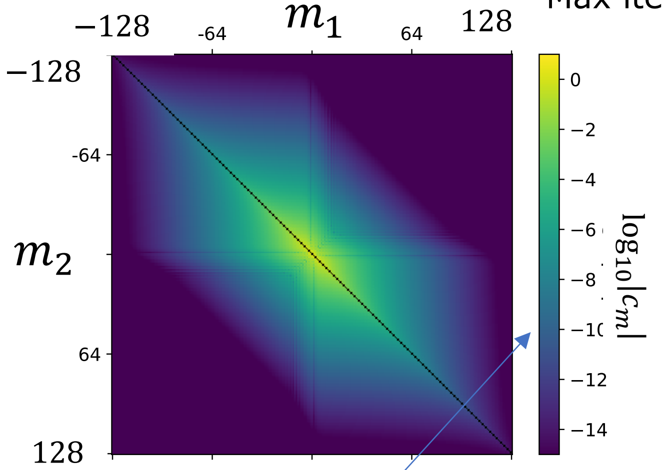
Kernel shapes @β=8.89 (1/1)

NM+ in prep

1st stage



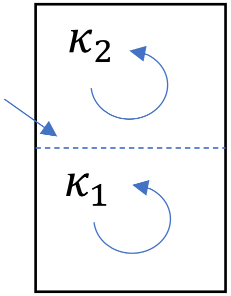
2nd stage



Solves with about an hour using GPU.
Max iteration count: ~9000

$$K_t = \sum_{\mathbf{m}} c_{t,\mathbf{m}} \cos(m_1\kappa_1 + m_2\kappa_2)$$

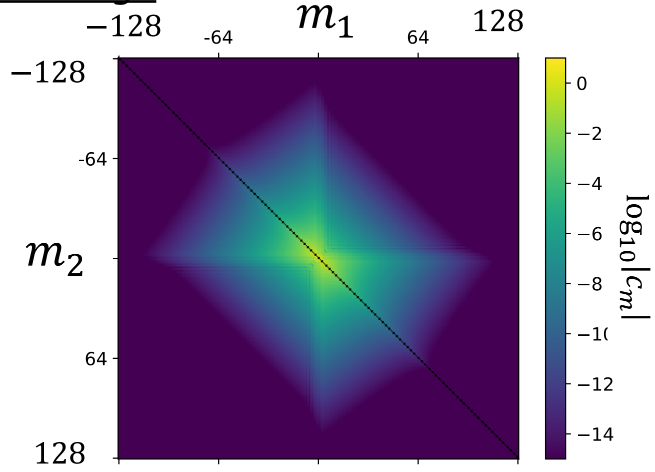
trivialized link



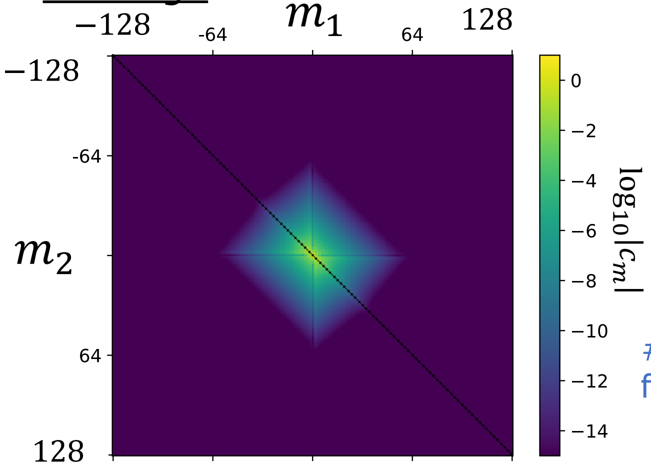
more spread out as $\beta \to \infty$

Due to higher-order loops in S_{eff}

3rd stage



4th stage

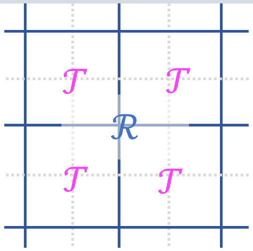


#(relevant loops) shrinks
for higher stages=coarse actions

- 2nd stage is the most expensive simply because ∃many terms.
- From $1/\beta$ expansion of the kernel, suppression of large winding is seemingly power-law.

Analyzing the tunneling (1/1)

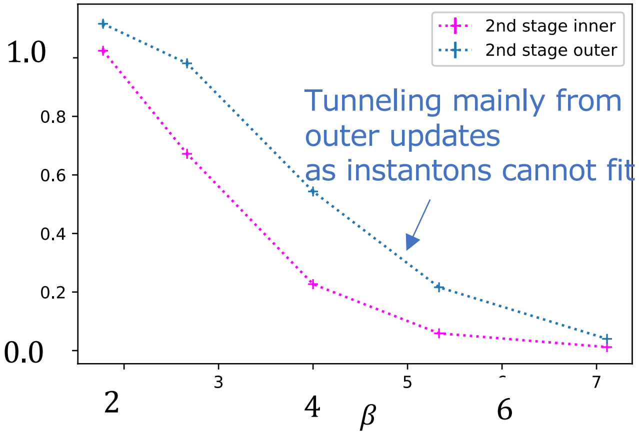
NM+ in prep



- By switching on/off the inner/outer updates alternatively, we investigate how tunneling is induced.

2nd stage

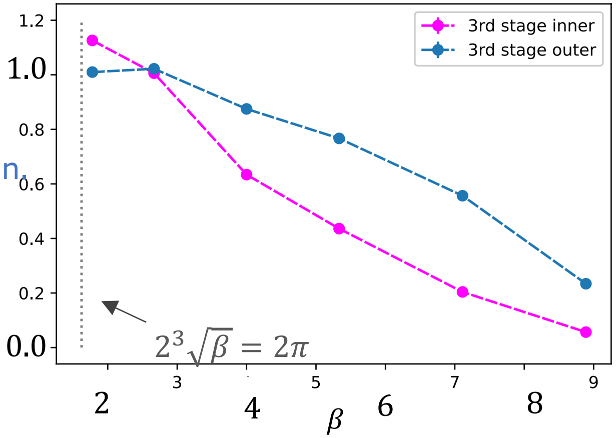
tunneling rate ($\equiv \langle |Q_n - Q_{n+1}| \rangle_{MC}$)



Tunneling mainly from outer updates as instantons cannot fit in.

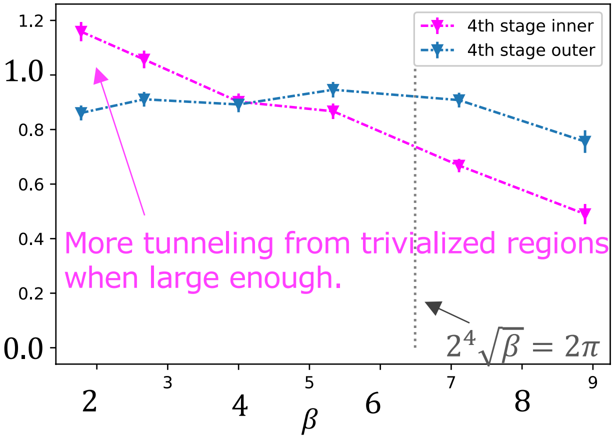
3rd stage

tunneling rate



4th stage

tunneling rate

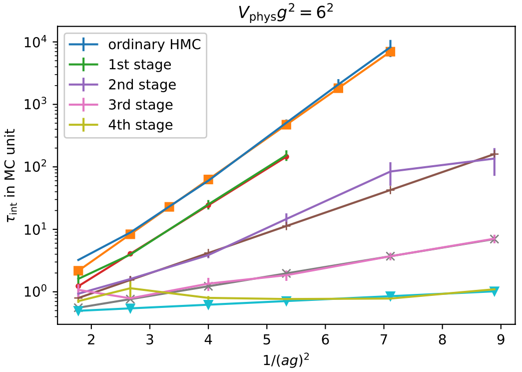


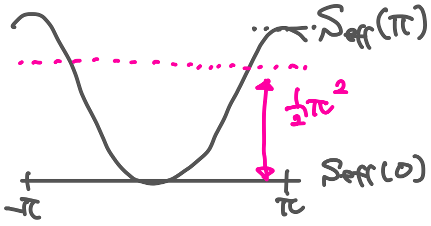
More tunneling from trivialized regions when large enough.

- At the large β regime, the ratio of the tunneling rates (in MC units) can be understood from the probability:

$$P\left(\frac{\pi^2}{2} > S_{\text{eff}}^{(\text{loc})}(\pi) - S_{\text{eff}}^{(\text{loc})}(0)\right), \pi \sim \mathcal{N}(0,1)$$

From fit	From prob
1: 0.886(52)	1: 0.856
2: 0.493(40)	2: 0.507
3: 0.235(14)	3: 0.242
4: 0.067(42)	4: 0.101





Aiming for large β, it seems more effective to get with field transformations a coarse-grained theory than enlarging completely trivialized regions.

Towards QCD (1/1)

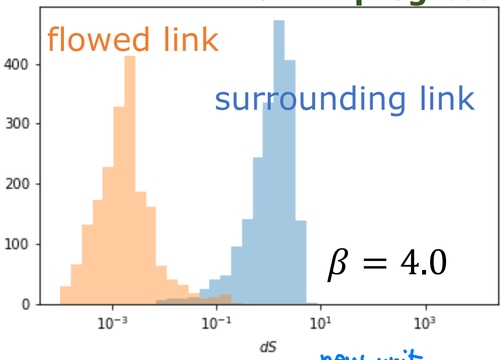
Including fermion

- We can expect exponential speed-up to remain when using exact S_{eff} in HMC (sometimes referred to as "FT-HMC")
  see Lüscher 09

  especially when fermion is present because of its additional cost.
  cf. Engel-Schaefer 11, *P.Boyle Plenary Tue*
- However, effect of this peculiar smearing on fermion is nontrivial.
  see also *J. Finkenrath Mon*

Forces (1^{st} stage, exact S_{eff})

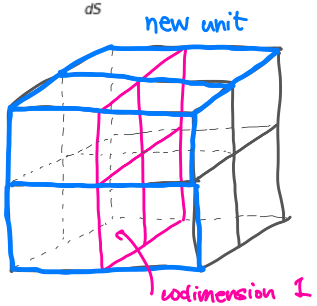
NM+ work in progress



Higher-dimension

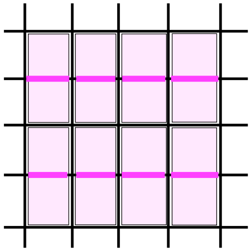
- trivializing map for codimension one surfaces → theory of 1x2 Wilson loops
  ∵ gauge invariance

  2D Wilson is special that links on a line are independent;
  much larger function space required for higher dimensions.



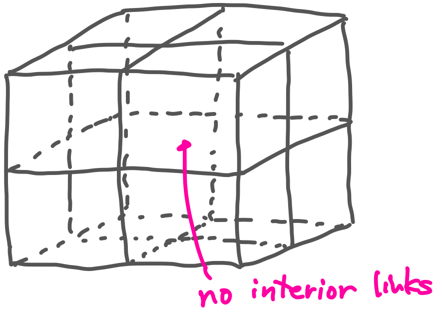
- Another possibility: freeze links surrounding local volume & trivialize interior.
  → "cage action", which can lower potential barriers for the remaining links.

⋮



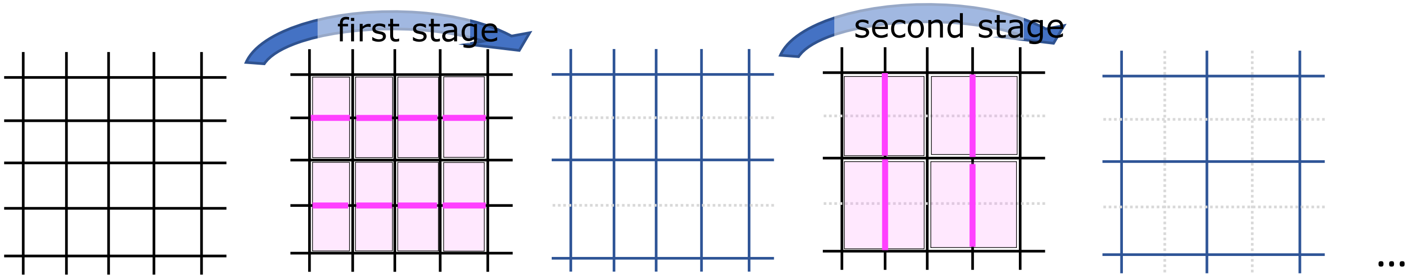
Non-Abelian groups

- We can work in the Wilson loop space to construct the function basis; labels may again be the winding numbers
  (though we need to take into account the noncommutativity and traces).
- Though there are Mandelstam constraints, **Mandelstam 79**
  use of overcomplete basis seems possible when using CG.

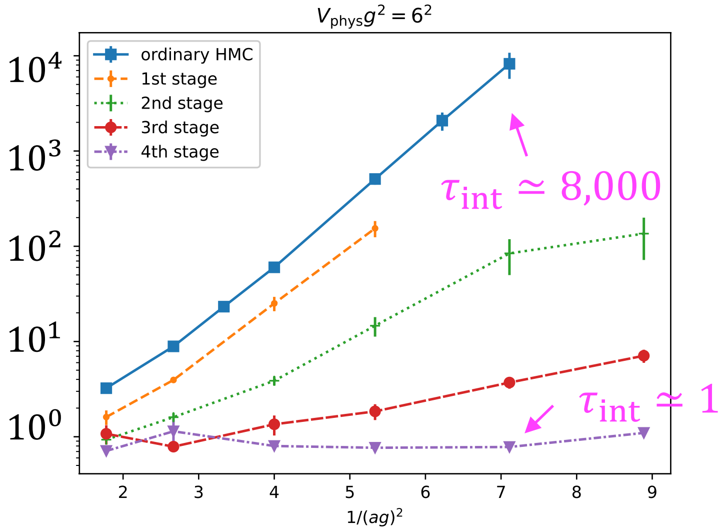


Summary (1/1)

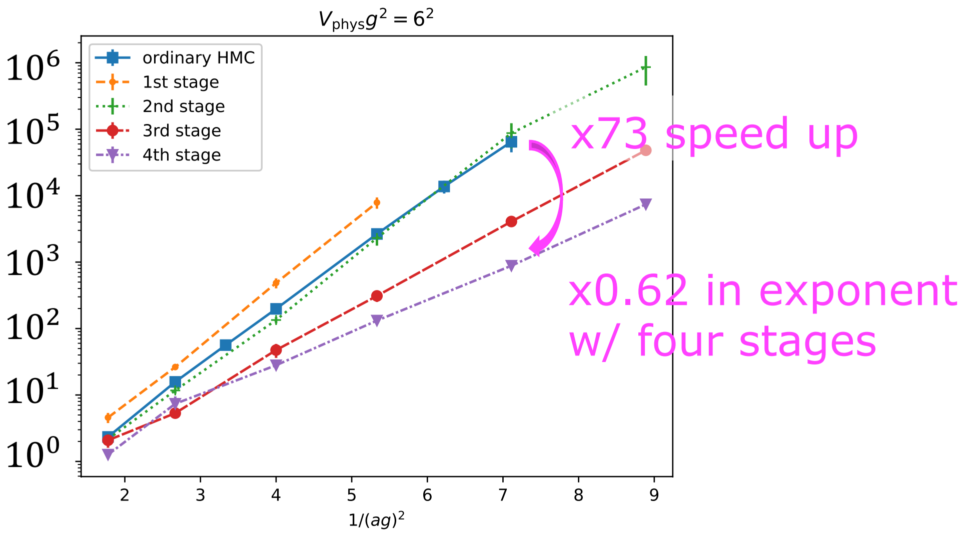
- We considered *decimation map* that can be regarded as a coarse-graining transformation.



$\tau_{\rm int}(Q)$ in MC unit



$\tau_{\rm int}(Q)$ in wall-clock time (no parallelization)



- It is true that the current investigation uses special features of 2D and U(1);

  however, we believe that having a method
  that works on this simplest model and has possible generalization directions
  will be a good starting point for developing algorithms for QCD.

Thank you.