Leapfrog Layers

A Trainable Framework for Effective Topological Sampling

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arXiv:2105.03418
bit.ly/l2hmc-lattice21
bit.ly/l2hmc-surprise
github.com/saforem2/l2hmc-qcd

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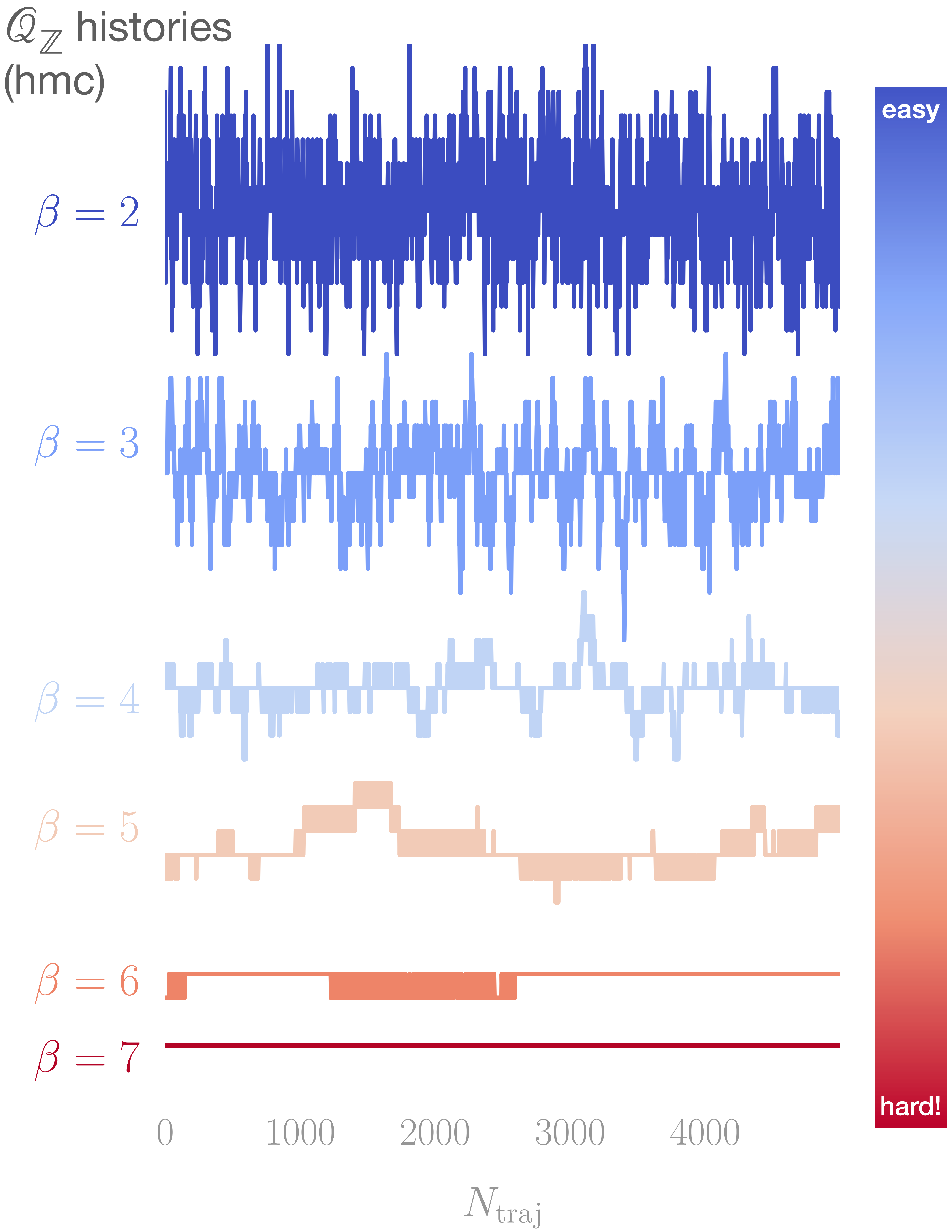
LATTICE 21
JULY 26-30 2021, ZOOM/GATHER@MIT

Critical Slowing Down

- Goal: Draw *independent samples* from target distribution $p(x)$.
  - Generating independent gauge configurations is a *major* bottleneck for LatticeQCD.
- **Topological Freezing**
  - As we approach the continuum limit $\beta \to \infty$, the MCMC updates get stuck in sectors of fixed gauge topology.
    - Number of trajectories needed to adequately sample different topological sectors **increases exponentially**



Hamiltonian Monte Carlo (HMC)

- Introduce $v \sim \mathcal{N}(0,\mathbb{I})$, then the target becomes:

$$p(x,v) = p(x)\cdot p(v) = e^{-Sx}\cdot e^{-v^T v/2}$$

- Evolve the joint $\xi \equiv (x,v)$ system using Hamilton's equations along $H = \text{const}$:

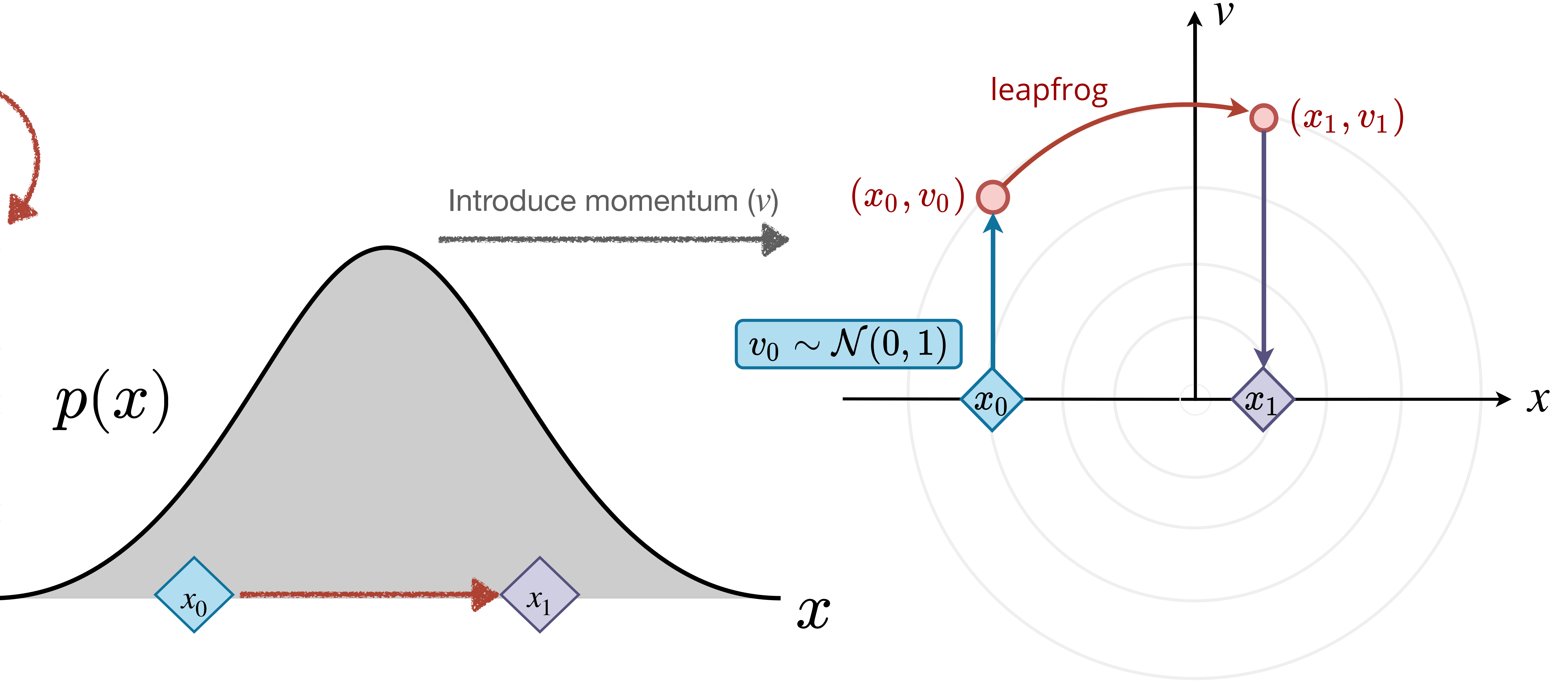
$$\boxed{\dot{x} = \frac{\partial H}{\partial v}, \quad \dot{v} = \frac{\partial H}{\partial v}}$$

- **Leapfrog Integrator:**

1. $\tilde{v} \leftarrow v - \varepsilon\cdot\partial_x S(x)/2$
2. $x' \leftarrow x + \varepsilon\tilde{v}$
3. $v' \leftarrow \tilde{v} - \varepsilon\partial_x S(x')/2$

- Accept / reject proposal x' using MH:

$$x_{i+1} \leftarrow \begin{cases} x' & \text{w/prob.} \quad A(\xi'|\xi) = \min\left\{1, \frac{p(\xi')}{p(\xi)}\left|\frac{\partial \xi'}{\partial \xi}\right|\right\}, \\ x_i & \text{w/prob.} \quad 1 - A(\xi'|\xi) \end{cases}$$



Leapfrog Layer

- Introduce persistent direction $d \sim \mathcal{U}(+,-)$ *(forward, backward).*
- **Target distribution:** $p(\xi) = p(x)\cdot p(v)\cdot p(d)$
- **kth-Leapfrog Layer:** $\xi_k \equiv (x_k, v_k, \pm) \longrightarrow (x''_k, v''_k, \pm) \equiv \xi_{k+1}$

(input) $\boxed{\xi_0 \to \xi_1 \to \cdots \to \xi_k \to \xi_{k+1} \to \cdots \to \xi_{N_{\mathrm{LF}}} \equiv \xi''}$ (proposal)

- Construct a *trajectory* by passing ξ_k through $k \in \{1, 2, \ldots, N_{\mathrm{LF}}\}$ leapfrog layers.

Invertible NN

momentum scaling

force scaling

translation

v **update:** ($d = +$)

$$v''_k = \Gamma^+(v_k; \boxed{\zeta_{v_k}}) \equiv v_k \odot \exp\left(\frac{\varepsilon_v^k}{2}\boxed{s_v^k(\zeta_{v_k})}\right) - \frac{\varepsilon_v^k}{2}\left[\partial_x S(x_k) \odot \exp\left(\varepsilon_v^k \boxed{q_v^k(\zeta_{v_k})}\right) + \boxed{t_v^k(\zeta_{v_k})}\right]$$

$$\boxed{\zeta_{v_k} = \left[x_k, \partial_x S(x_k)\right]}$$

x **update:** ($d = +$)

$$x''_k = \Lambda^+(x_k; \boxed{\zeta_{v_k}}) \equiv x_k \odot \exp\left(\varepsilon_x^k \boxed{s_x^k(\zeta_{x_k})}\right) + \varepsilon_x^k\left[v'_k \odot \exp\left(\varepsilon_x^k \boxed{q_x^k(\zeta_{x_k})}\right) + \boxed{t_x^k(\zeta_{x_k})}\right]$$

$$\boxed{\zeta_{x_k} = \left[\bar{m}^k \odot x_k, v_k\right]}$$

l2hmc: Generalized Leapfrog

- **Leapfrog Step:** $\xi_k \rightarrow \xi''_k$

Invertible NN

1. Half-step v update:

$$v'_k = \Gamma^{\pm}(v_k; \zeta_{v_k})$$

2. Full-step, ***half-*** x update:

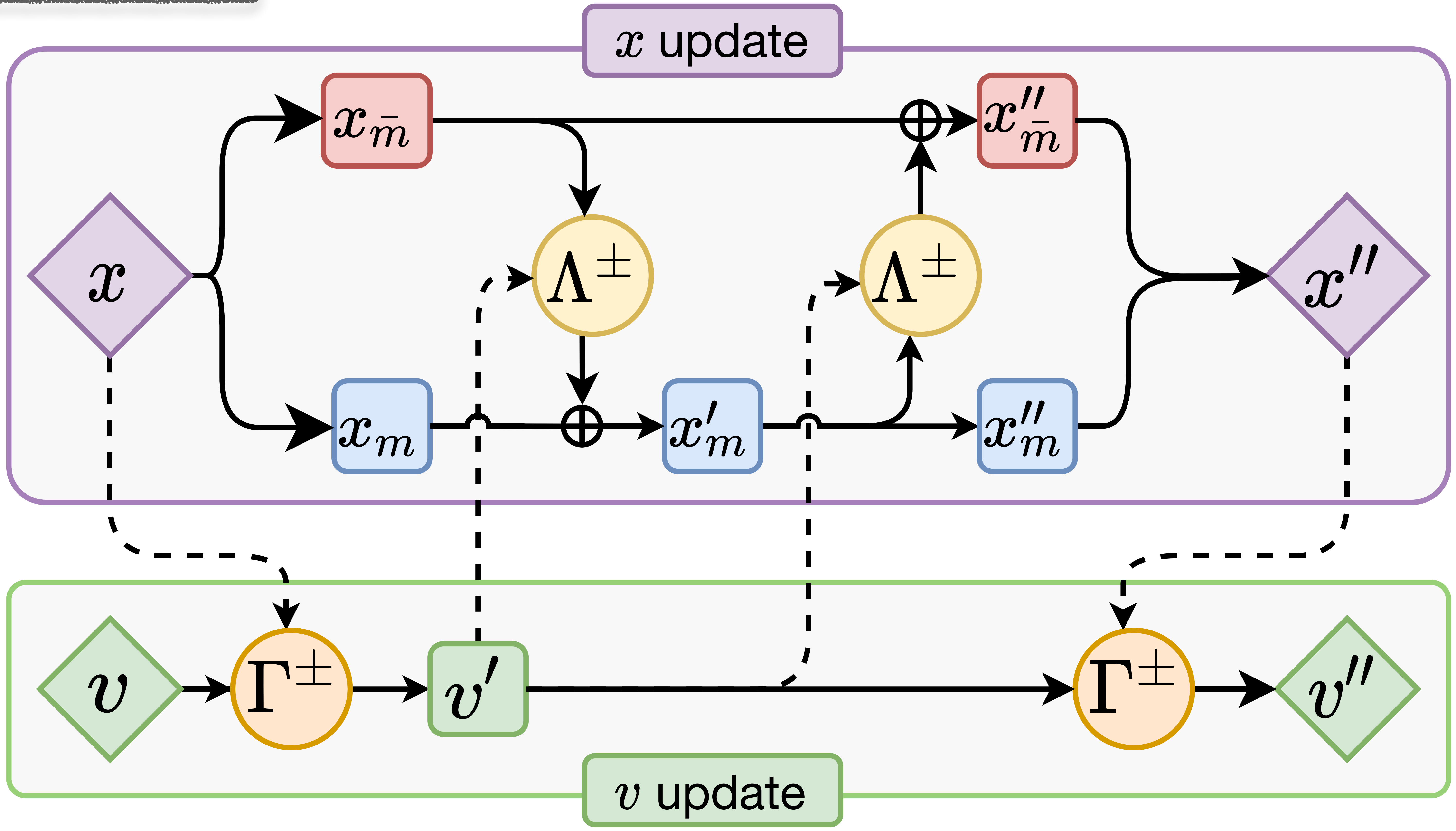
$$x'_k = m^k \odot x_k + \bar{m}^k \odot \Lambda^{\pm}(x_k; \zeta_{x_k})$$

3. Full-step, ***half-*** x update:

$$x''_k = \bar{m}^k \odot x'_k + m^k \odot \Lambda^{\pm}(x'_k; \zeta_{x'_k})$$

4. Half-step v update:

$$v''_k = \Gamma^{\pm}(v'_k; \zeta_{v_k})$$



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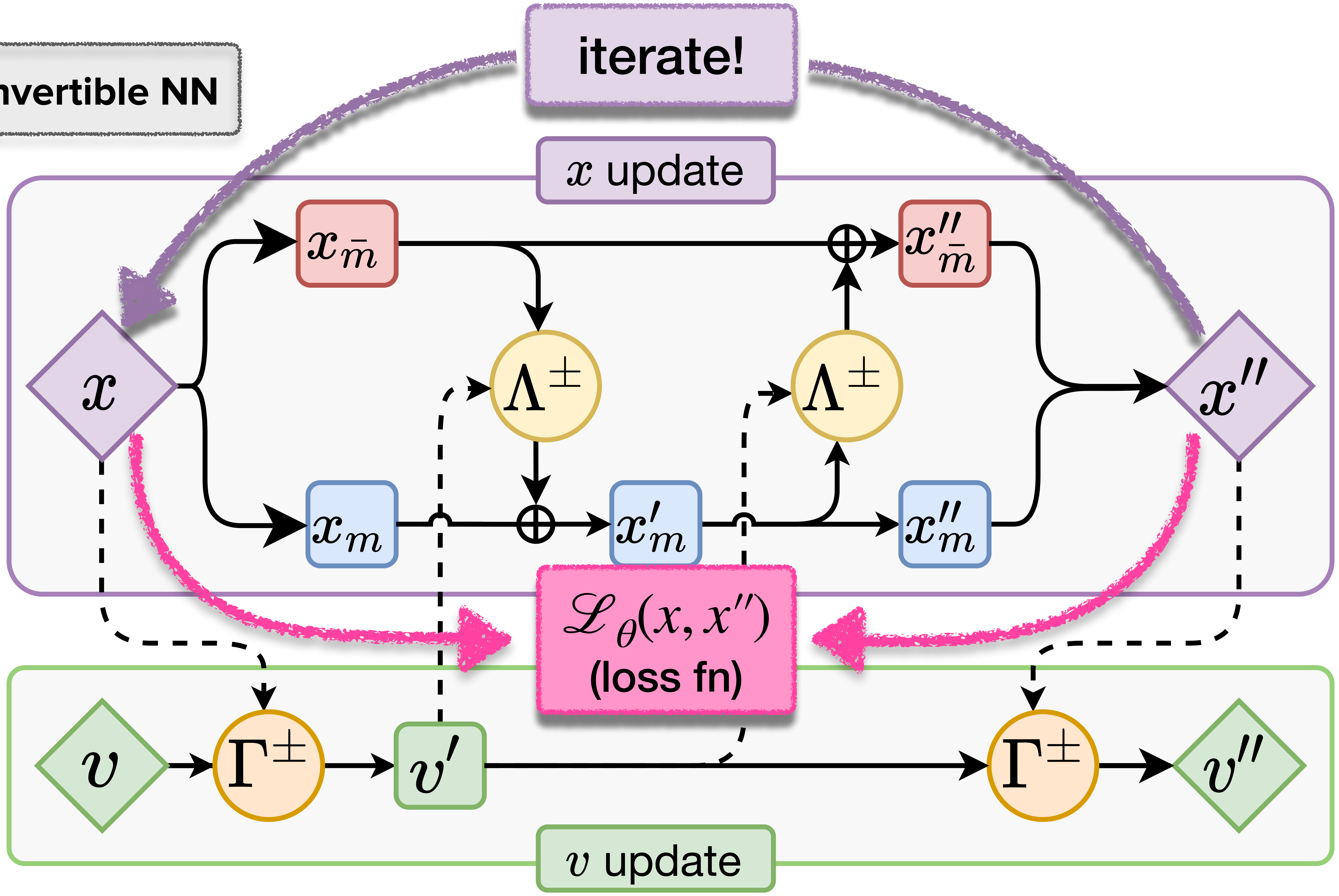
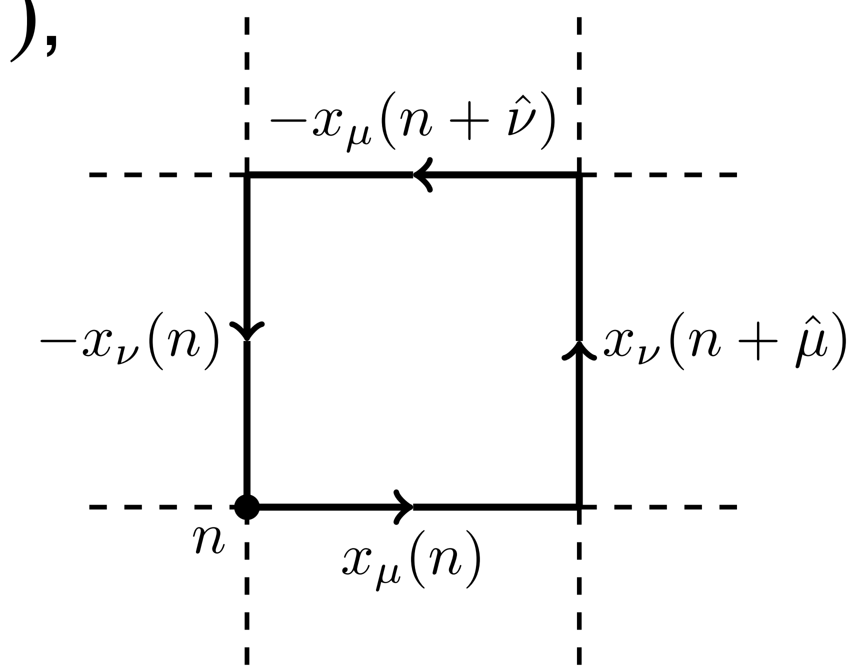


2D $U(1)$ Lattice Gauge Theory

- Link variables $U_\mu(n) = e^{ix_\mu(n)} \in U(1)$,

  with $x_\mu(n) \in [-\pi, \pi]$.



- **Wilson action:**
  - $S_\beta(x) = \beta \sum_P 1 - \cos x_P,$
  - $x_P = x_\mu(n) + x_\nu(n+\hat{\mu}) - x_\mu(n+\hat{\nu}) - x_\nu(n)$

- **Topological charge:**
  - $\mathcal{Q}_\mathbb{R} = \frac{1}{2\pi} \sum_P \sin x_P \in \mathbb{R}$

    continuous, differentiable

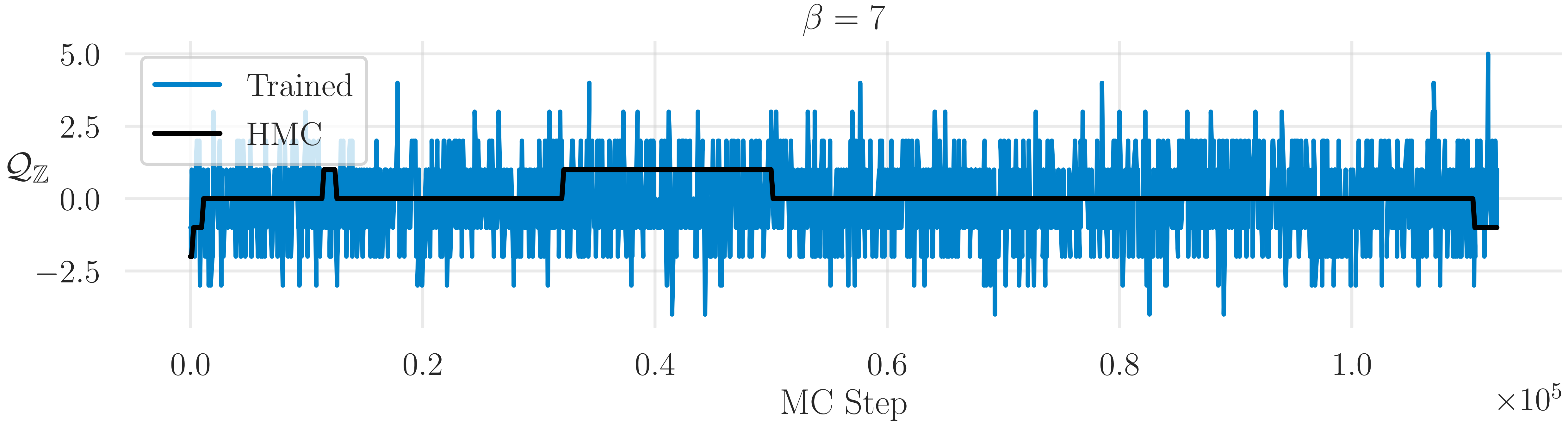
  - $\mathcal{Q}_\mathbb{Z} = \frac{1}{2\pi} \sum_P \lfloor x_P \rfloor \quad \in \mathbb{Z}$

    discrete, hard to work with

    $\lfloor x_P \rfloor = x_P - 2\pi \left\lfloor \frac{x_P + \pi}{2\pi} \right\rfloor$

Loss function, $\mathscr{L}(\theta)$

- We maximize the *expected squared charge difference:*
  - $\boxed{\mathscr{L}(\theta) = \mathbb{E}_{p(\xi)} \left[-\delta \mathcal{Q}^2_\mathbb{R}(\xi', \xi) \cdot A(\xi' | \xi) \right]}$
  - $\delta \mathcal{Q}^2_\mathbb{R}(\xi', \xi) = \left(\mathcal{Q}_\mathbb{R}(x') - \mathcal{Q}_\mathbb{R}(x) \right)^2$ *(squared charge diff.)*
  - $A(\xi' | \xi) = \min \left\{ 1, \frac{p(\xi')}{p(\xi)} \left| \frac{\partial \xi'}{\partial \xi^T} \right| \right\}$ *(acceptance prob.)*



Simulated Annealing

- Introduce an **annealing schedule** during the training phase:
  - $\boxed{\left\{\gamma_t\right\}_{t=0}^{N} = \left\{\gamma_0, \gamma_1, \ldots, \gamma_{N-1}, \gamma_N\right\},}$ ex: $\{0.1, 0.2, 0.3, \ \ldots, 0.9, 1.0\}$
  - $\gamma_0 < \gamma_1 < \cdots < \gamma_N \equiv 1,$ increasing
  - $\delta_\gamma \equiv \|\gamma_{t+1} - \gamma_t\| \ll 1$ varied *slowly*
- For $\|\gamma_t\| < 1$, this helps to rescale *(shrink)* the energy barriers between isolated modes
  - Allows sampler to explore previously inaccessible regions of the target distribution.
- Target distribution becomes:
  - $\boxed{p_t(x) \propto e^{-\gamma_t S_\beta(x)}, \text{ for } t = 0,1,\ldots,N}$

Training Algorithm

```
input:
    1. Loss function, L_θ(ξ', ξ, A(ξ'|ξ))
    2. Batch of initial states, x
    3. Learning rate schedule, {α_t}_{t=0}^{N_train}
    4. Annealing schedule, {γ_t}_{t=0}^{N_train}
    5. Target distribution, p_t(x) ∝ e^{-γ_t S_β(x)}
Initialize weights θ
for 0 ≤ t < N_train :
  | resample  v ~ N(0, 𝟙)
  | resample  d ~ U(+, −)
  | construct  ξ_0 ≡ (x_0, v_0, d_0)
  | for 0 ≤ k < N_LF :
  |   | propose (leapfrog layer)  ξ'_k ← ξ_k
  | compute  A(ξ'|ξ) = min{1, p(ξ')/p(ξ) |∂ξ'/∂ξ^T|}
  | update  L ← L_θ(ξ', ξ, A(ξ'|ξ))
  | backprop  θ ← θ − α_t ∇_θ L
  | assign  x_{t+1} ← { x'  with probability A(ξ'|ξ)
  |                   { x   with probability (1 − A(ξ'|ξ)).
```

re-sample
momentum
+ direction

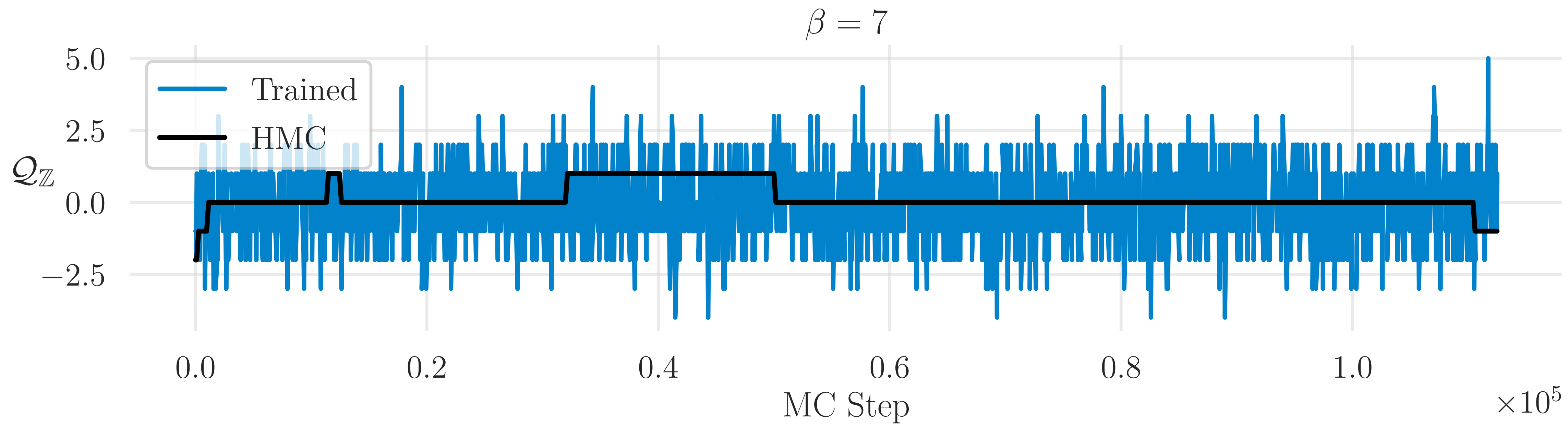
construct
trajectory

Compute loss
+ backprop

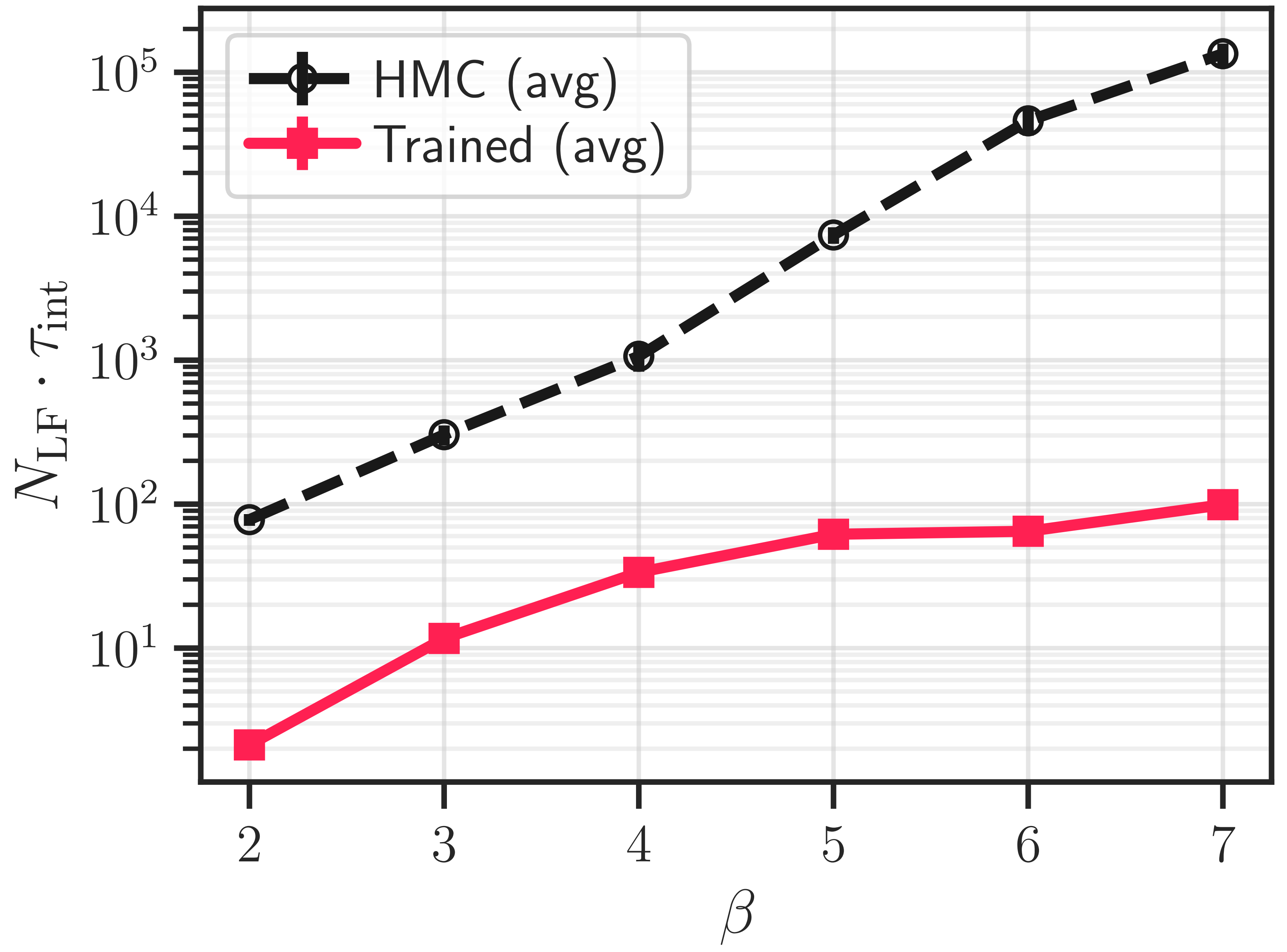
Metropolis-Hastings
accept/reject

Results

- Want to calculate $\langle \mathcal{O} \rangle \propto \int [\mathcal{D}x]\, \mathcal{O}(x) e^{-S(x)}$
- If we had *independent* configurations, we could approximate by
  - $\langle \mathcal{O} \rangle \simeq \frac{1}{N} \sum_{n=1}^{N} \mathcal{O}(x_n) \rightarrow \sigma^2 = \frac{1}{N} \mathrm{Var}\left[\mathcal{O}(x)\right]$
- Accounting for *autocorrelation*: $\sigma^2 = \frac{\tau_{\mathrm{int}}^{\mathcal{O}}}{N} \mathrm{Var}\left[\mathcal{O}(x)\right]$
- We measure the performance of our model by looking at the *integrated autocorrelation time*, τ_{int} of the topological charge $\mathcal{Q}_{\mathbb{Z}}$.
- For generic HMC, it is known that τ_{int} grows exponentially as $\beta \rightarrow \infty$ **(critical slowing down)**



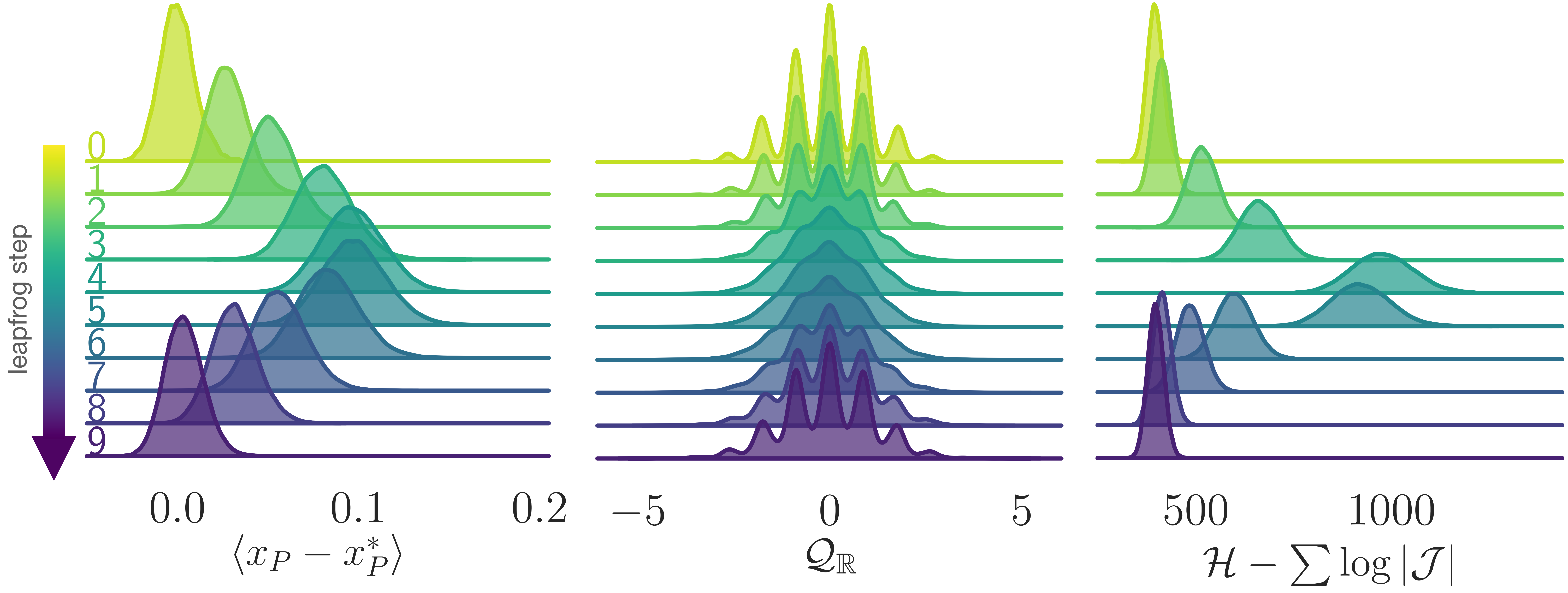
(d.) Plot of the topological charge history $\mathcal{Q}_{\mathbb{Z}}$ vs MC Step



(c.) Estimate of the integrated autocorrelation time τ_{int} vs β for both the trained model and generic HMC.

Interpretation

- Look at how different quantities evolve over the course of a trajectory (N_{LF} leapfrog layers)
  - See that the sampler artificially *increases the energy* during the first half of the trajectory

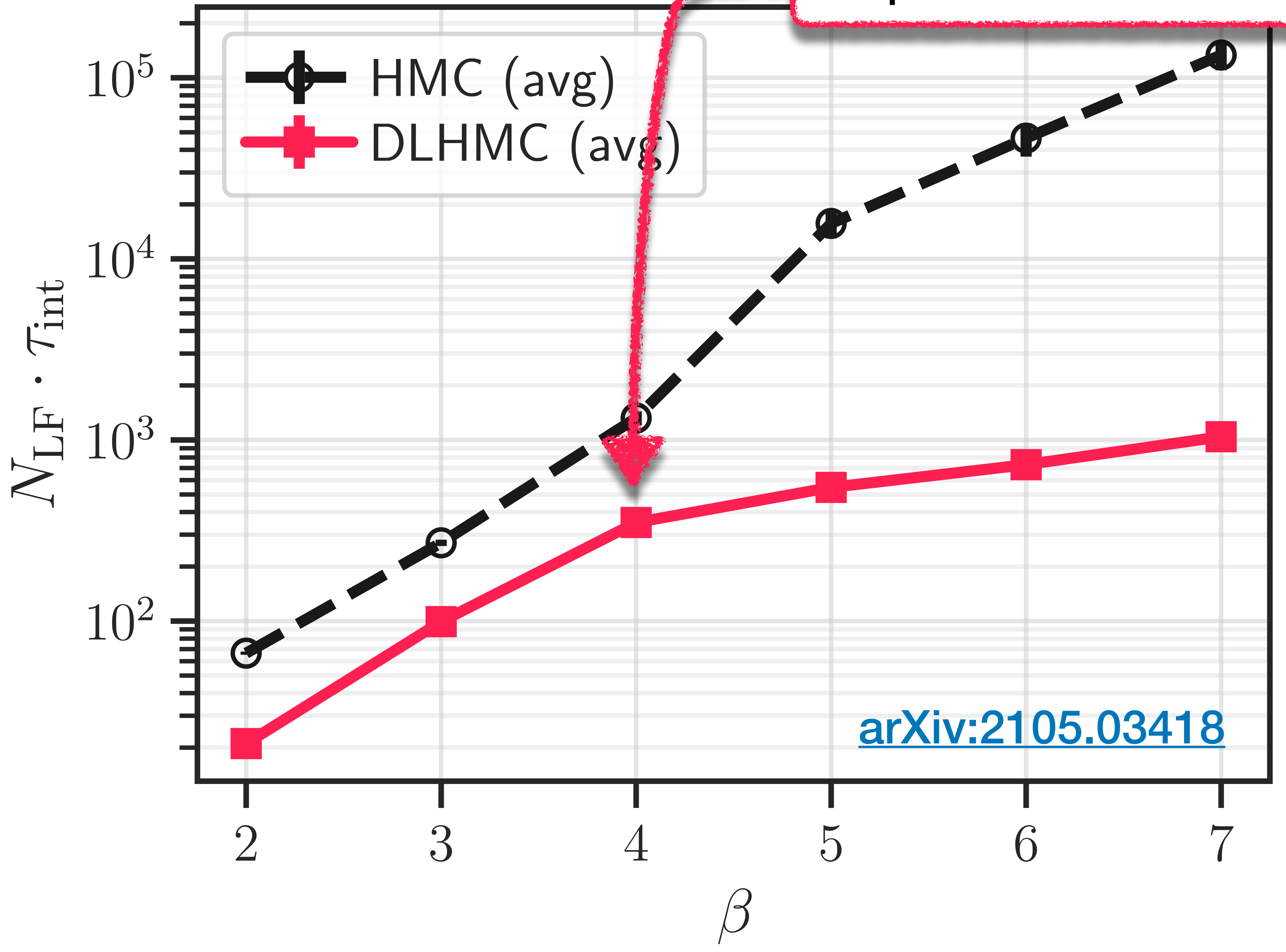


(a.) Deviation in the average plaquette, x_P

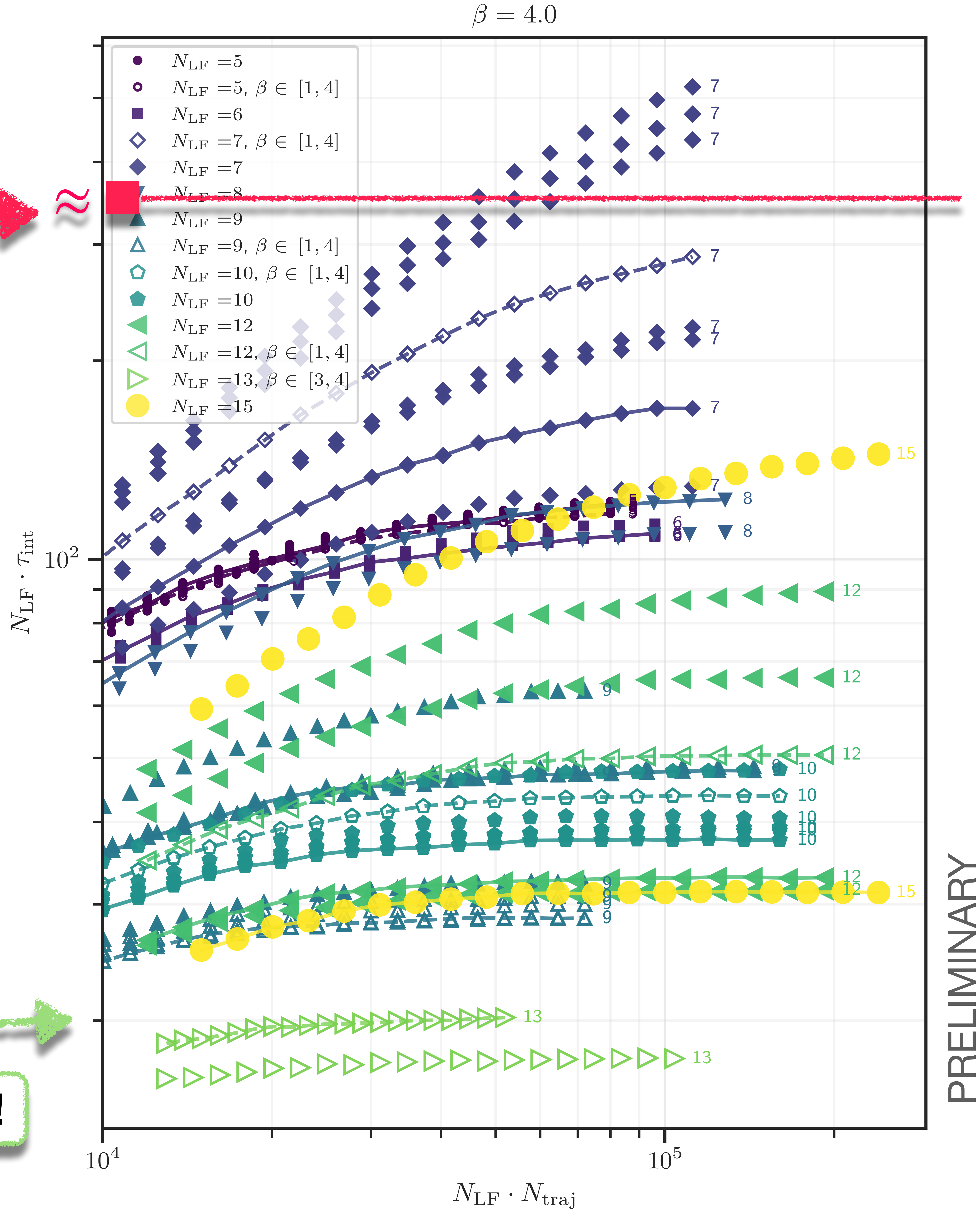
(b.) Evolution of the continuous charge $\mathcal{Q}_{\mathbb{R}}$

(c.) Evolution of the effective energy

New Results



this point would be here

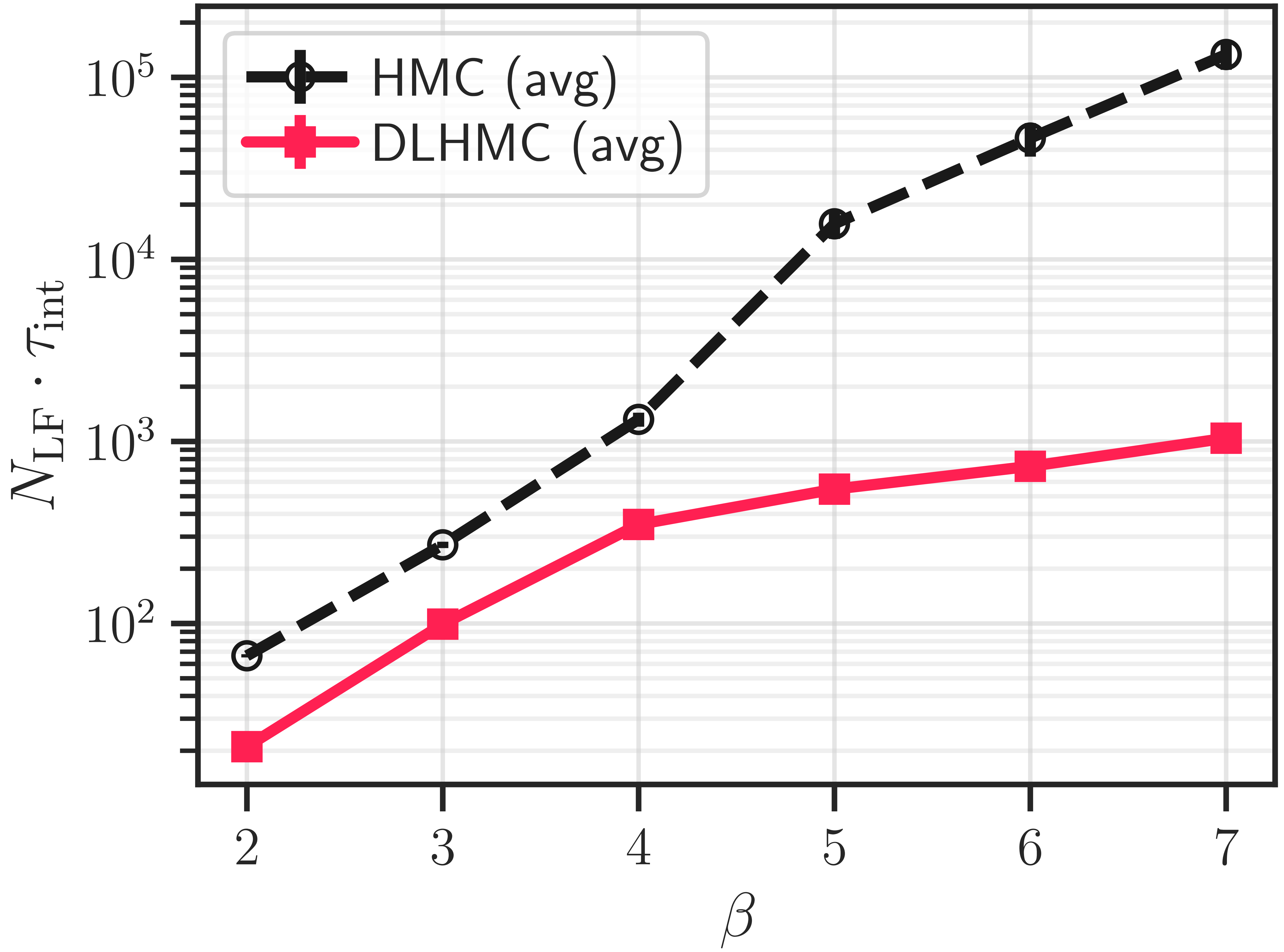


- **Better performance:** $\approx$**10** $\times$ previous results

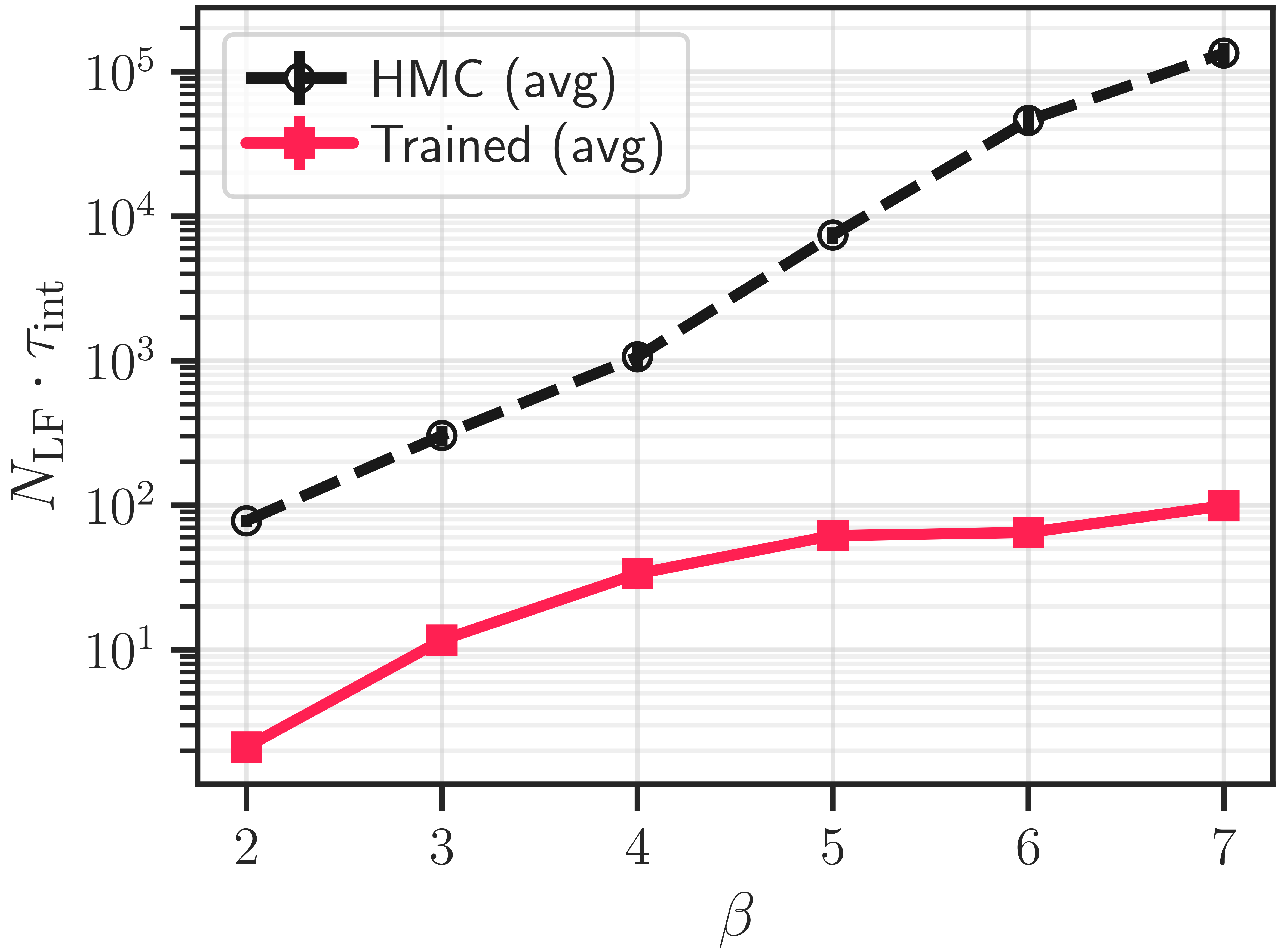
New networks!

Comparison

previous (from arXiv:2105.03418)



new (preliminary)



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EXASCALE COMPUTING PROJECT

l2hmc-qcd

Sam Foreman*, Xiao-Yong Jin, & James C. Osborn

A trainable framework for accelerating HMC on lattice gauge models.

[arXiv:2105:03418](https://arxiv.org/abs/2105.03418) bit.ly/l2hmc-lattice21 github.com/saforem2/l2hmc-qcd

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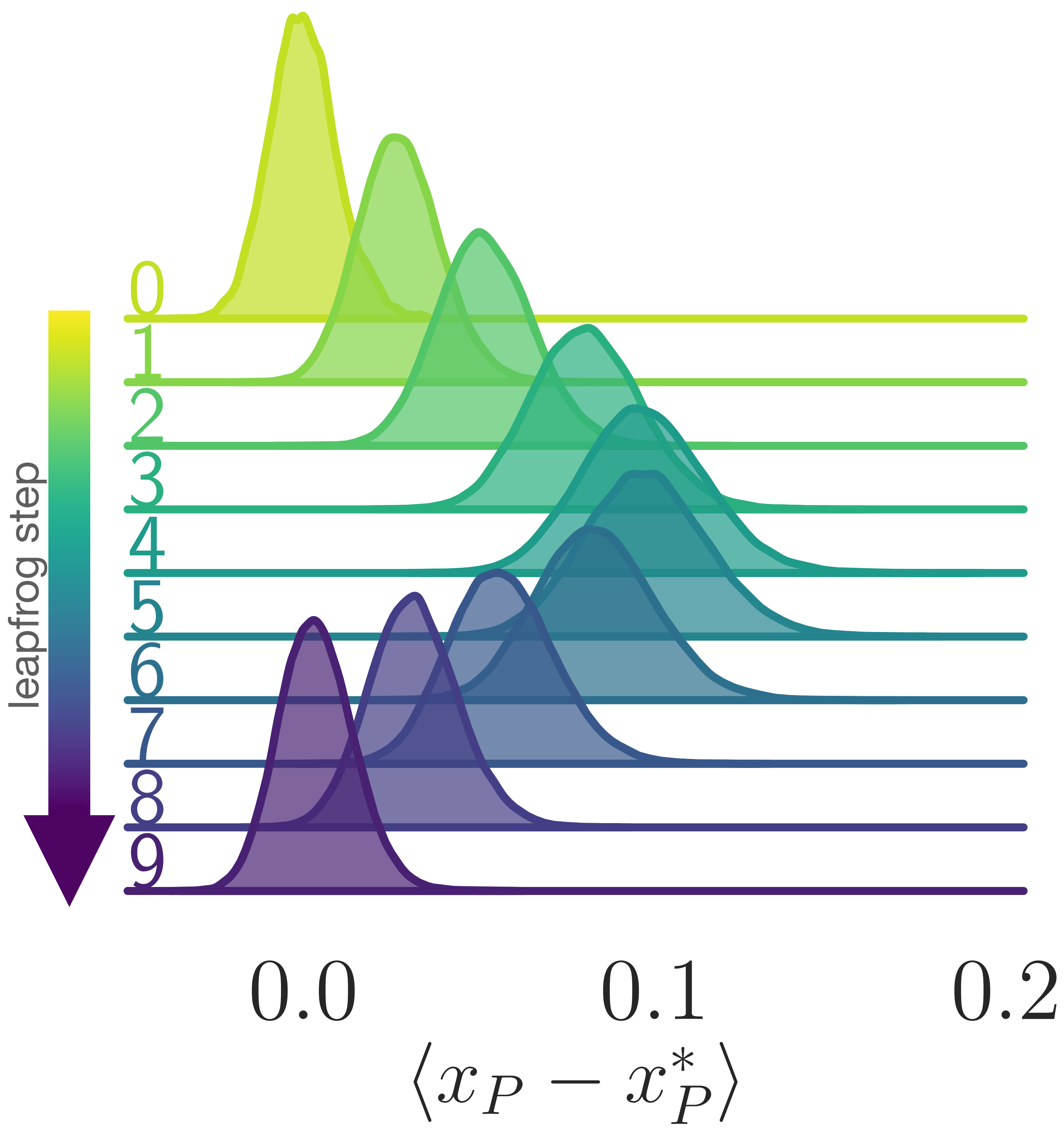
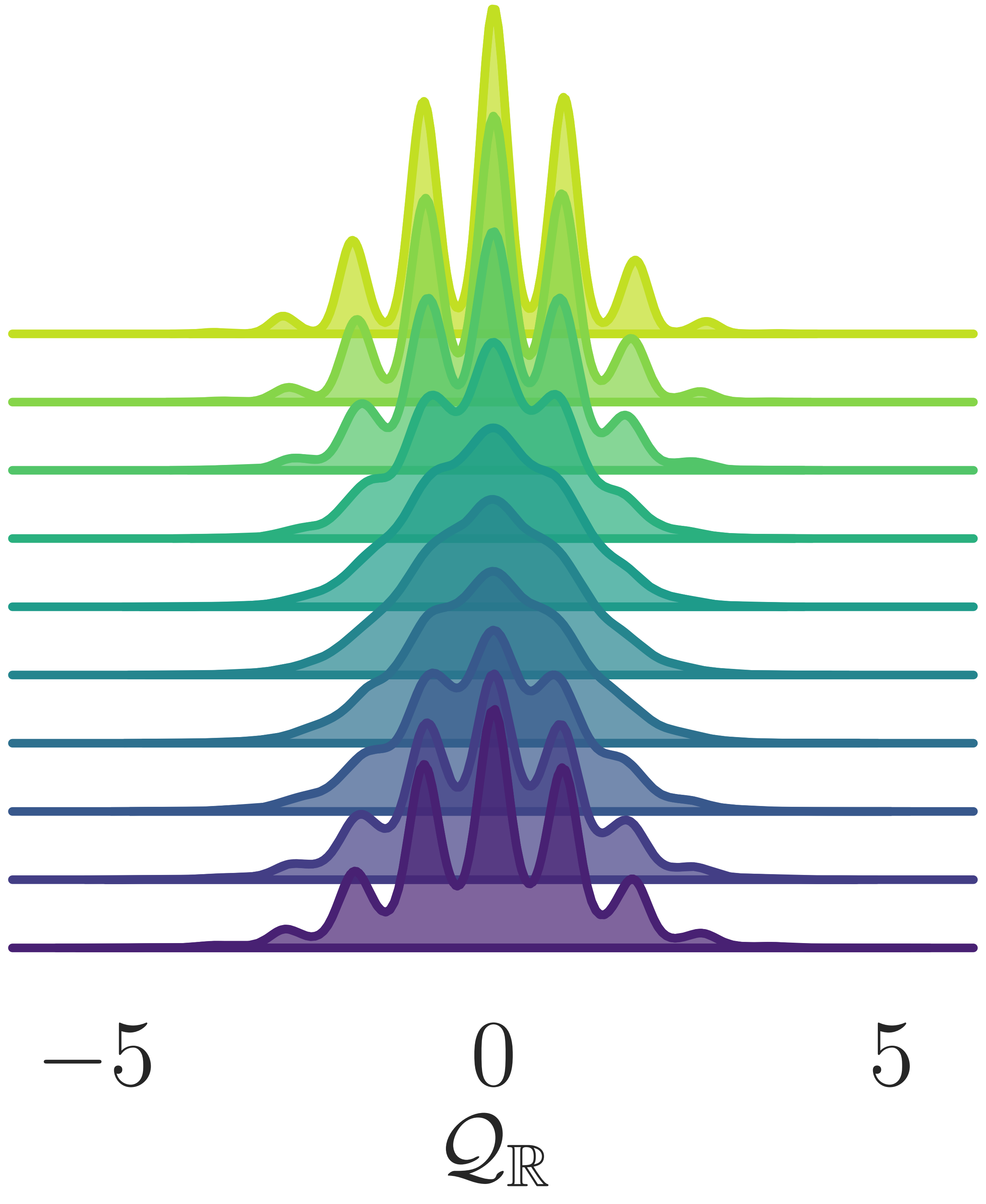
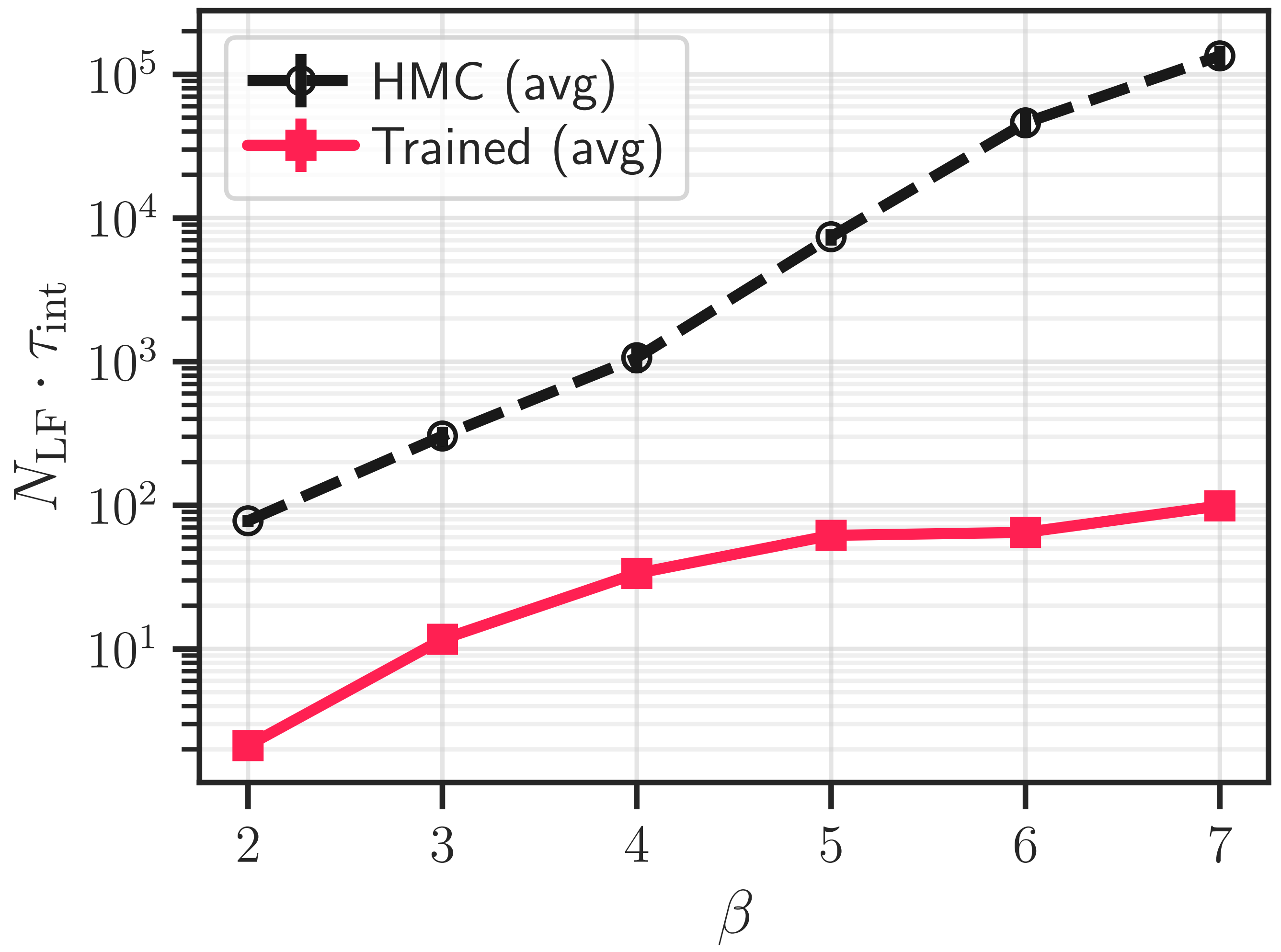


(a.) Deviation in the average plaquette, x_P over a single trajectory.

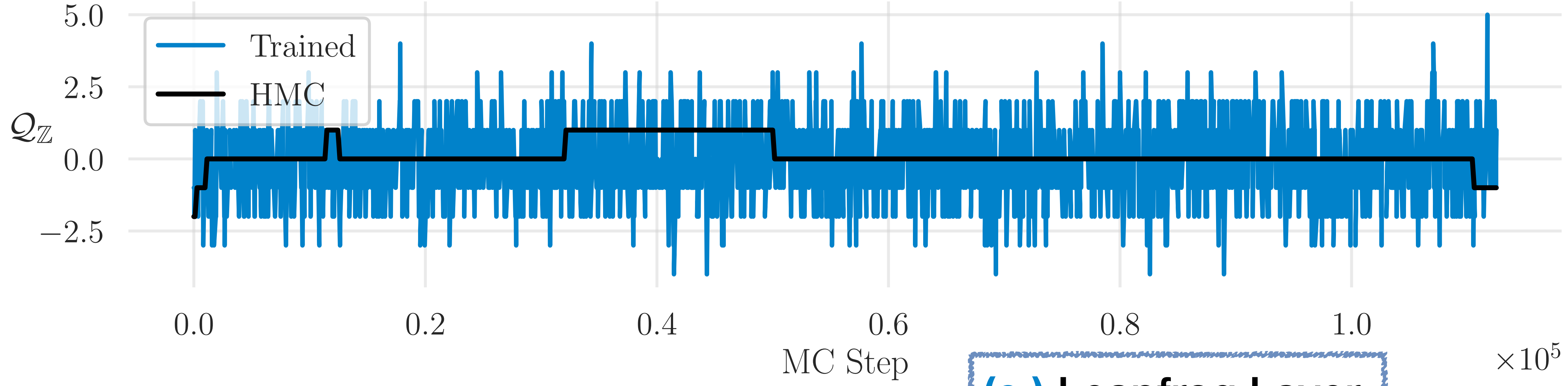


(b.) Evolution of $\mathcal{Q}_{\mathbb{R}} = \frac{1}{2\pi}\sum_P \sin x_P \in \mathbb{R}$

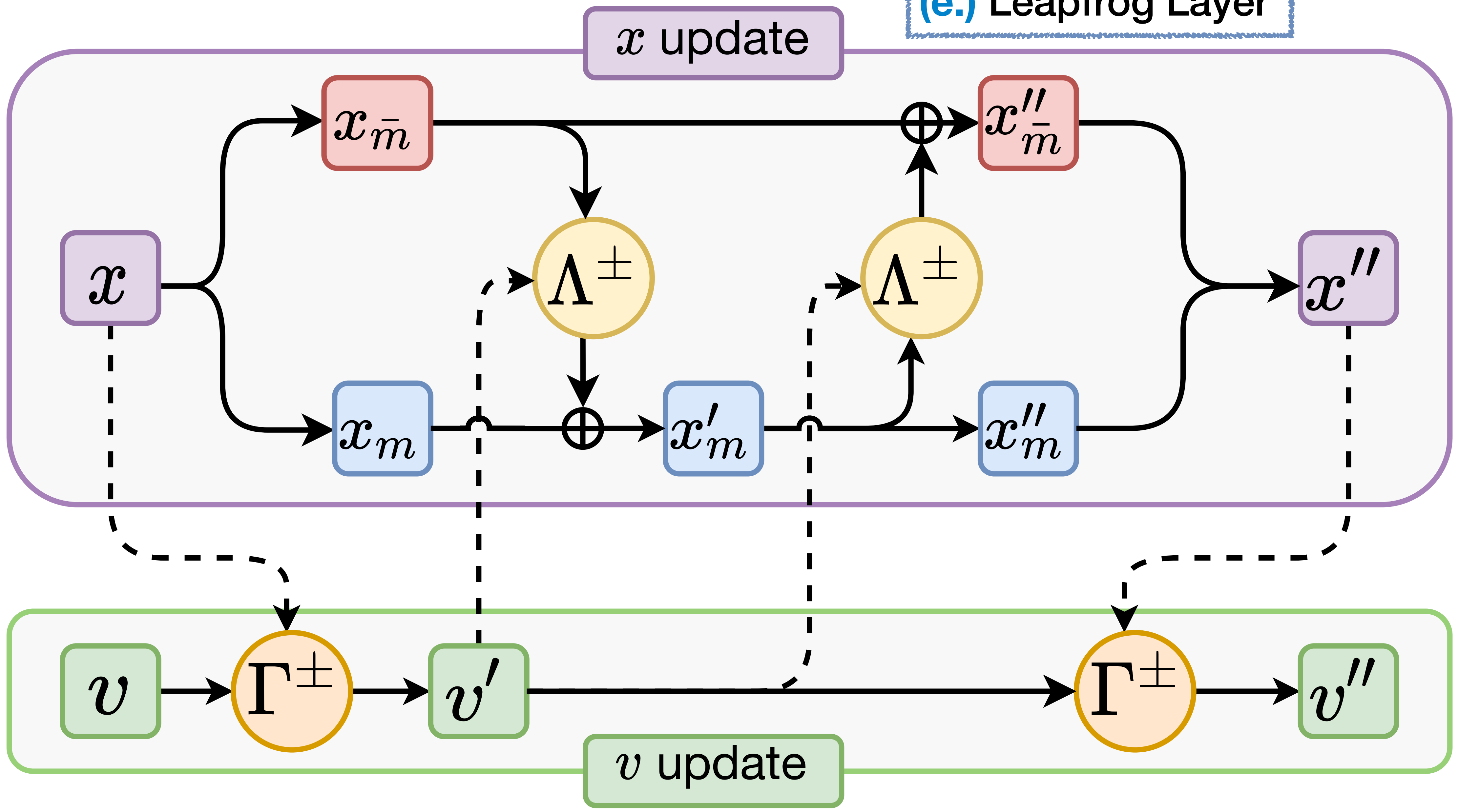


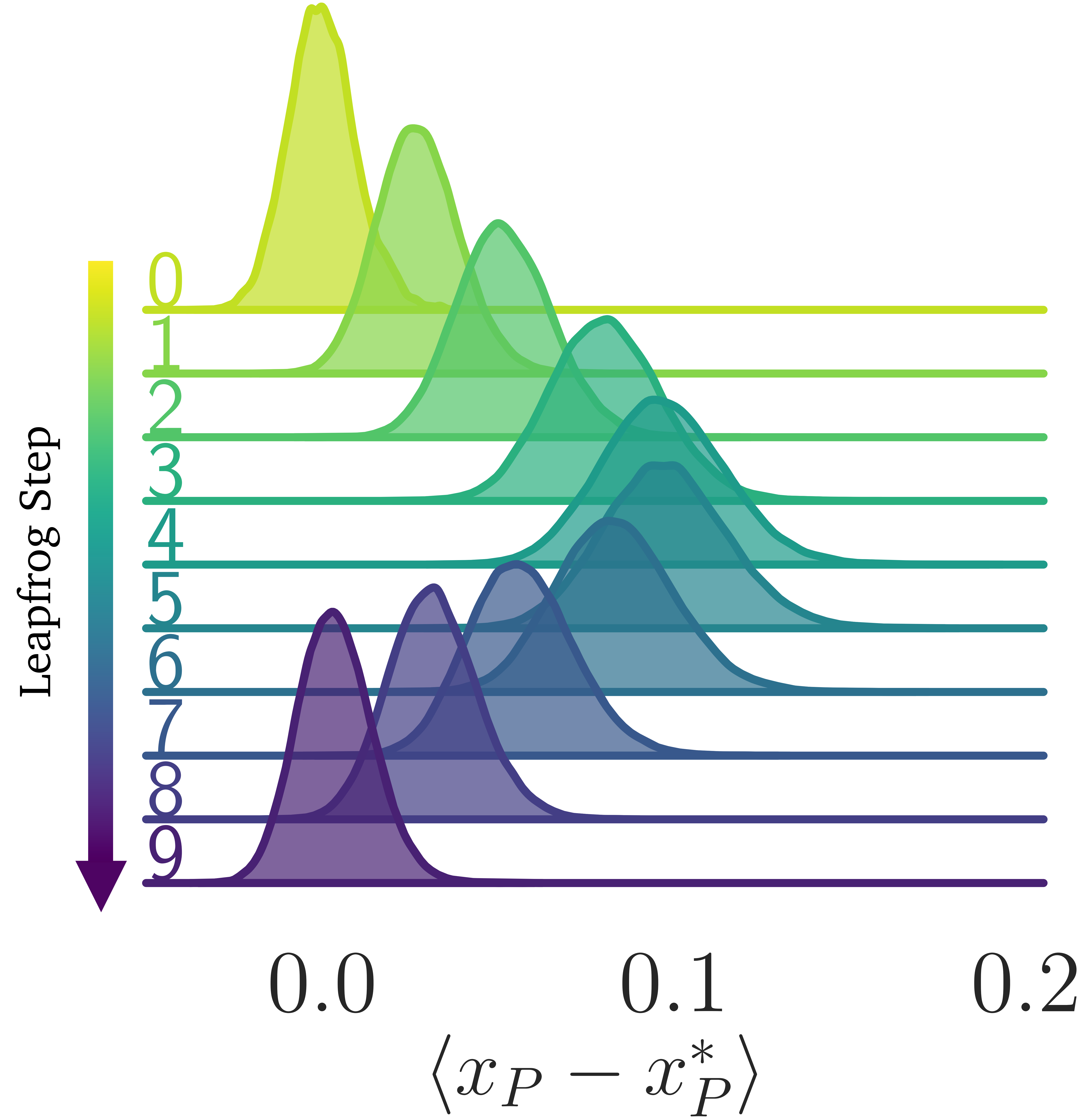
(c.) Estimate of the integrated autocorrelation time τ_{int} of $\mathcal{Q}_{\mathbb{Z}} \in \mathbb{Z}$

(d.) Topological charge history



(e.) Leapfrog Layer





Leapfrog Step
0
1
2
3
4
5
6
7
8
9
0.0
0.1
0.2
$\langle x_P - x_P^* \rangle$