28.07.2026 — College Park, Md

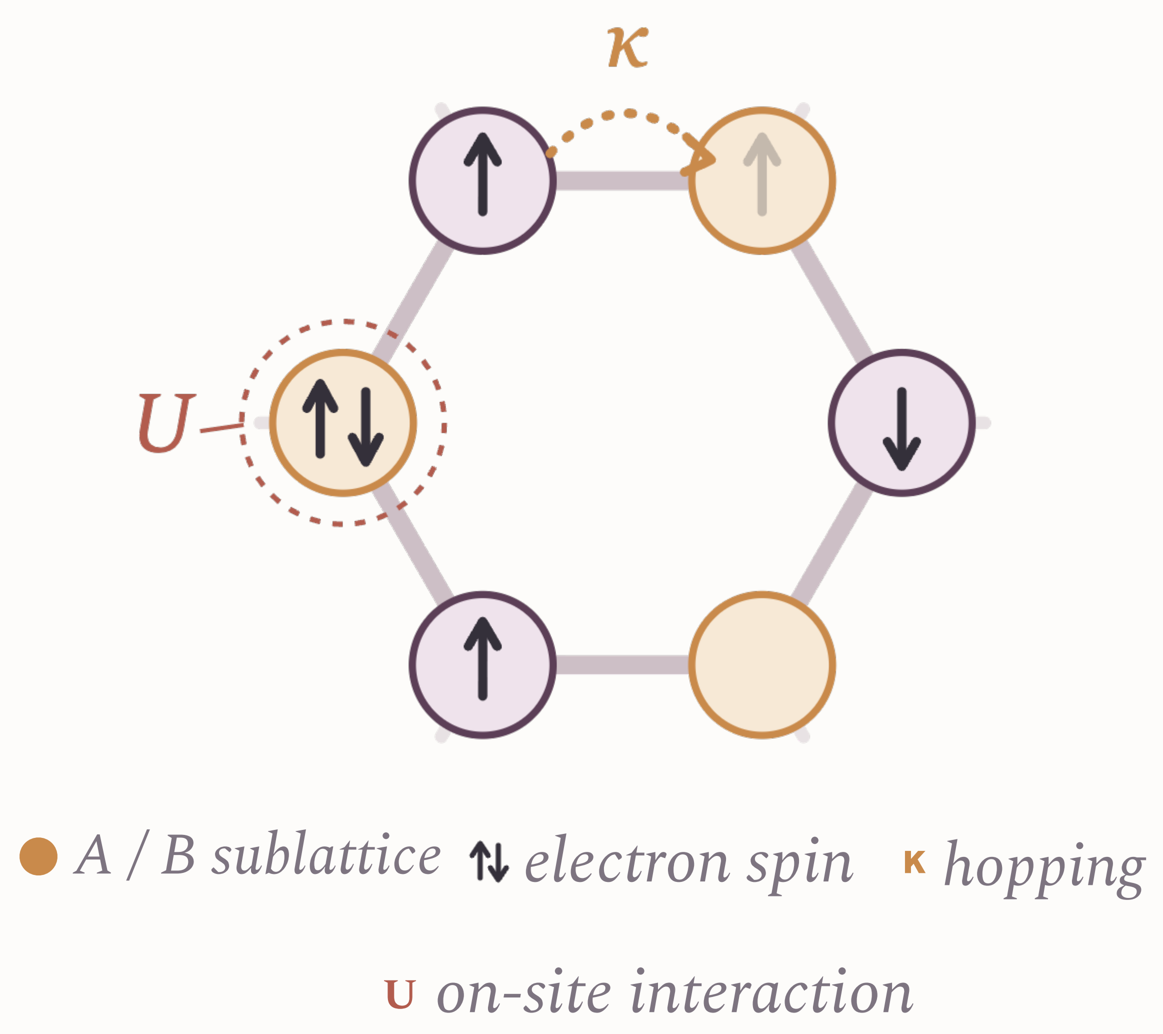
Tackling the Sign Problem in the Doped Hubbard Model with Normalizing Flows

Dominic Schuh

University of Bonn · TRA Matter · Helmholtz-Institute for Radiation and Nuclear Physics

The Hubbard Model

$$H = -\kappa \sum_{\langle x,y \rangle} \left(a^\dagger_{x,\uparrow} a_{y,\uparrow} + a^\dagger_{x,\downarrow} a_{y,\downarrow} \right) - \frac{U}{2} \sum_x \left(n_{x,\uparrow} - n_{x,\downarrow} \right)^2 - \mu \sum_x q_x$$



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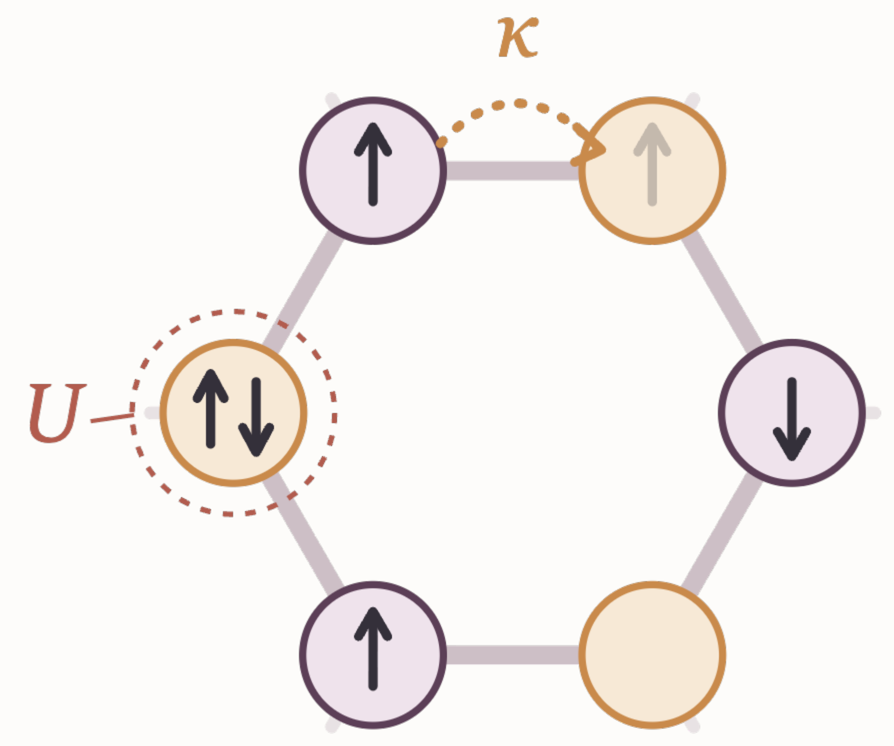
- **Mott insulator**
- **Magnetism**
- **Superconductivity**



● *A / B sublattice* ⇅ *electron spin* κ *hopping*

U *on-site interaction*

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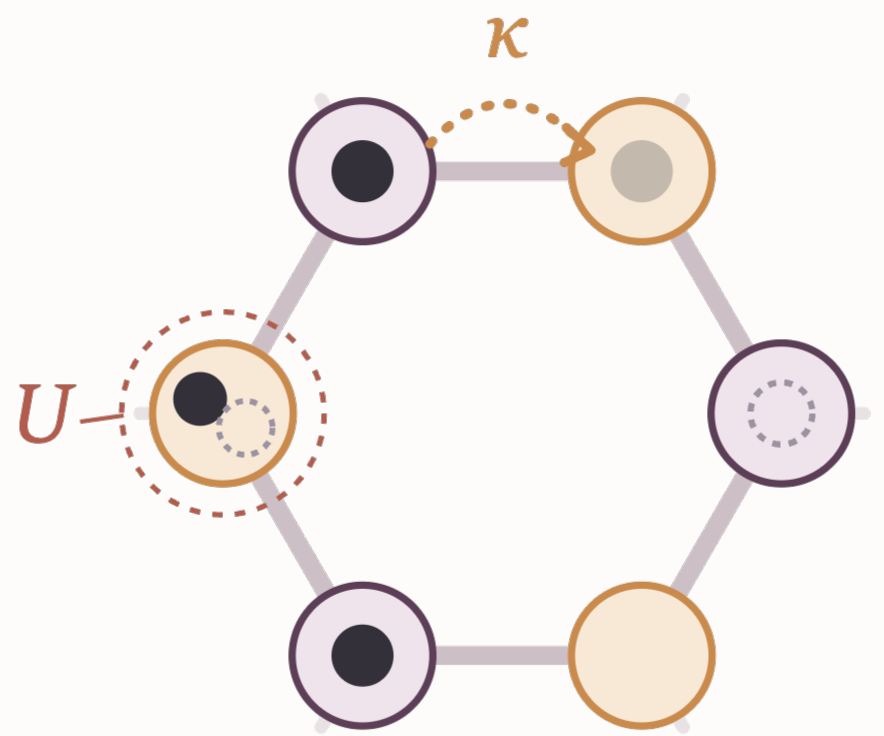

A / B sublattice *particle / hole* κ *hopping*

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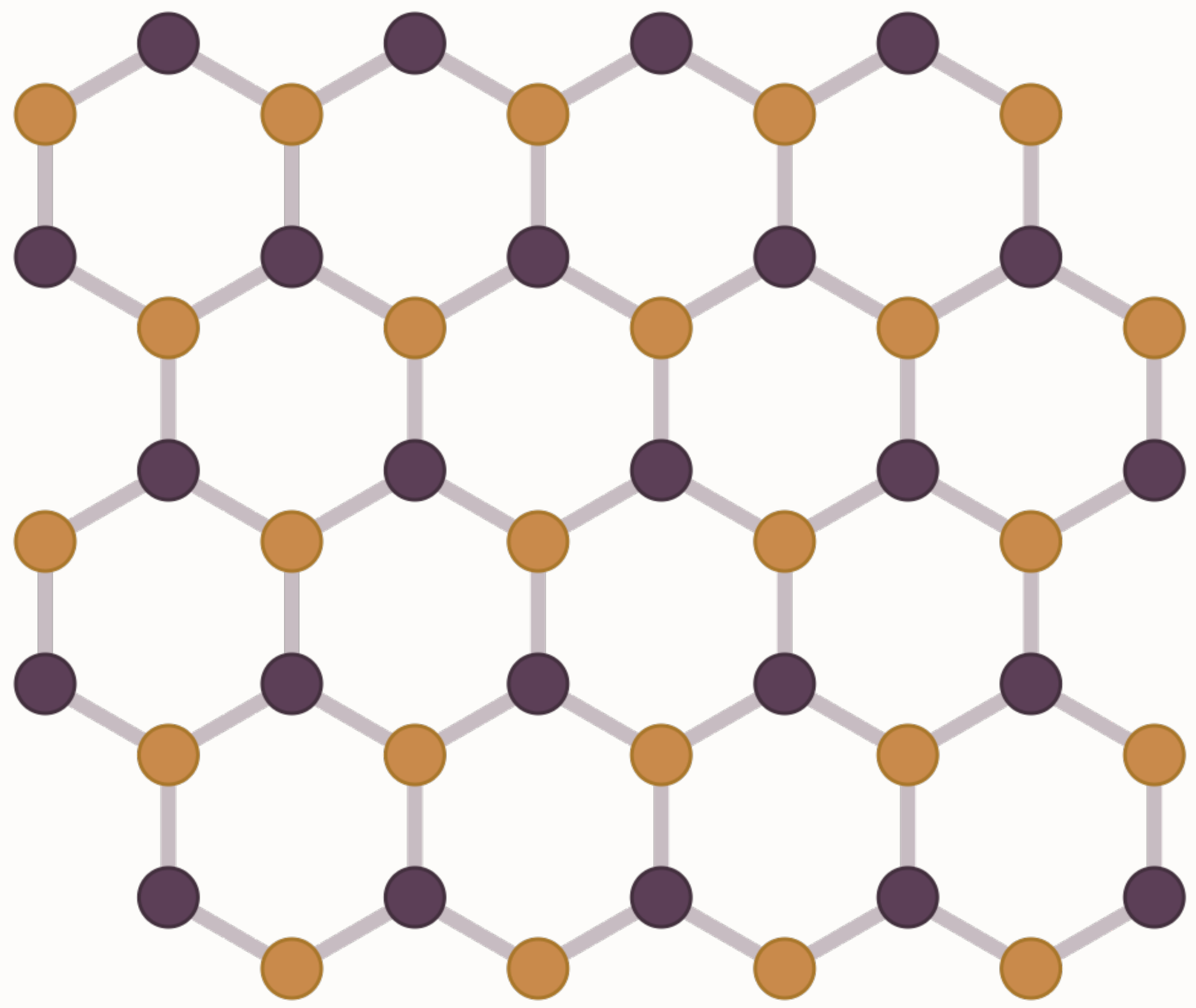
$$\Big\downarrow \ \text{Hubbard-Stratonovich transformation}$$

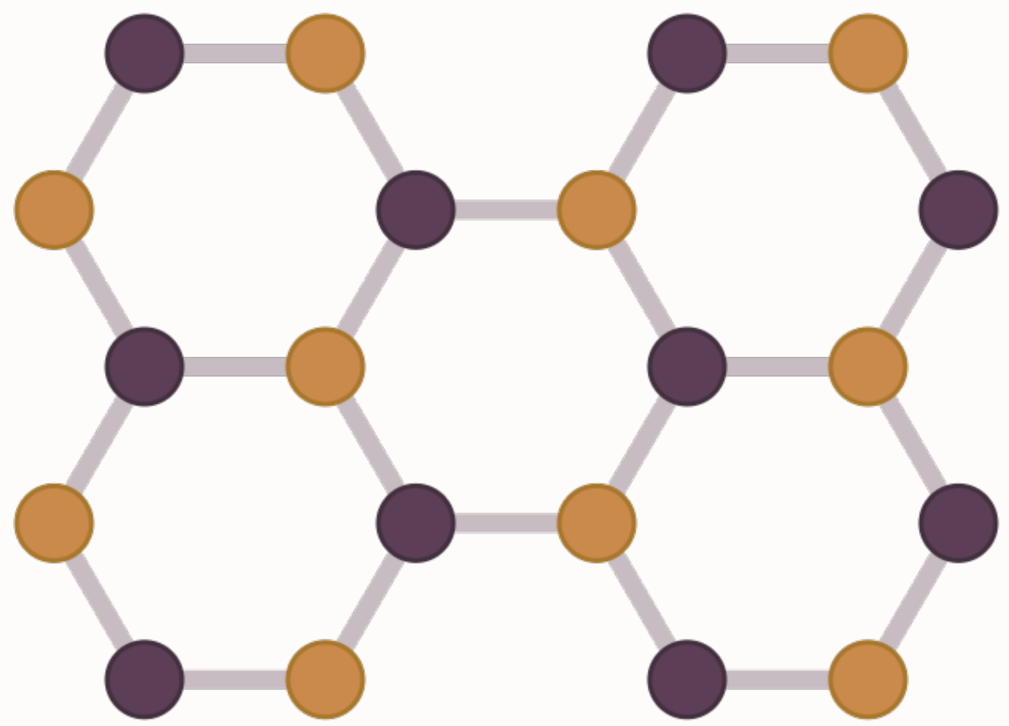
$$S[\phi] = \frac{1}{2\tilde{U}} \sum_{x,t} \phi^2_{x,t} - \log\det M[\phi \,|\, \mu] - \log\det M[-\phi \,|\, \mu]$$

Carbon-based systems



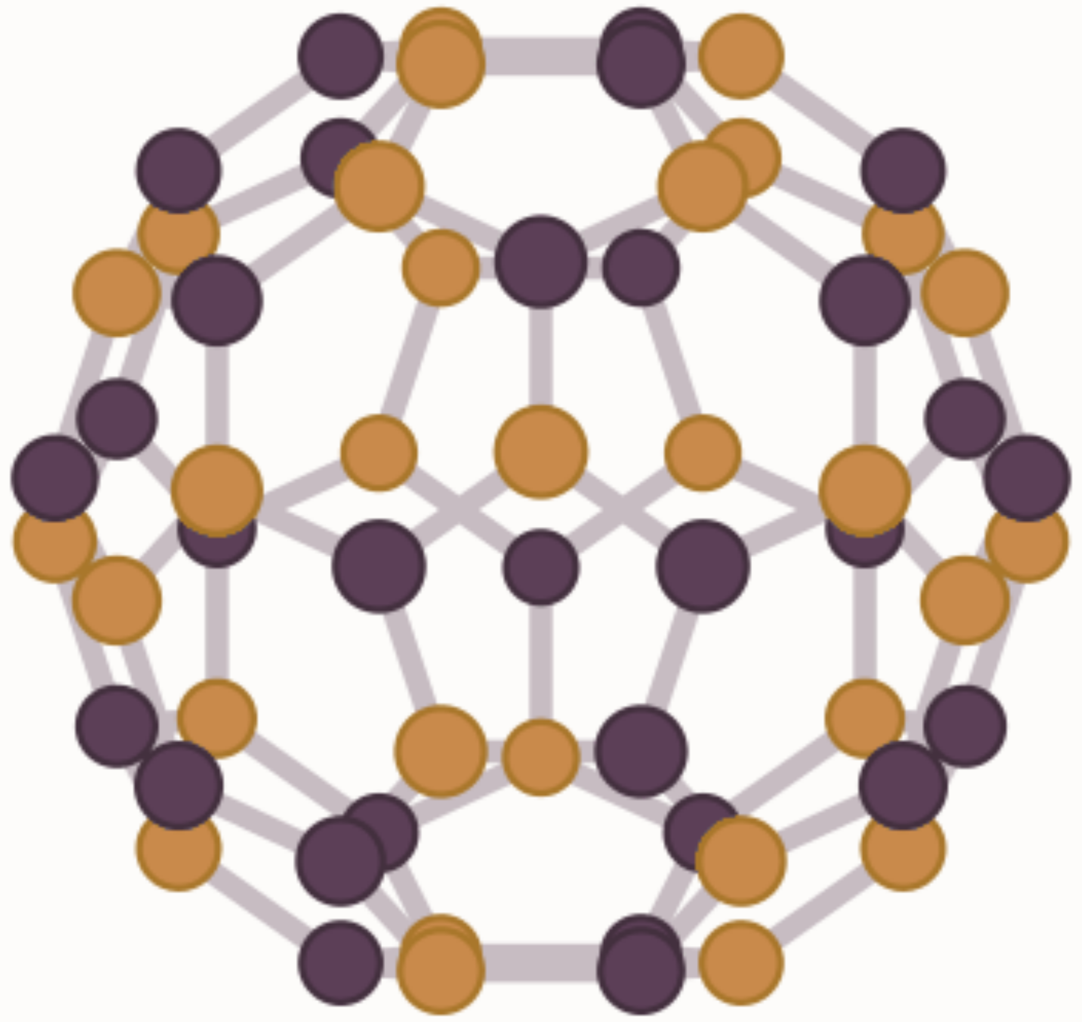
Graphene

Ostmeyer, et al. PRB 2021



$C_{20}H_{12}$

Rodekamp, et al. EPJB 2025

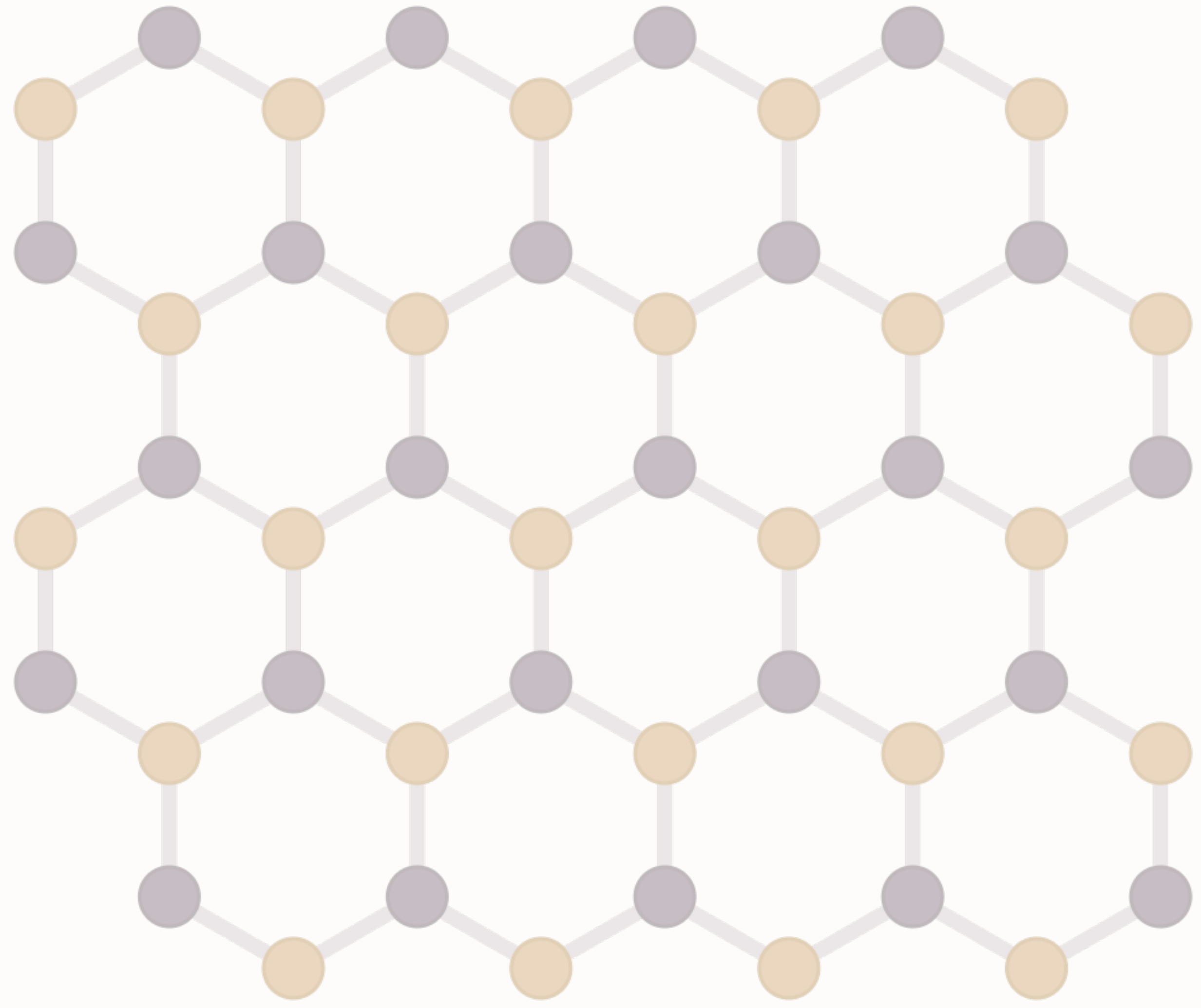


C_{60} Fullerene

Gäntgen, et al. PRB 2024

Carbon-based systems

Talk by
Janik Kreit!



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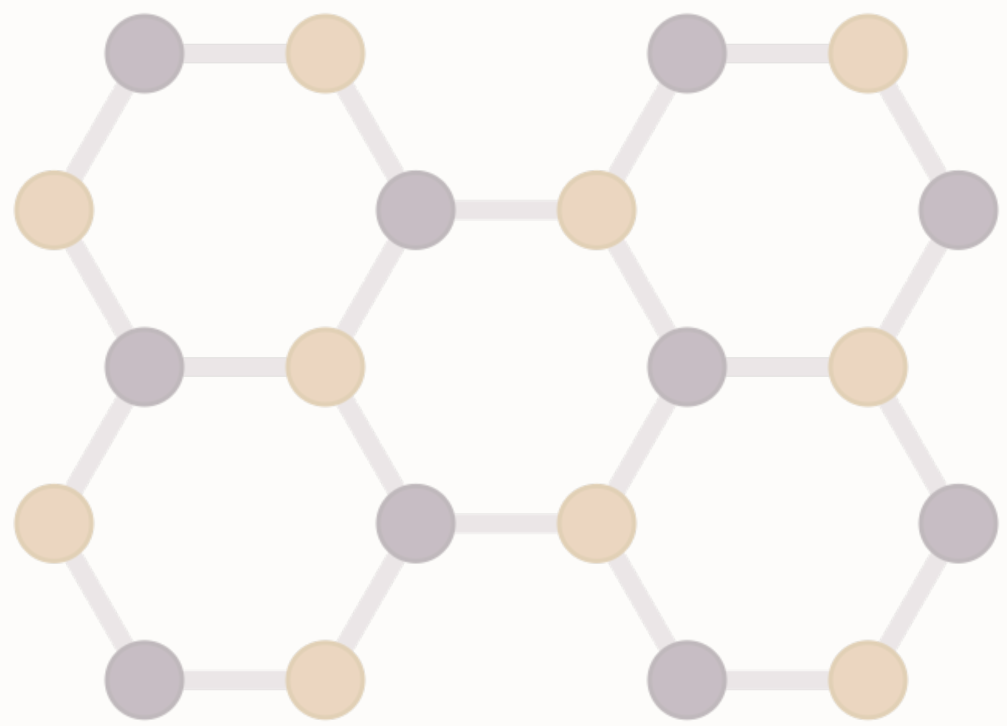

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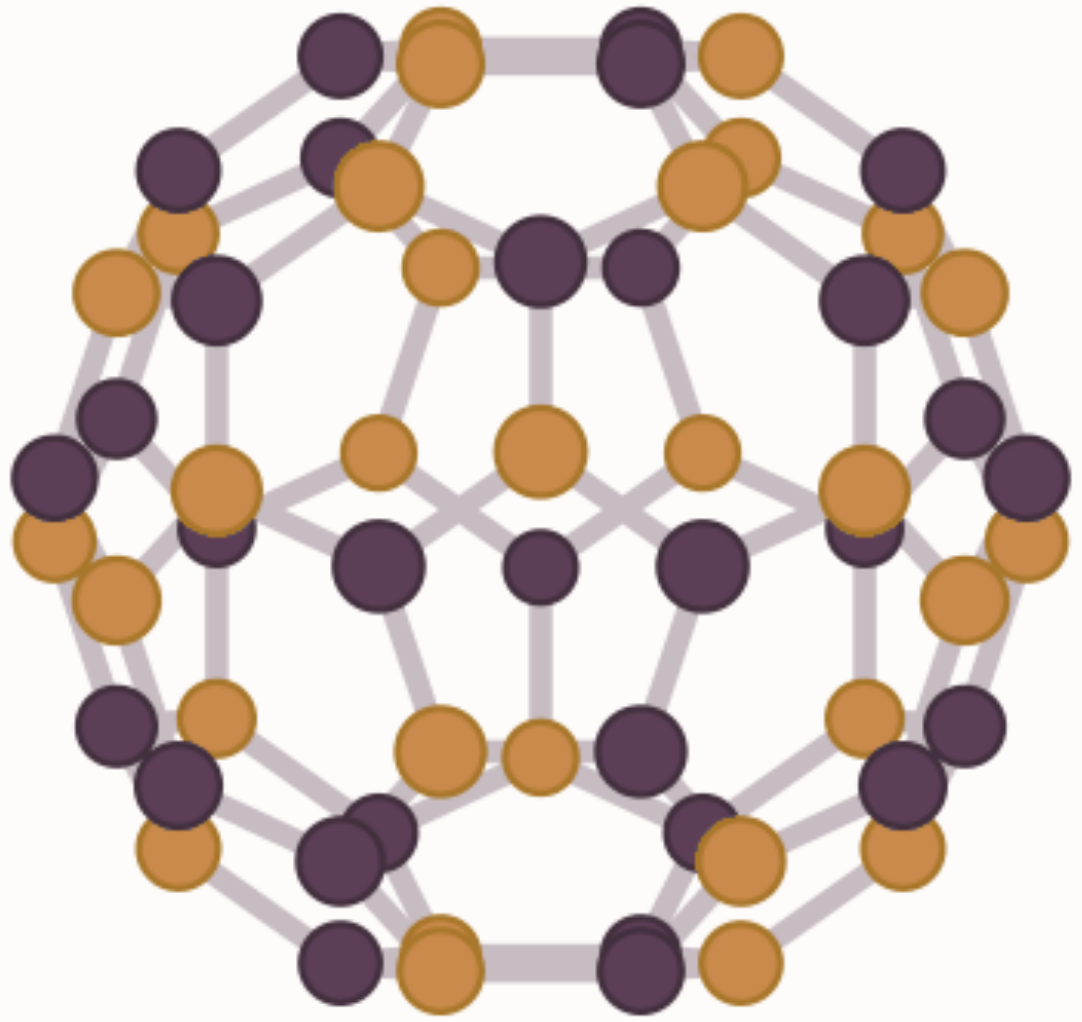

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Flow-based generative sampling

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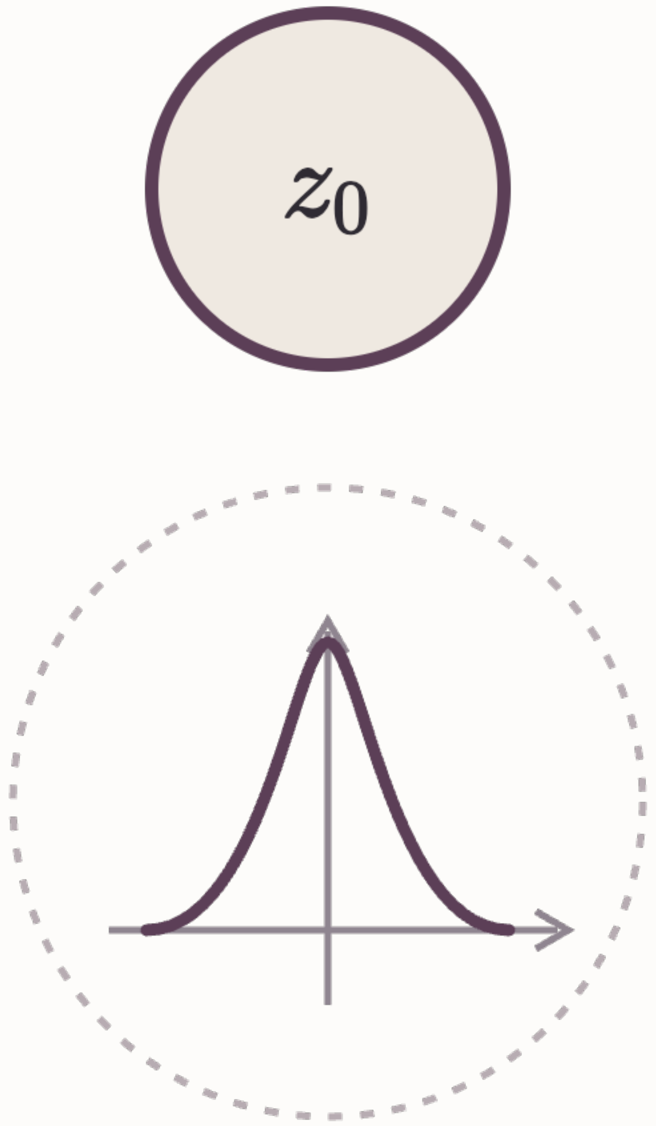
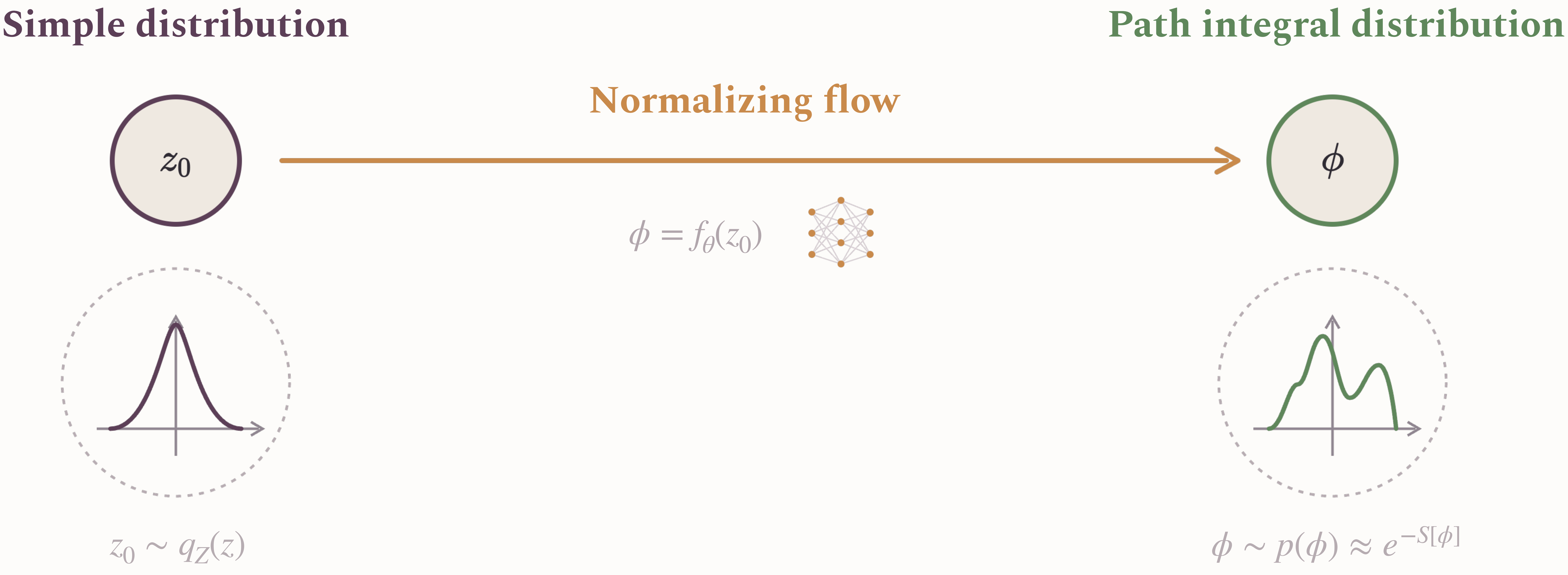
Simple distribution



$z_0 \sim q_Z(z)$

D. Rezende & S. Mohamed, ICML 2016 · M. Albergo et al., PRD 2019

Flow-based generative sampling



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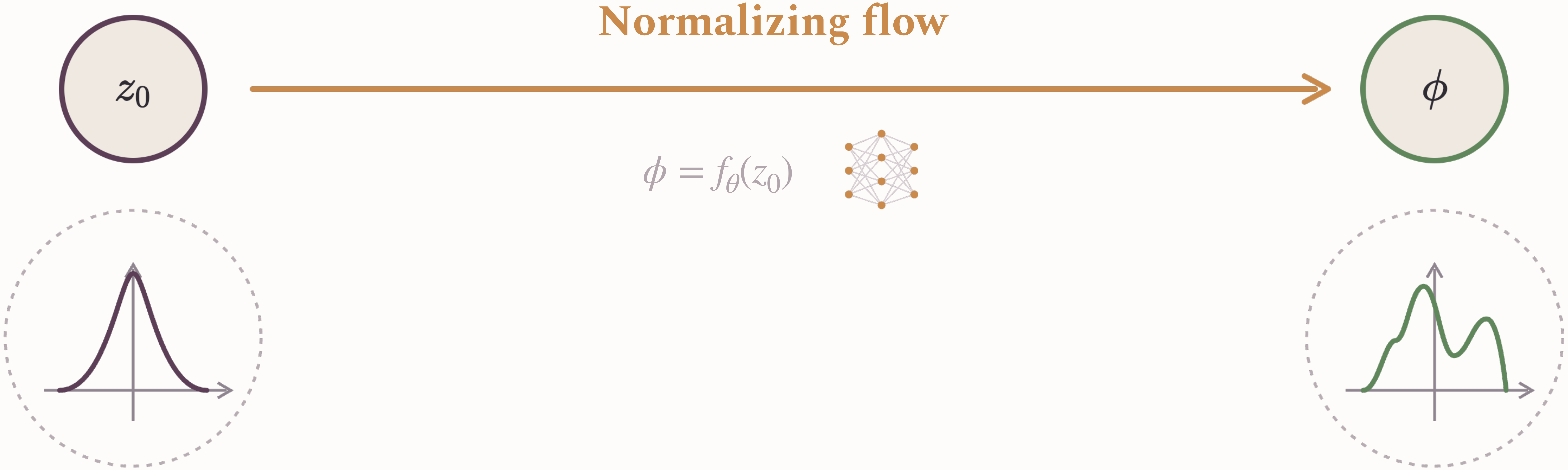
(Approximate) Path integral distribution

Normalizing flow



$z_0 \sim q_Z(z)$

$\phi \sim p(\phi) \approx e^{-S[\phi]}$

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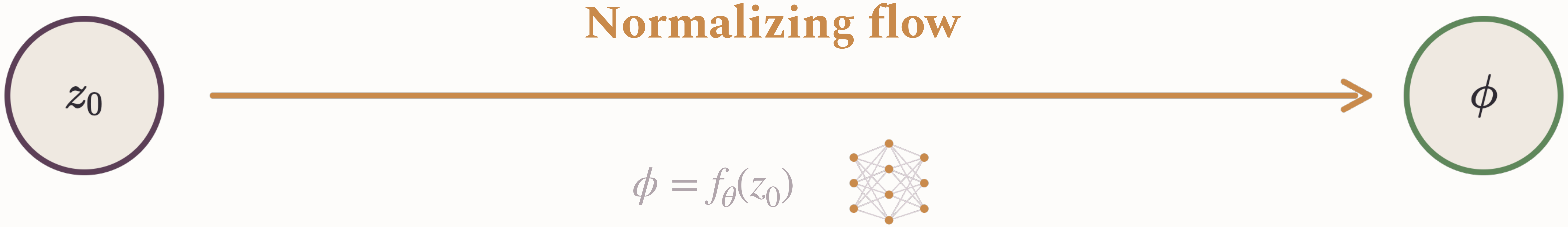

> Invertibility allows for tractable and exact probability estimation, enabling reweighting and and an ***asymptotically unbiased*** estimator.

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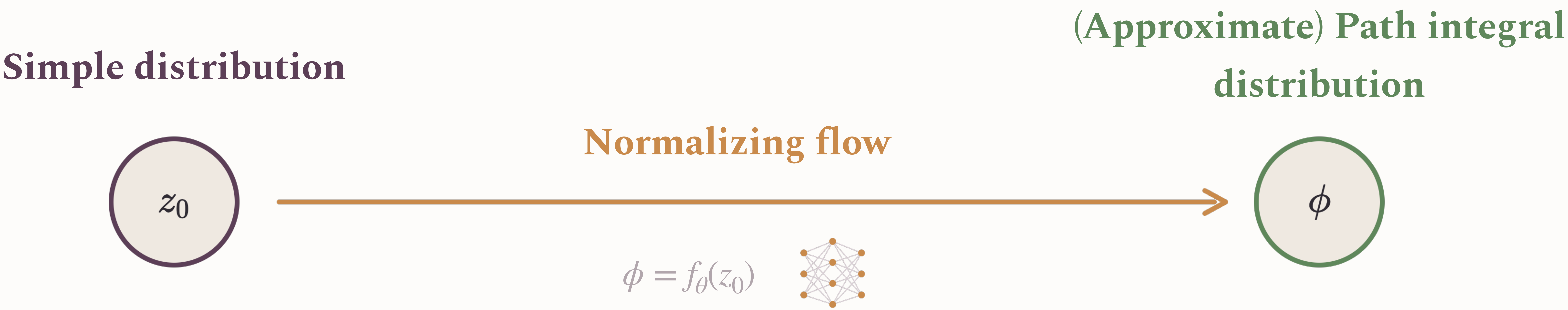

Invertibility allows for tractable and exact probability estimation, enabling reweighting and and an ***asymptotically unbiased*** estimator.

- Sampling is i.i.d. and highly parallelizable
- Data free training

D. Rezende & S. Mohamed, ICML 2016 · M. Albergo et al., PRD 2019 · K. Nicoli et al., PRE 2019

The sign problem in the Hubbard model

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Finite chemical potential μ breaks the charge symmetry that kept the probability weight positive and real.

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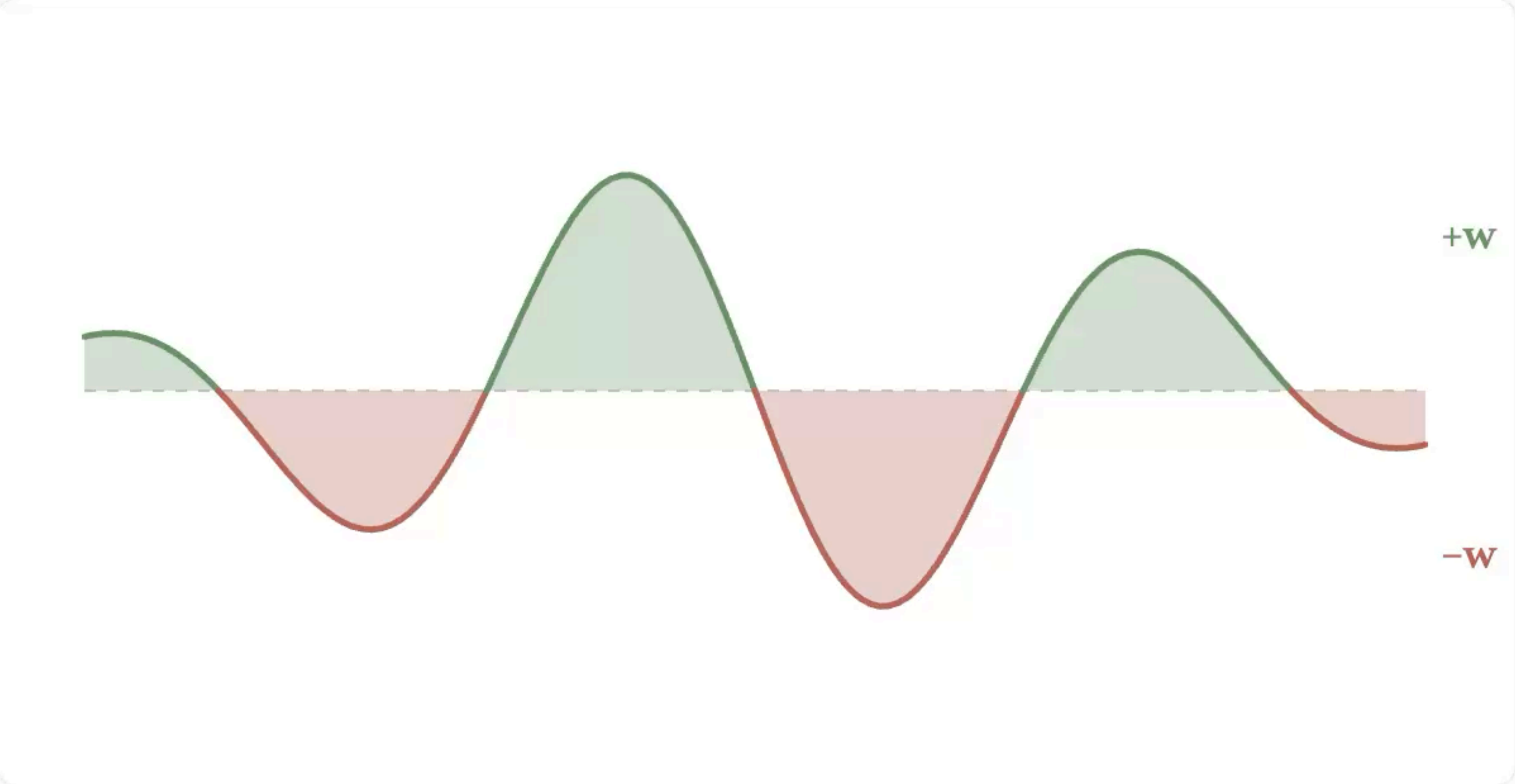

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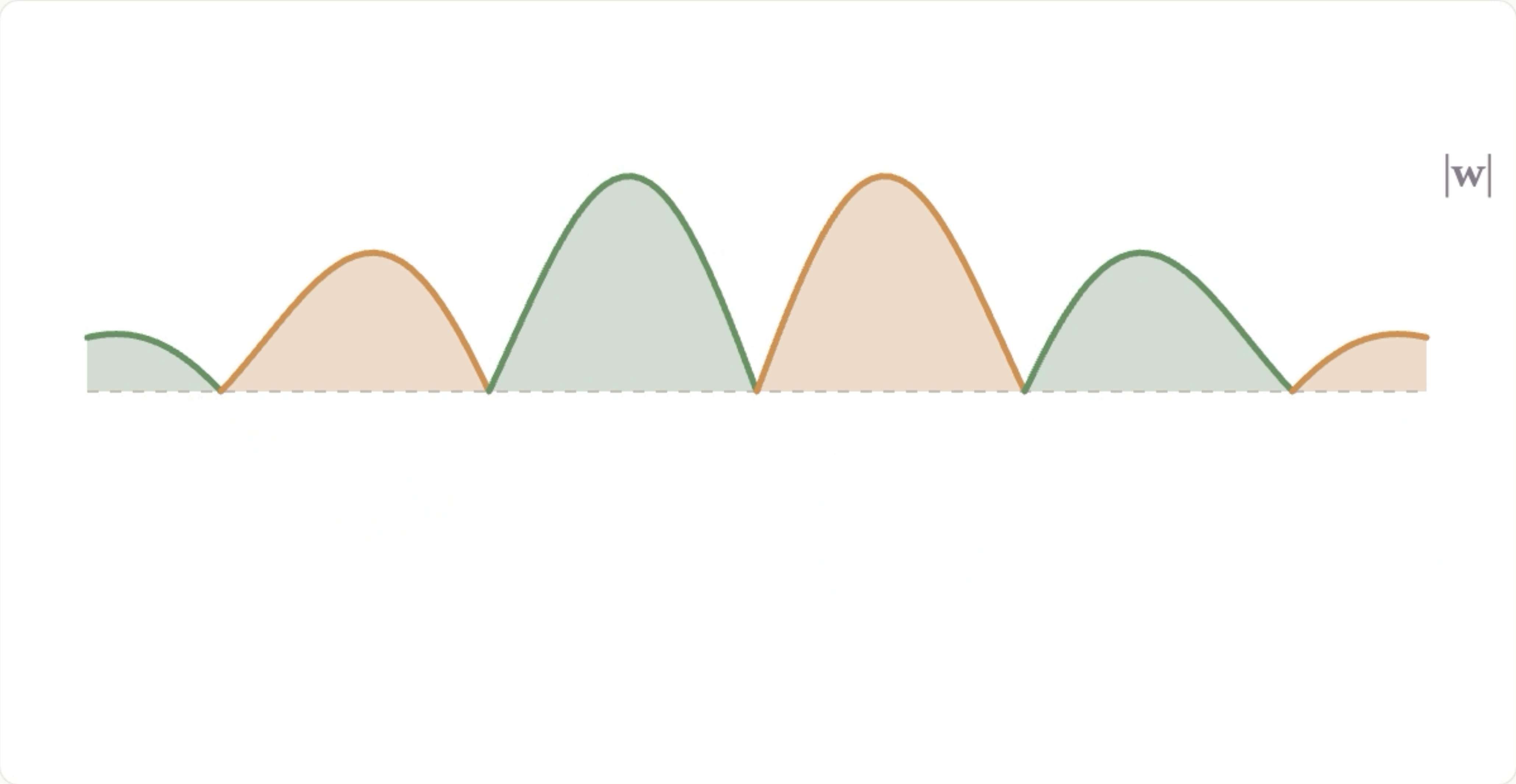

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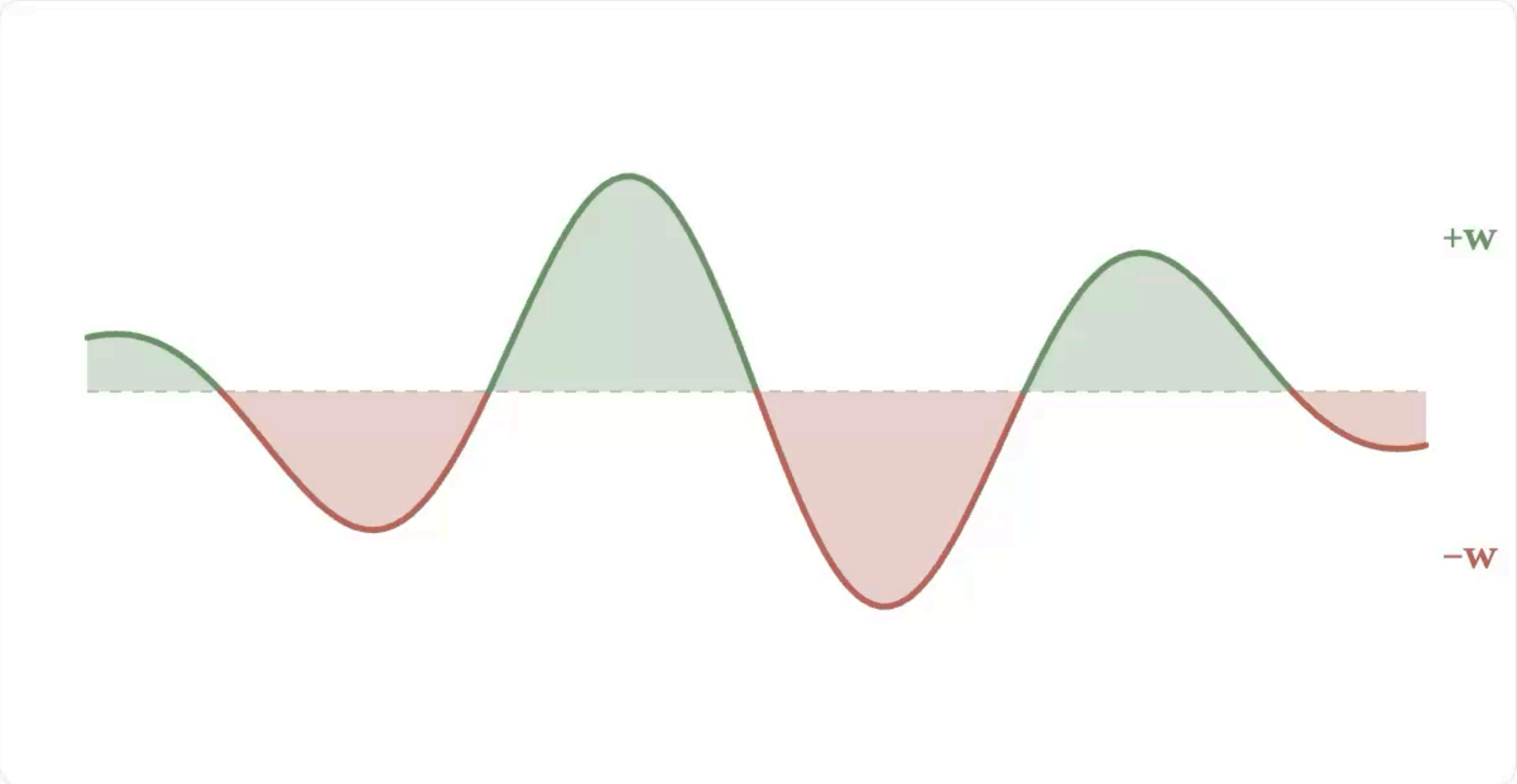

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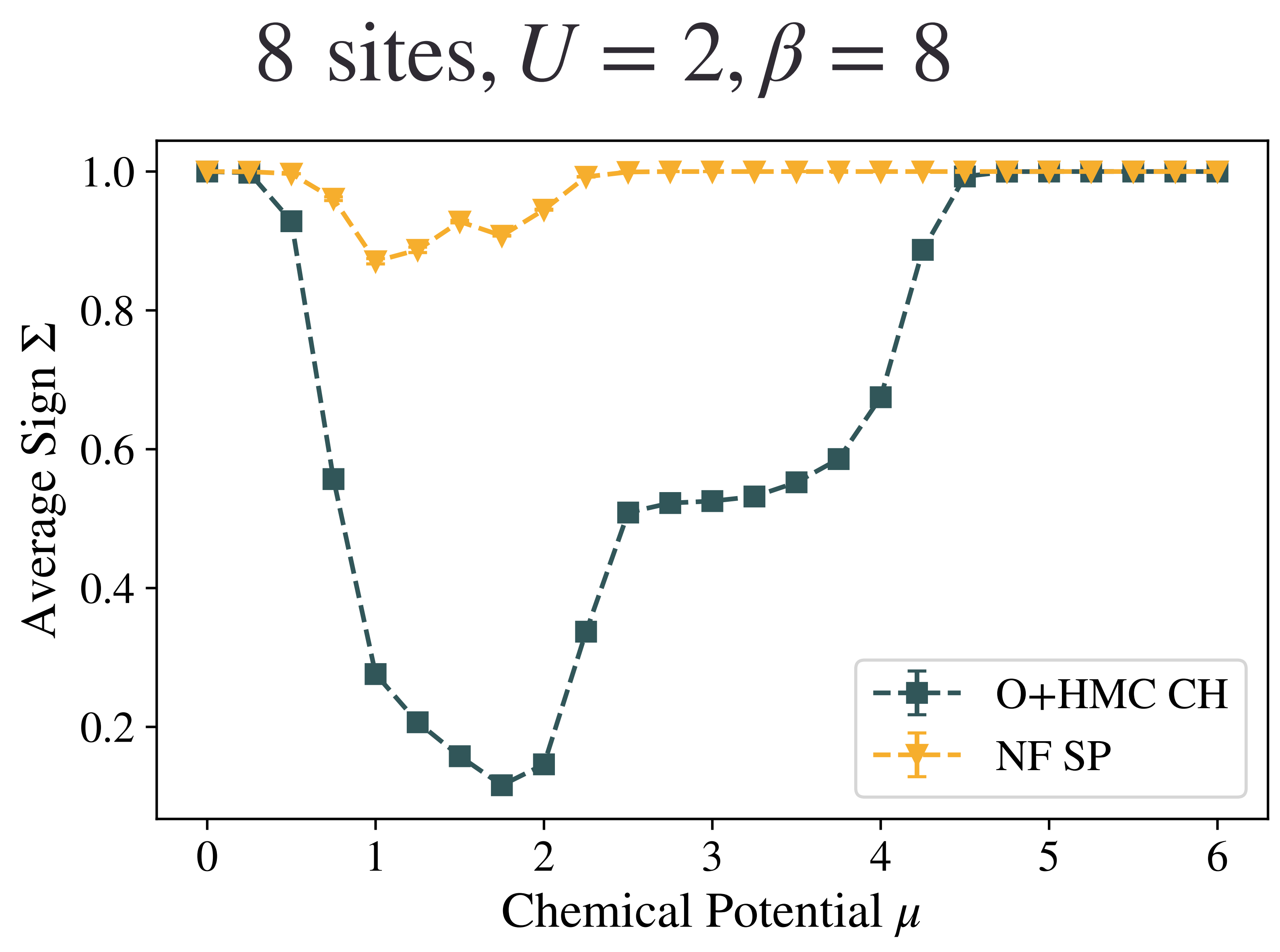

DS et al., 2026 · HMC from Gäntgen et al., PRB 2024

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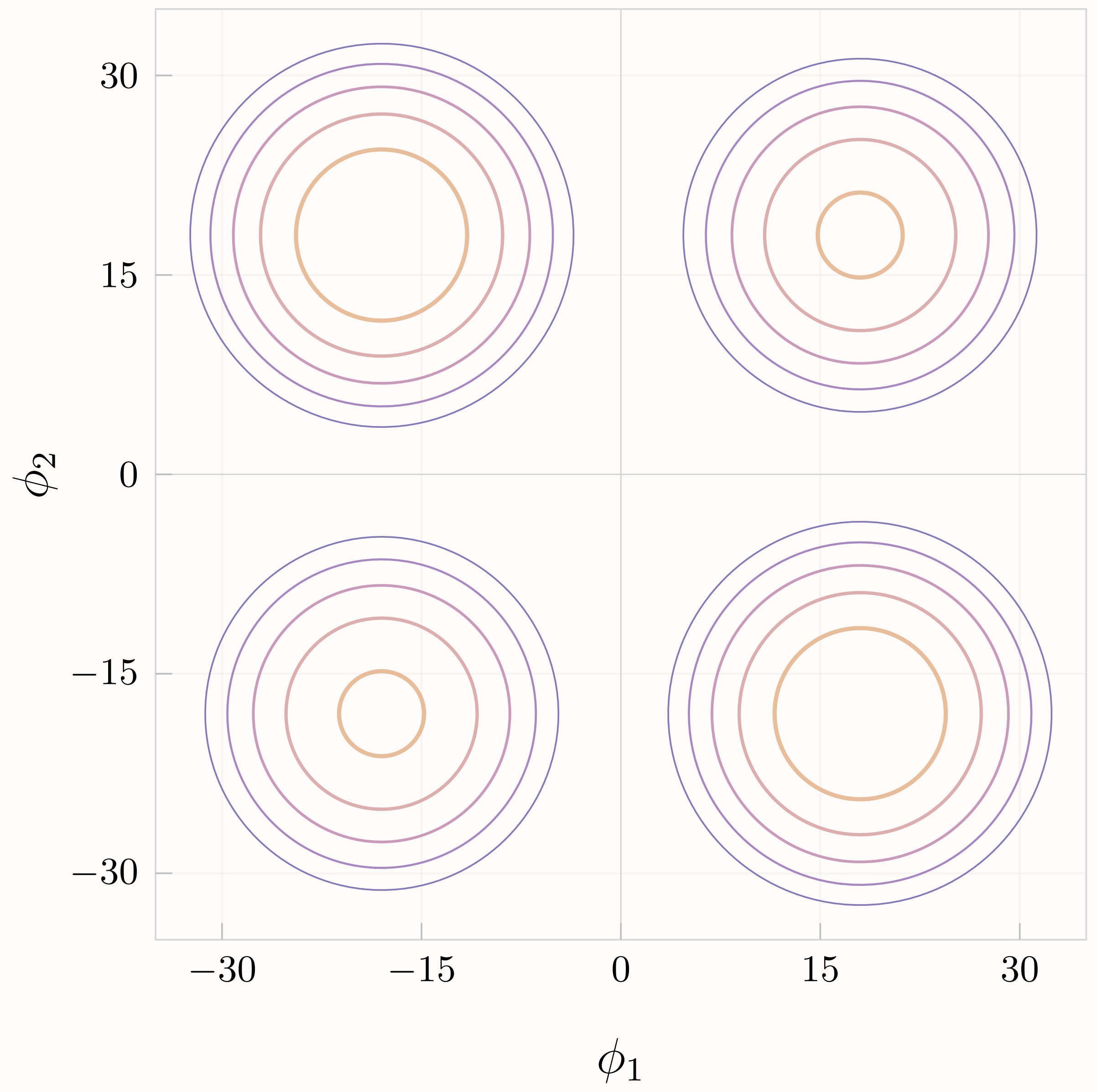

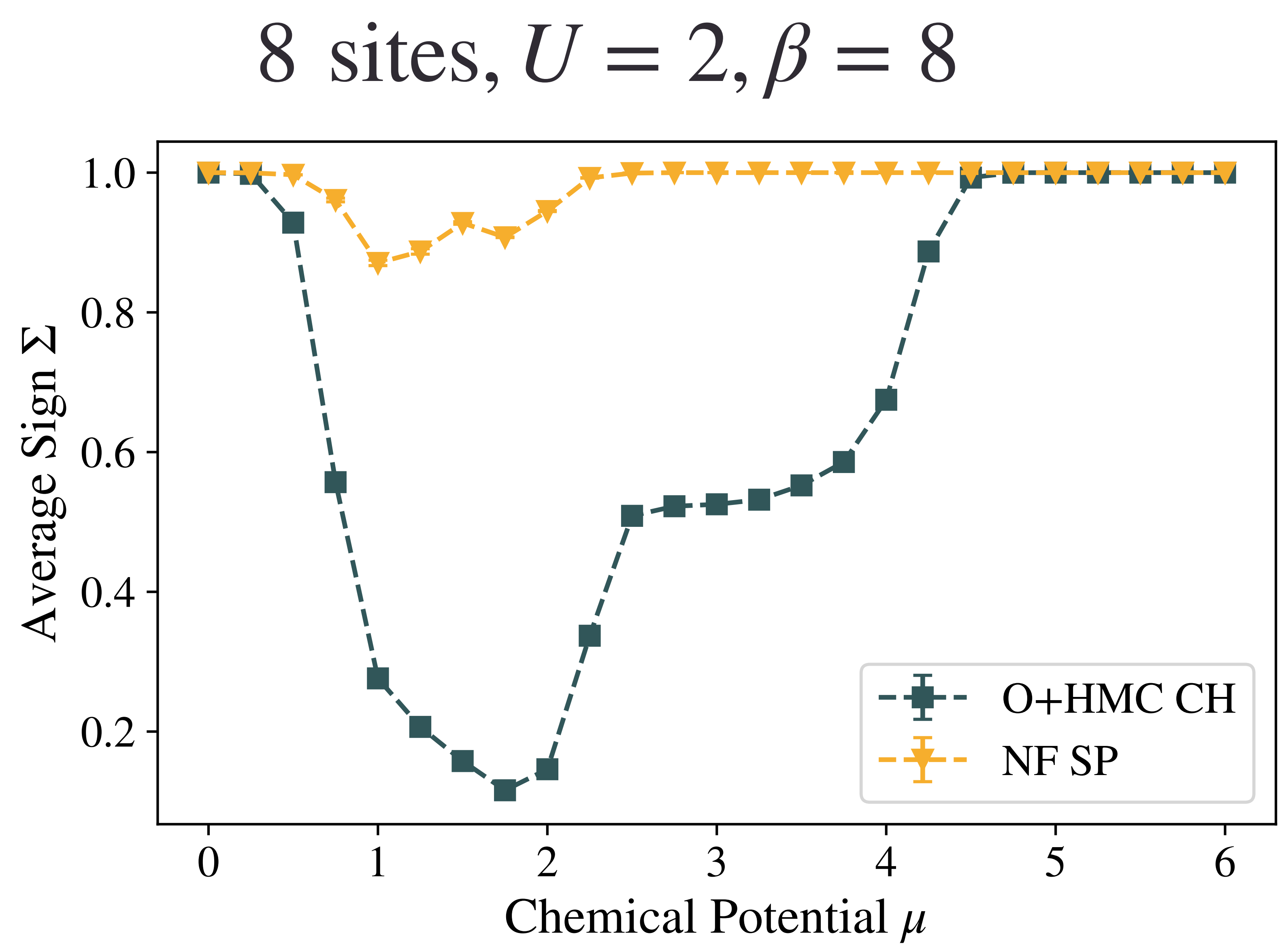

SPIN-BASIS TRADEOFF

Sign problem is structurally milder, but ergodicity concerns limit its applicability.

DS et al., 2026 · HMC from Gäntgen et al., PRB 2024

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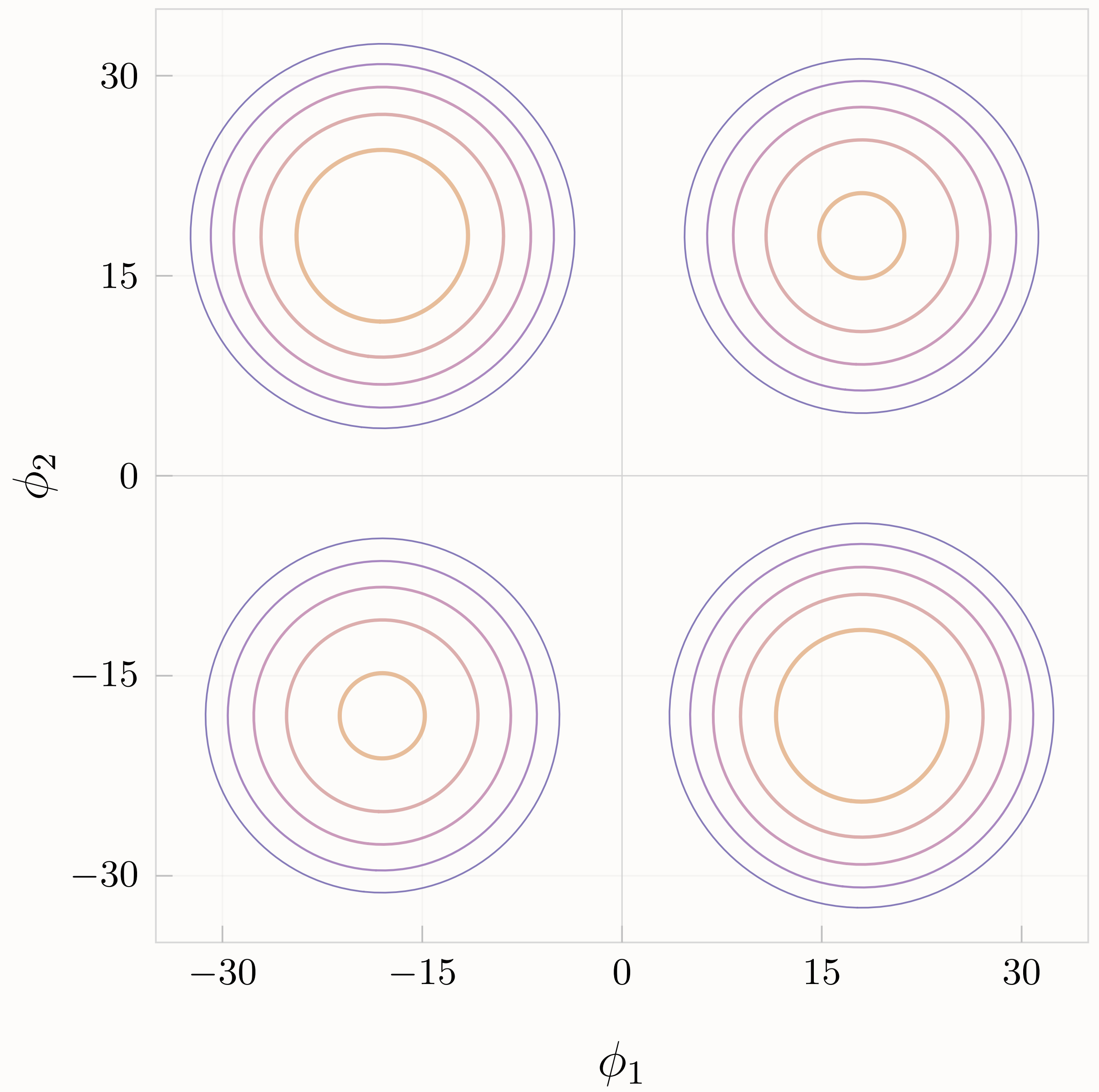

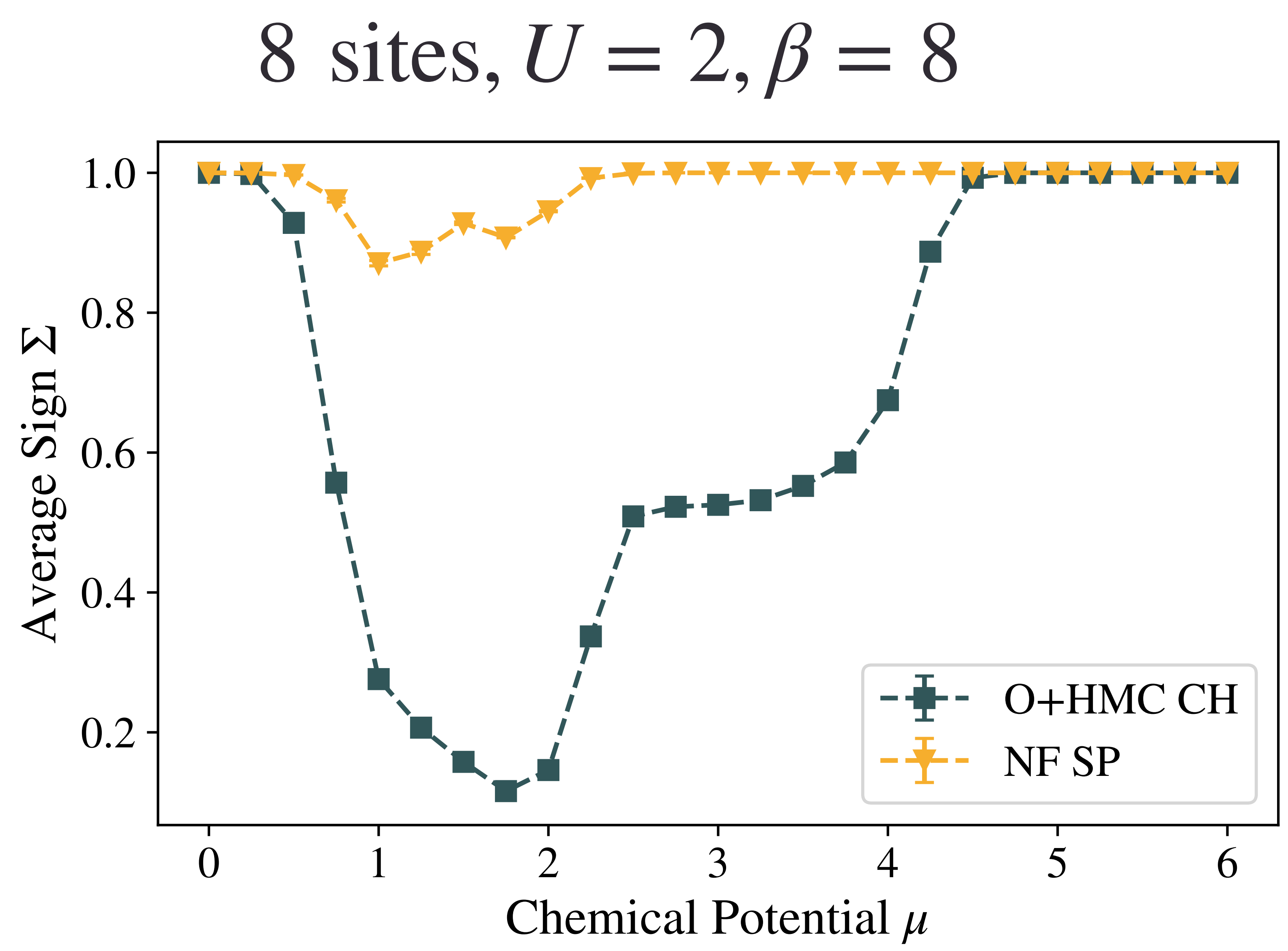

SPIN-BASIS TRADEOFF

Sign problem is structurally milder, but ergodicity concerns limit its applicability.

GOAL

Find a way to ergodically simulate the spin basis at intermediate couplings and finite density.

DS et al., 2026 · HMC from Gäntgen et al., PRB 2024

Annealing to the target distribution

Goal: get training signal from every mode, without deterministic symmetry transformations.

$$S_q[\phi] = \sum_{x,t\in\Lambda} \frac{\phi_{x,t}^2}{2\tilde{U}} - \log \left|\det\left(M[\phi]M[-\phi]\right)\right|$$

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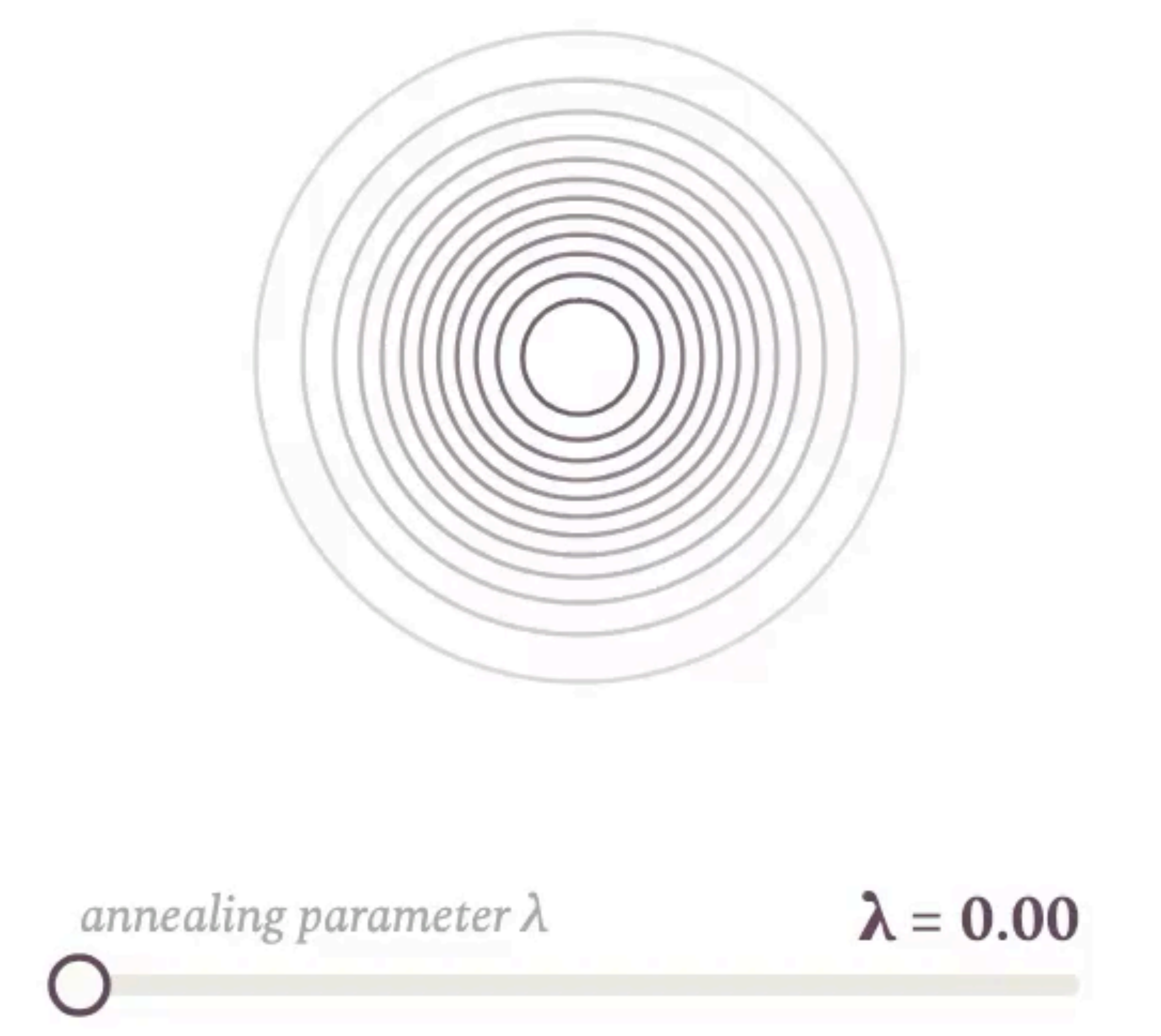
Smoothly introduce multimodality by slowly ramping fermionic contributions from $\lambda = 0$ to $\lambda = 1$ at the beginning of training.



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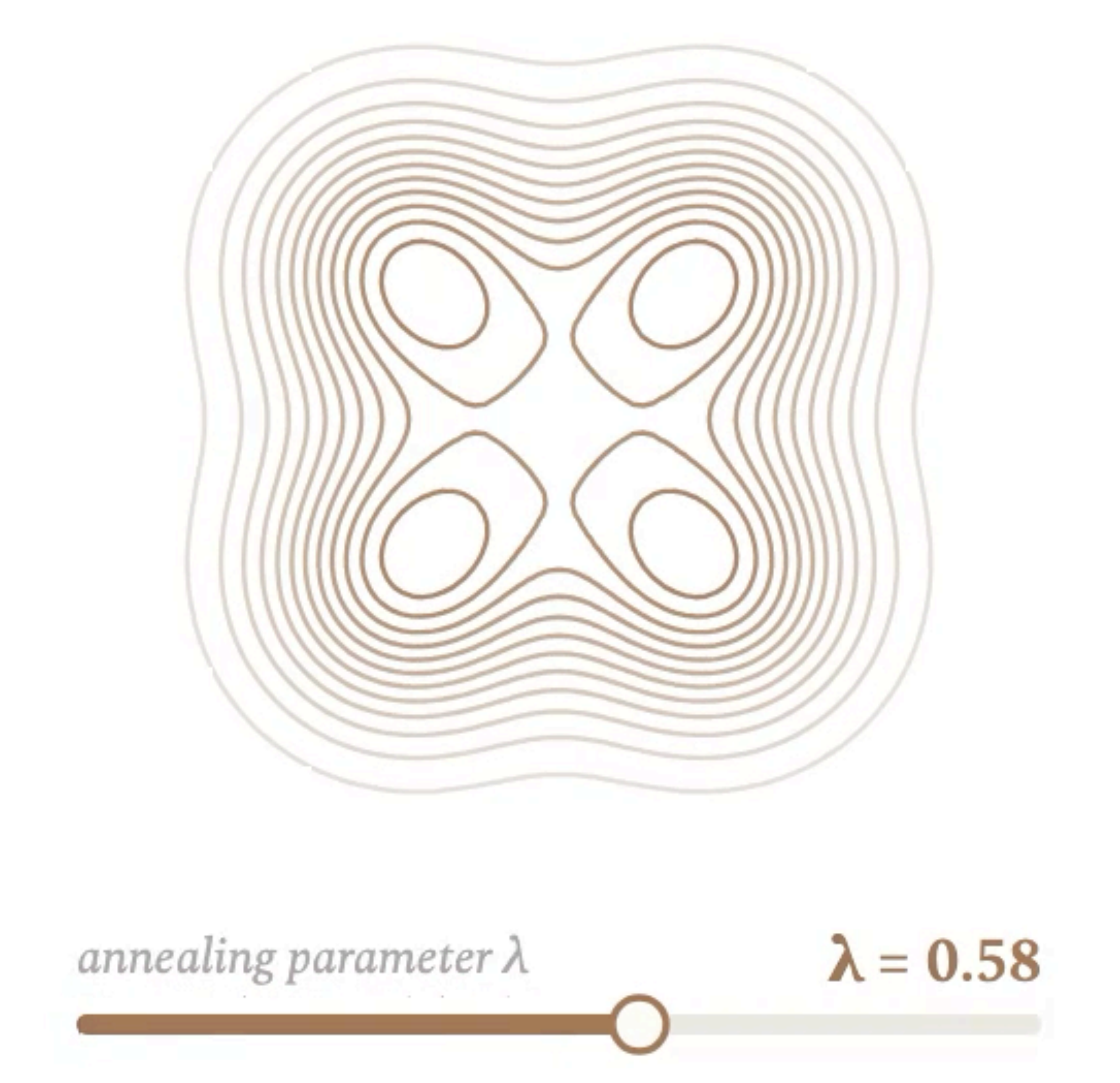

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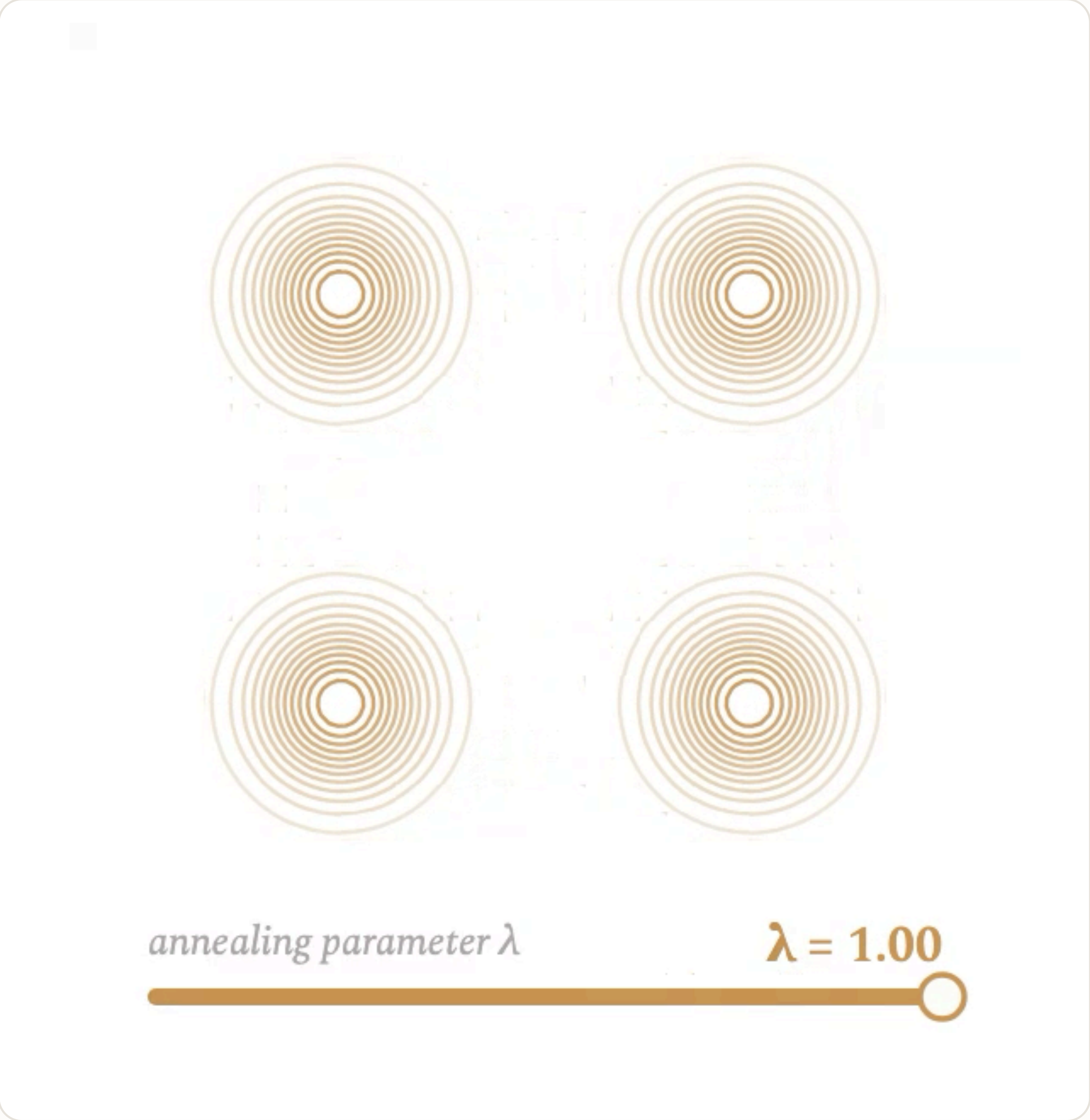

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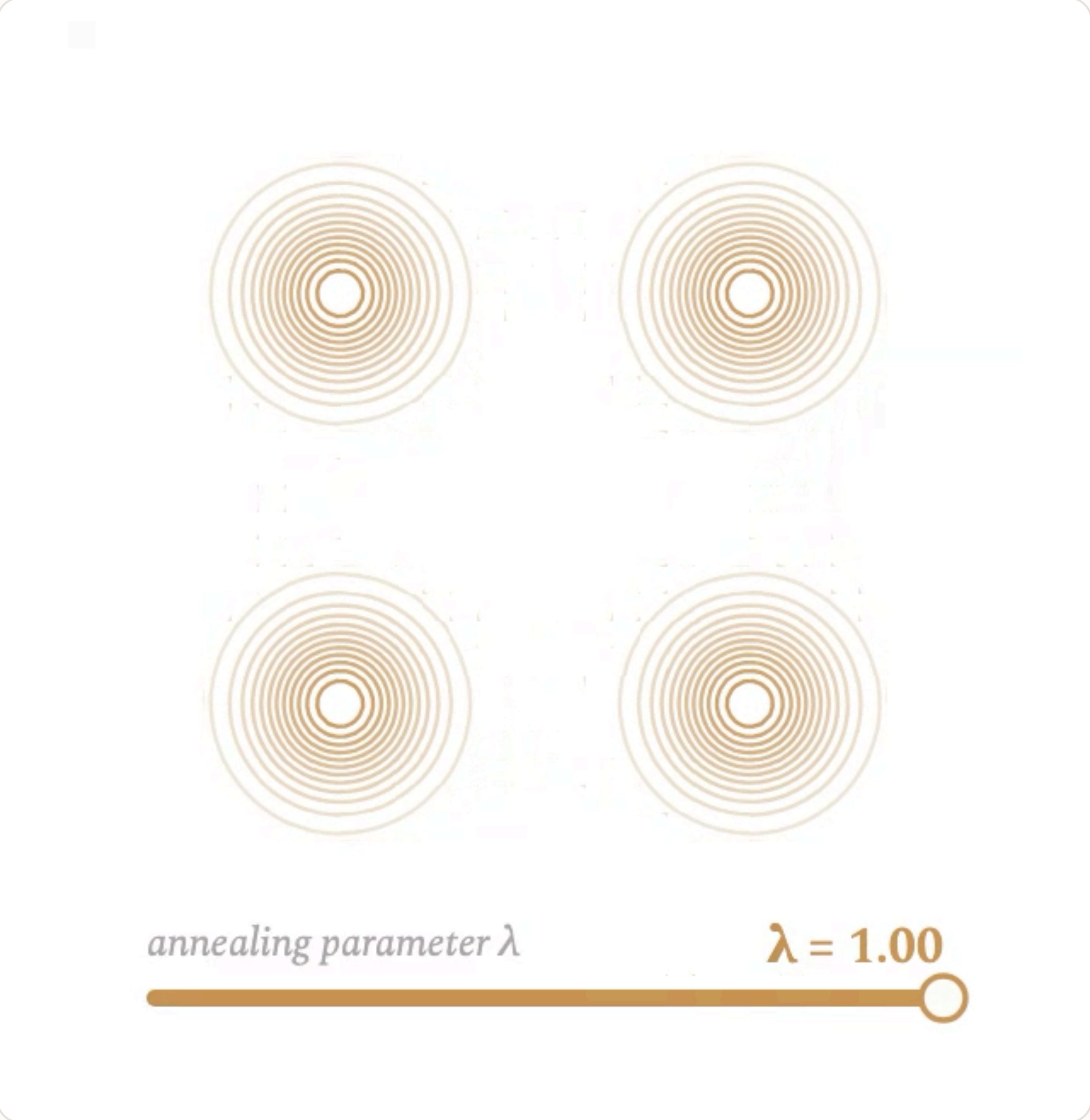

> Signal from ***every mode*** — independent of volume and parameter regime.

One-body correlation function

$$C_{xy}(t) = \left\langle a_x(t)\, a_y^\dagger(0) \right\rangle$$

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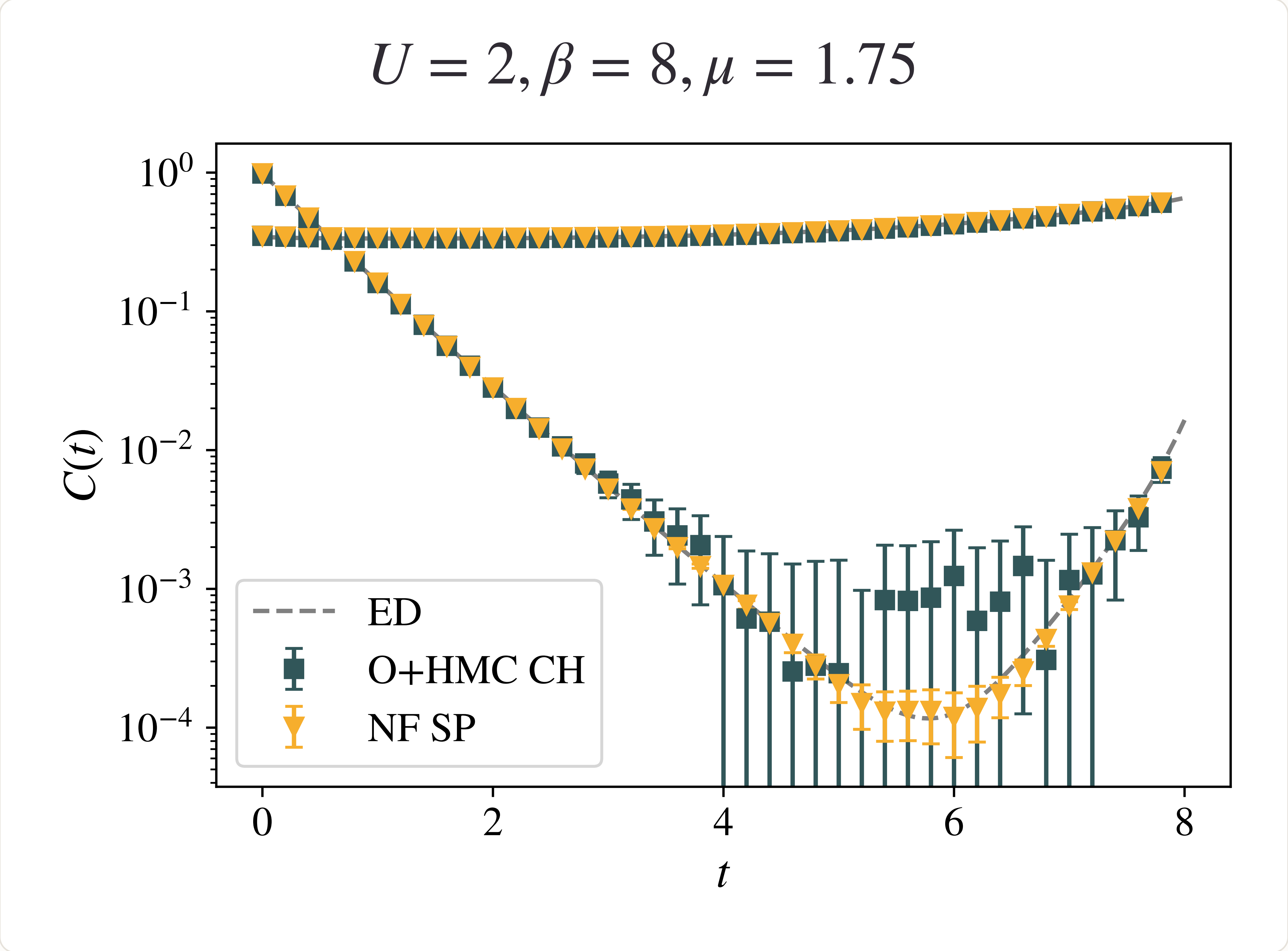
$$C_{xy}(t) = \left\langle a_x(t)\, a_y^\dagger(0) \right\rangle = \left\langle M^{-1}_{(x,t);(y,0)}[\phi] \right\rangle$$

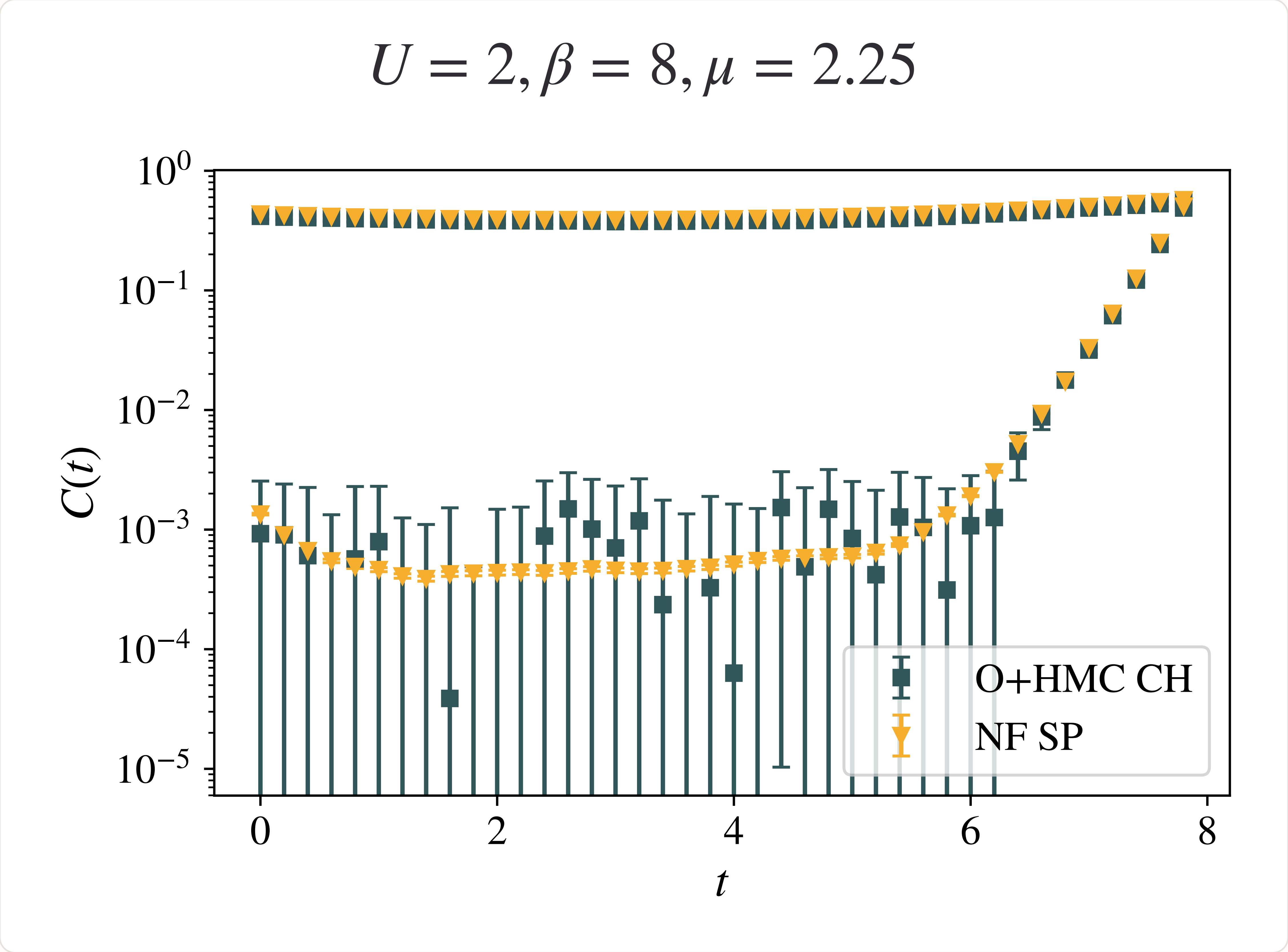
8-sites correlator



$C(t)$ vs. Euclidean time — orange ∇: NF (spin basis); dark ▪: HMC with optimized shifts (particle/hole basis)

DS et al., 2026

18-sites correlator



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Conclusion

Conclusion & outlook

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Extension towards **larger systems** and **lower temperatures**.

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In collaboration with

Janik Kreit

Lena Funcke

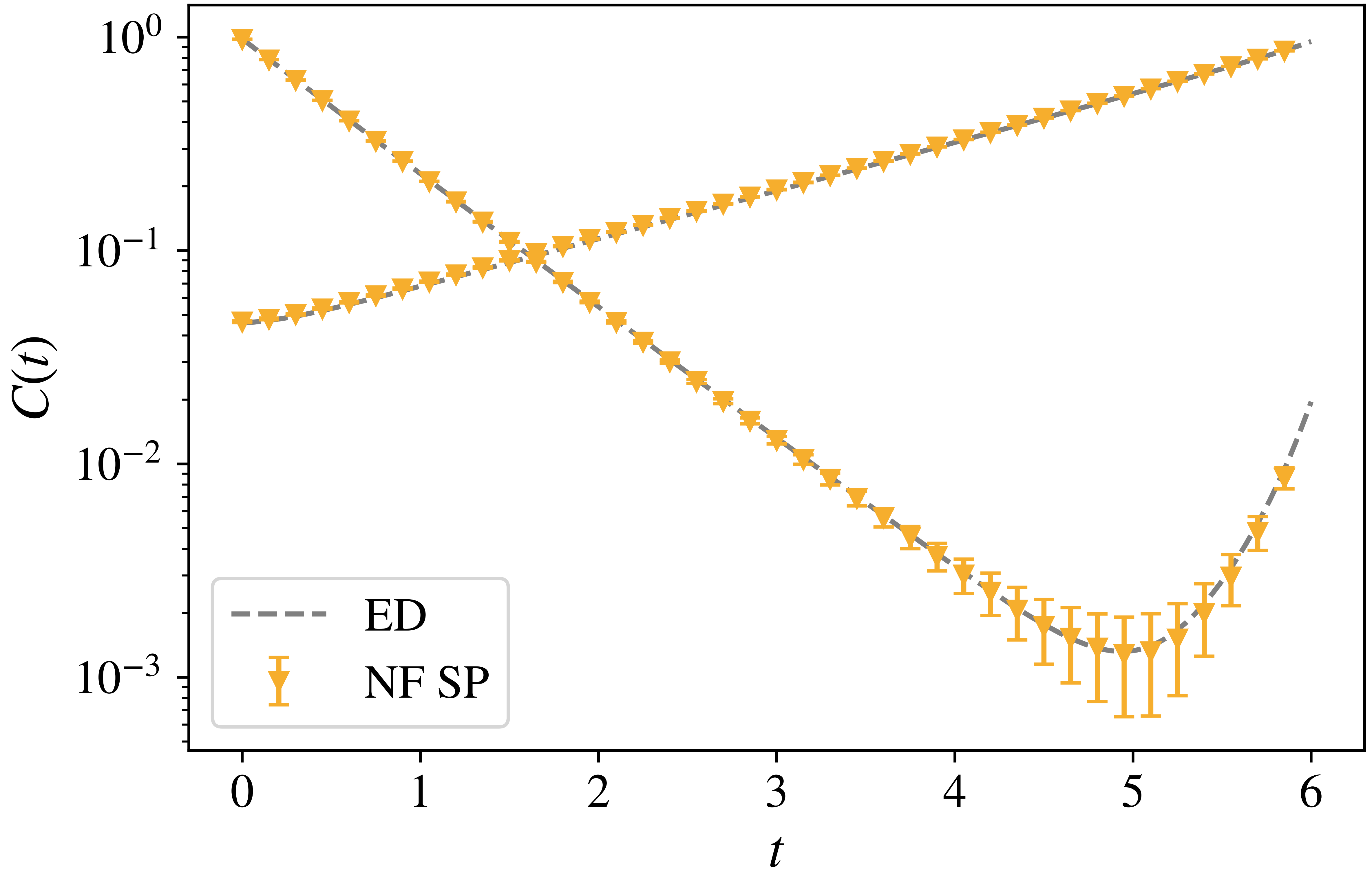
Thomas Luu

Simran Singh

Thank You!

Backup

Annealing 8-sites $U = 3$



Annealing HMC comparison 8-sites $U = 2$