Machine Learning techniques in lattice QCD

towards challenges RHIC faces

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Recent reviews for references:

- *R. Gupta, T. Bhattacharya, B. Yoon, AI and Theoretical Particle Physics, arXiv:2205.05803*
- *D. Boyda, S. Calì, S. Foreman, L. Funcke, D. C. Hackett, Y. Lin, G. Aarts, A. Alexandru, X.-Y.Jin, B. Lucini, P. E. Shanahan, Applications of Machine Learning to Lattice Quantum Field Theory, arXiv:2202.05838*

Outline

- ML for LQCD in RHIC
- Examples of ML-based approaches for
  - “faster” solutions
  - “better” solutions
- Outlook

lattice QCD contribution to RHIC science

- Study Equation of States (EoS)
- QCD phase diagram
- QCD critical point
- Fluctuations of conserved charges
- Extracting freeze-out parameters
- Transport properties of QCD matter

Challenges
- Higher chemical potential
- More precision
- Increasing signal to nose ratio
- Inverse problems

ML for LQCD challenges

could help but should be used with caution

- Uncertainties must be qualified and kept under control
- Exactness guarantee must be done
  - ➢ Mathematical proof is required, heuristic approach is not enough
- ML approach should be useful: be “faster” or “better”
  - ➢ <u>bad</u> ML model => results correct and slow and/or uncertainties diverge
  - ➢ <u>good</u> ML model => results correct and faster and/or with smaller uncertainties

Examples of ML-based approaches to obtain solution <u>“faster”</u>

Universal tools

used both in measurements and generation

- Tunning hyperparameters of lattice QCD algorithms
- Development of neural preconditioners
- Improving stochastic estimators

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- *D. Boyda, S. Calì, S. Foreman, L. Funcke, D. C. Hackett, Y. Lin, G. Aarts, A. Alexandru, X.-Y.Jin, B. Lucini, P. E. Shanahan, Applications of Machine Learning to Lattice Quantum Field Theory, arXiv:2202.05838*

Can we get more precise result with improved algorithms?

Measurements

observable regression

B. Yoon, T. Bhattacharya, R. Gupta, Phys. Rev. D 100, 014504 (2019)

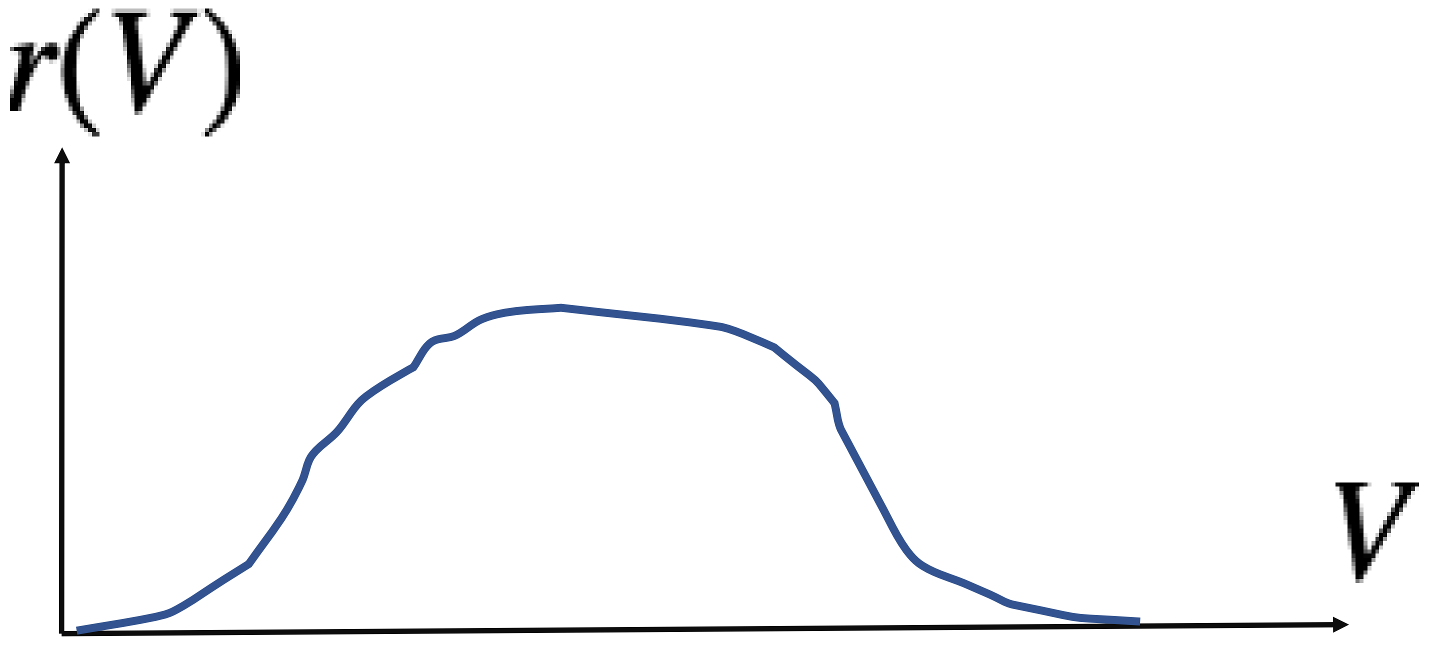
- Observables calculation takes similar or larger than generation resources
- Use ML regression to compute them faster
  - N *configurations,* $N_{train} + N_{bs}$*measurements of* O, N_{train} *measurements are used for training*
  - *effective samples size is increased from* $N_{train} + N_{bs}$ *to* N
- Correct bias

$$\bar{O} = \frac{1}{N - N_{train} - N_{bc}} \sum O_i^{ML} + \frac{1}{N_{bc}} \sum (O_j - O_j^{ML})$$

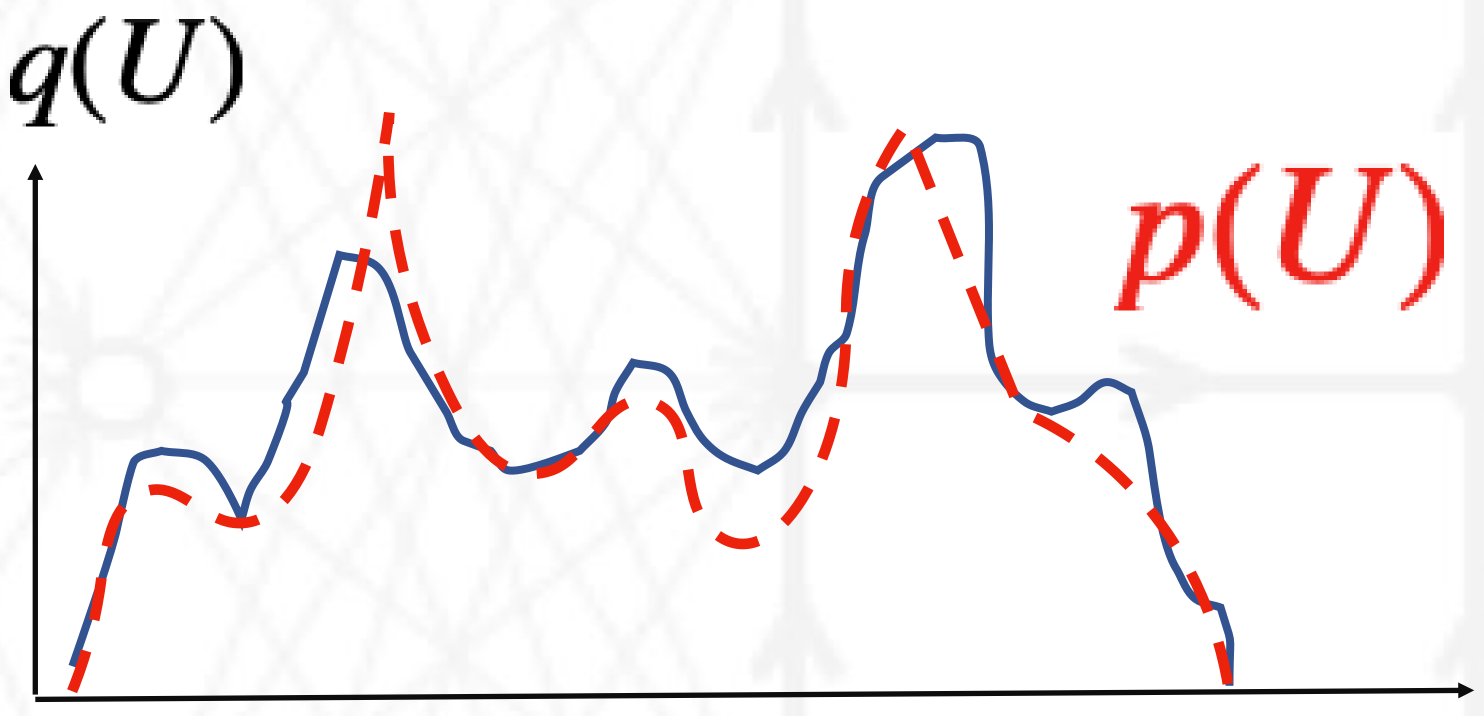
Can we decrease time for observable measurements and get higher statistics?

Configuration generation with normalizing flows

Flow-based models learn a change-of-variables that transforms a known distribution to the desired one



$$U = f(V)$$



$$\int r(V)dV$$

$$\underbrace{\int r(V)\left|\det\frac{\partial f^{-1}(U)}{\partial U}\right|dU}_{}$$

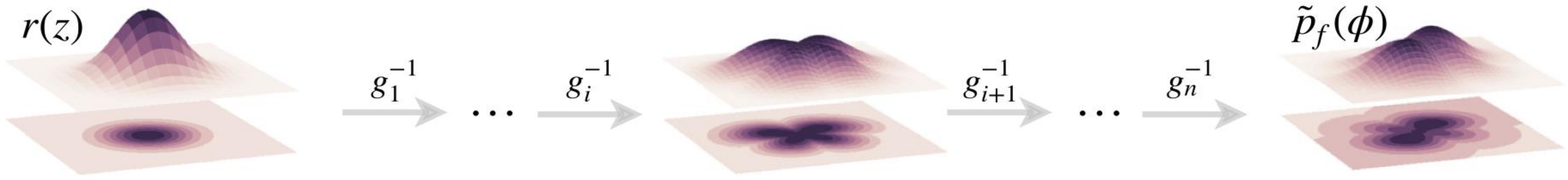
$$\boxed{q(U) \xrightarrow{\text{train/optimize}} p(U)}$$

Exactness guarantee is done via correction $q(U)$ to $p(U)$ using reweighting of building MCMC chain

Coupling layer based normalizing flows

Flow-based models learn a change-of-variables that transforms a known distribution to the desired one
[Rezende & Mohamed 1505.05880]

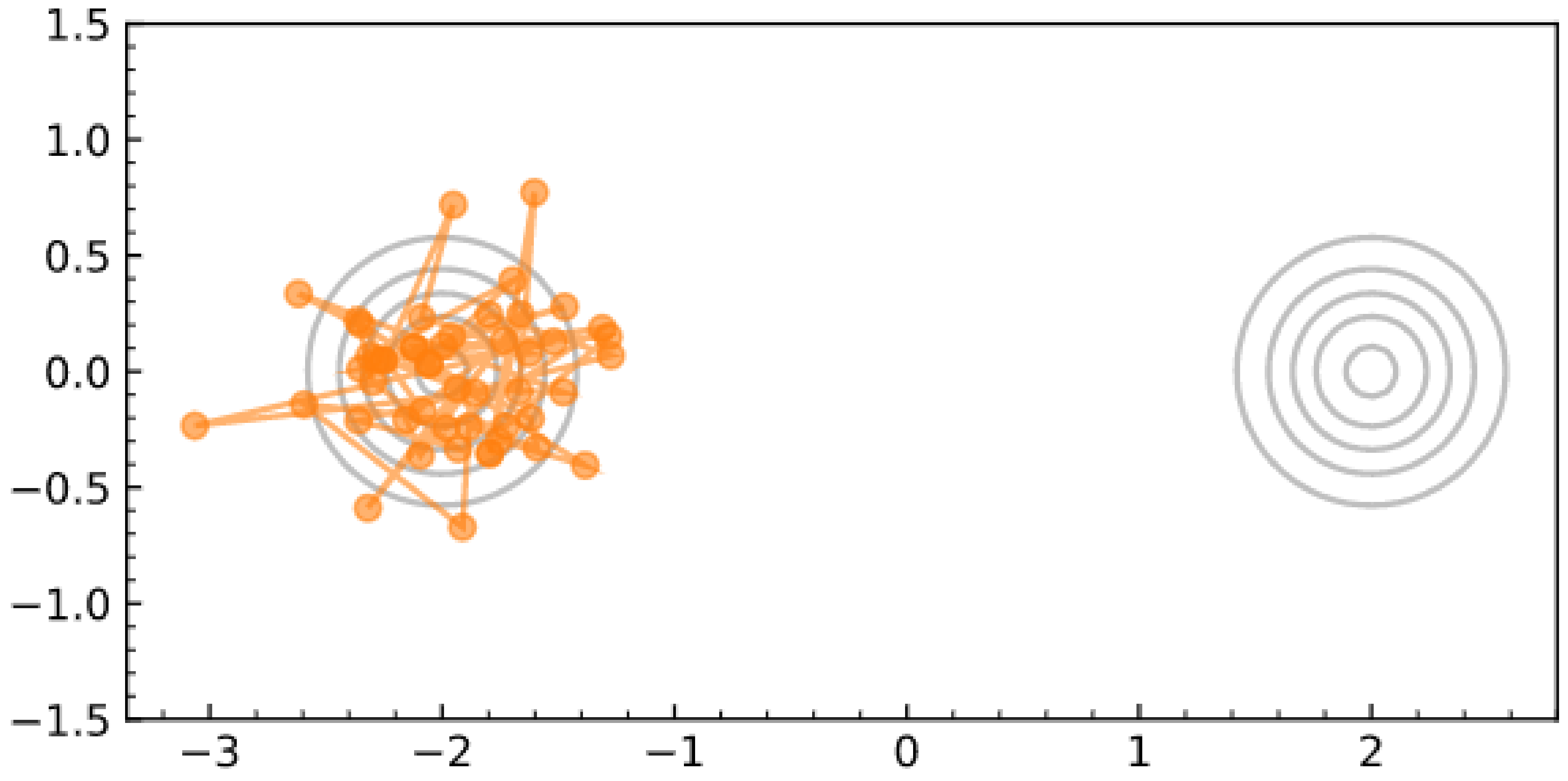
- $U = f(V)$
- Some conditions to f apply
- f parametrized with NN
- Self training – no expensive samples needed



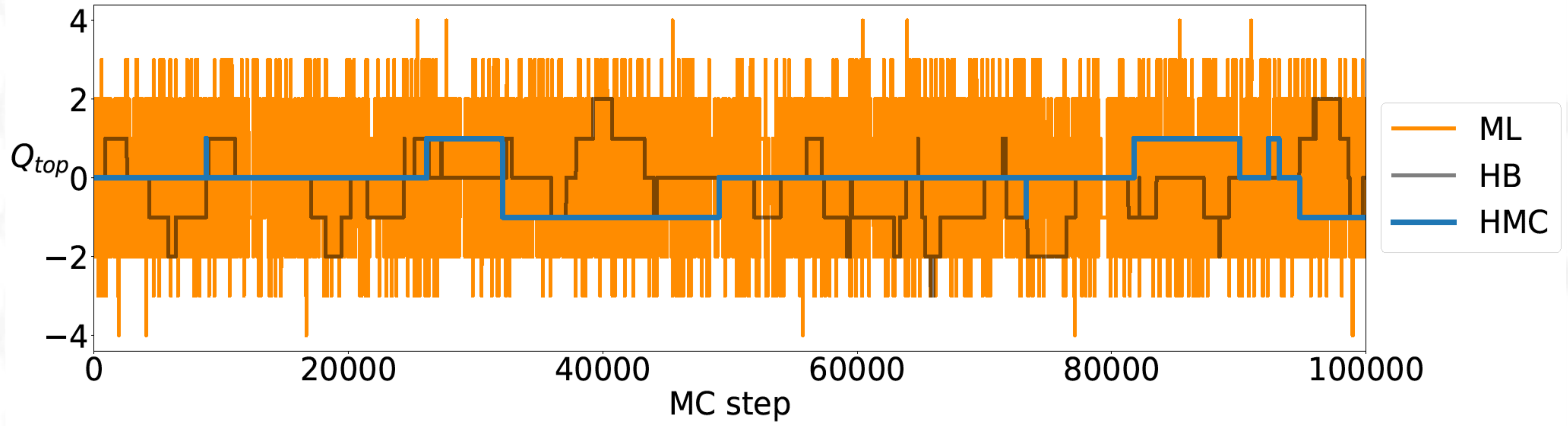
Normalizing flows: better mixing

U(1) lattice gauge theory in 2D

Example of under sampling of some region of target probability density



Example of improving topological sampling with NF comparing to other techniques (HB, HMC) in U(1) LGT in 2D

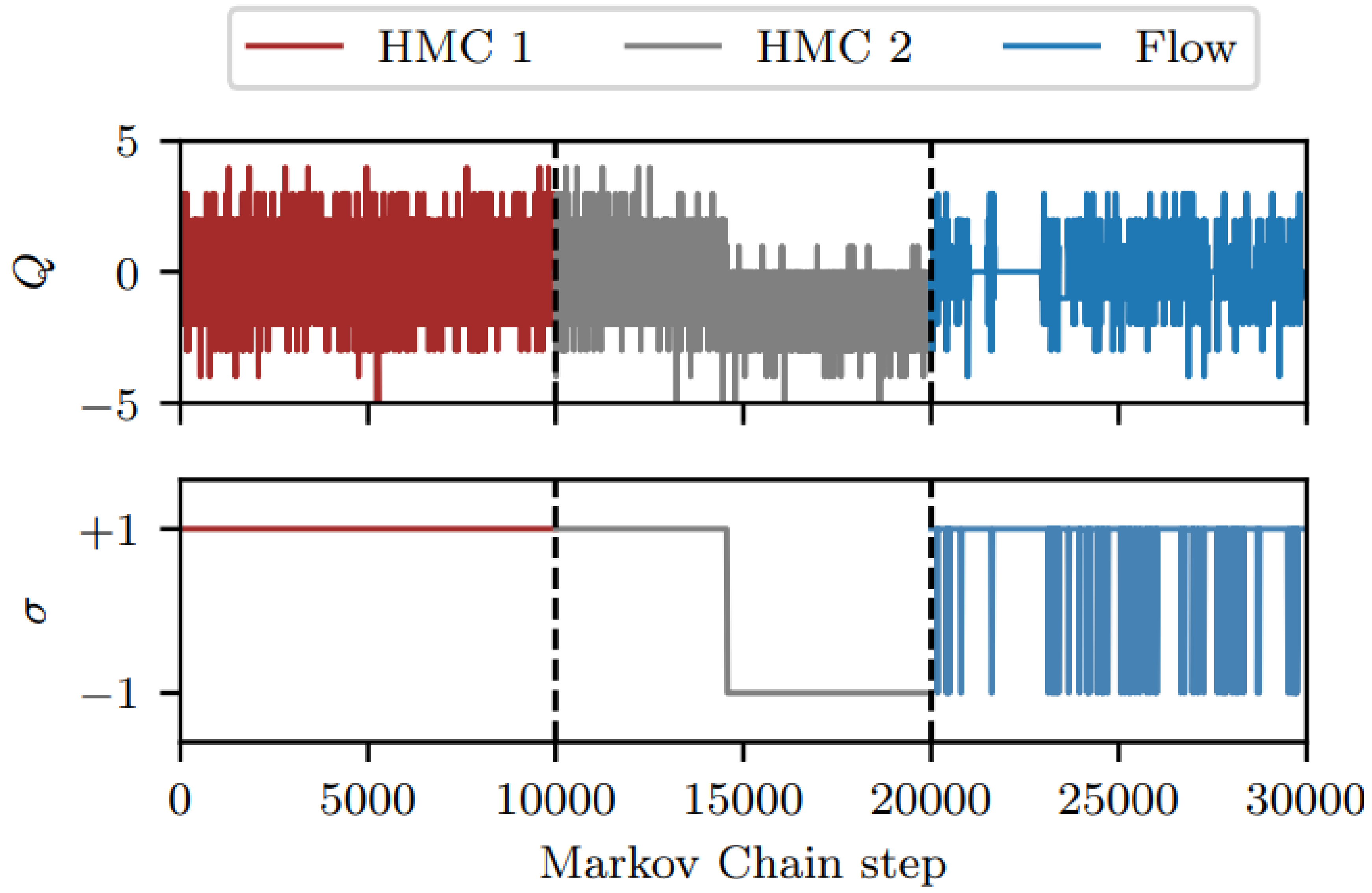


Phys. Rev. Lett. 125, 121601 (2020)

Normalizing flows: better uncertainty qualification at finite statistics

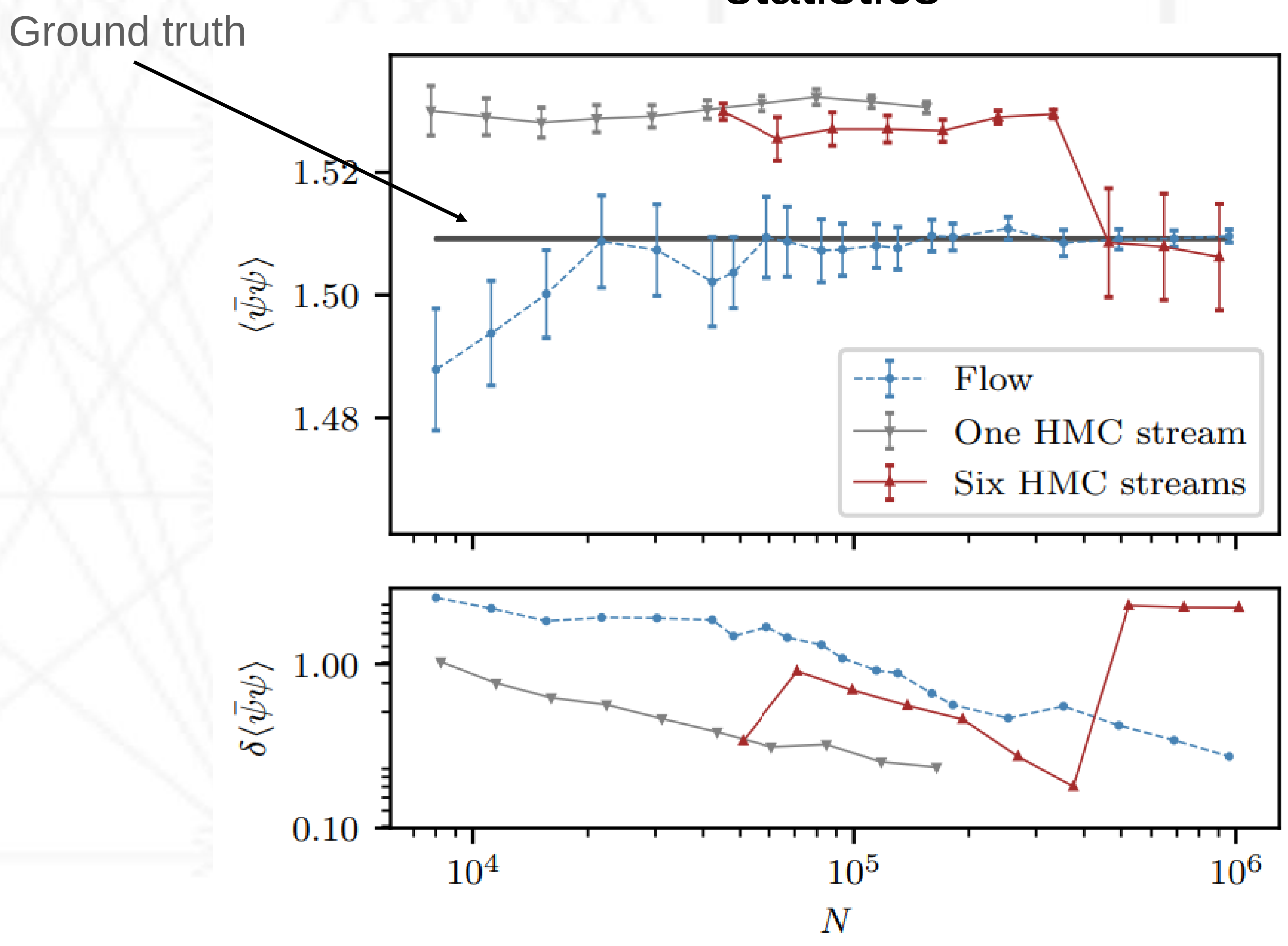
Lattice Schwinger model near criticality

Determination of topological mixing is difficult due to UV fluctuations



arXiv:2202.11712

Example of improving uncertainty estimation for finite statistics



arXiv:2202.11712

Normalizing flows is a promising technique from ML for solving challenges LQCD for RHIC faces

Can we generate ensembles with larger lattice in temporal direction?
Can we decrease lattice spacing?
Can we get better mixing and use reweighting more efficiently?

Examples of ML-based approaches to obtain “better” solution

Thermodynamical properties of QGP and EoS with normalizing flows

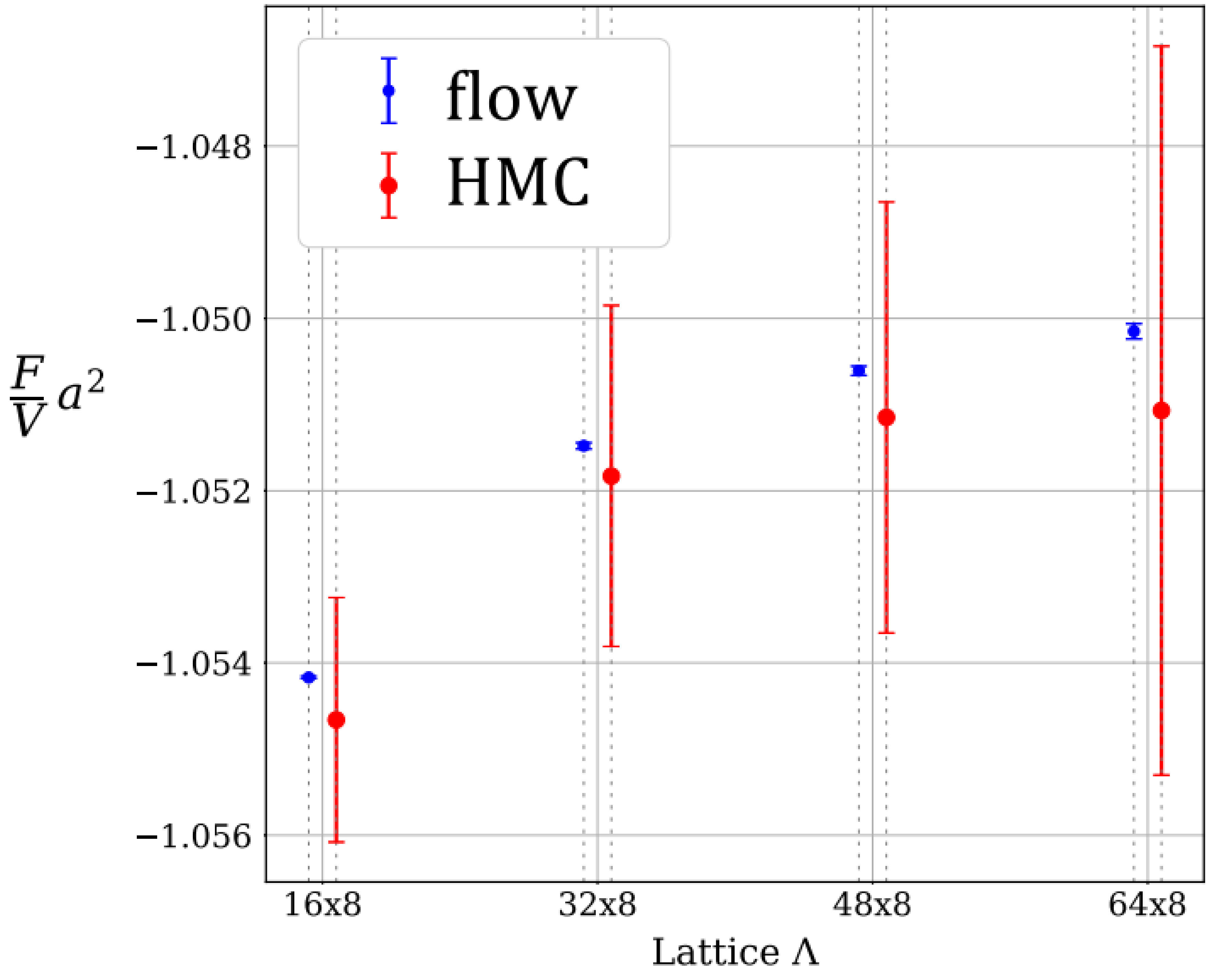
Lattice scalar field theory

The fundamental difficulty is that MCMC is not able to directly estimate the partition function of the lattice field theory.

Normalizing flows have direct access to partition function

$$Z = \int D\phi q_\theta(\phi) \frac{e^{-S(\phi)}}{q_{\theta(\phi)}} = \left\langle \frac{e^{-S(\phi)}}{q_{\theta(\phi)}} \right\rangle_{q_{\theta(\phi)}}$$

Example free energy computation



K. A. Nicoli, C. J. Anders, L.Funcke, T. Hartung, K. Jansen, P. Kessel, S. Nakajima, P. Stornati, Phys. Rev. Lett. 126, 032001 (2021)

Can we compute QCD EoS with higher precision?

Compute QCD phase diagram in (T, mu) with normalizing flows

Direct MCMC simulations of QCD at nonzero chemical potential is not tractable due to Sign Problem

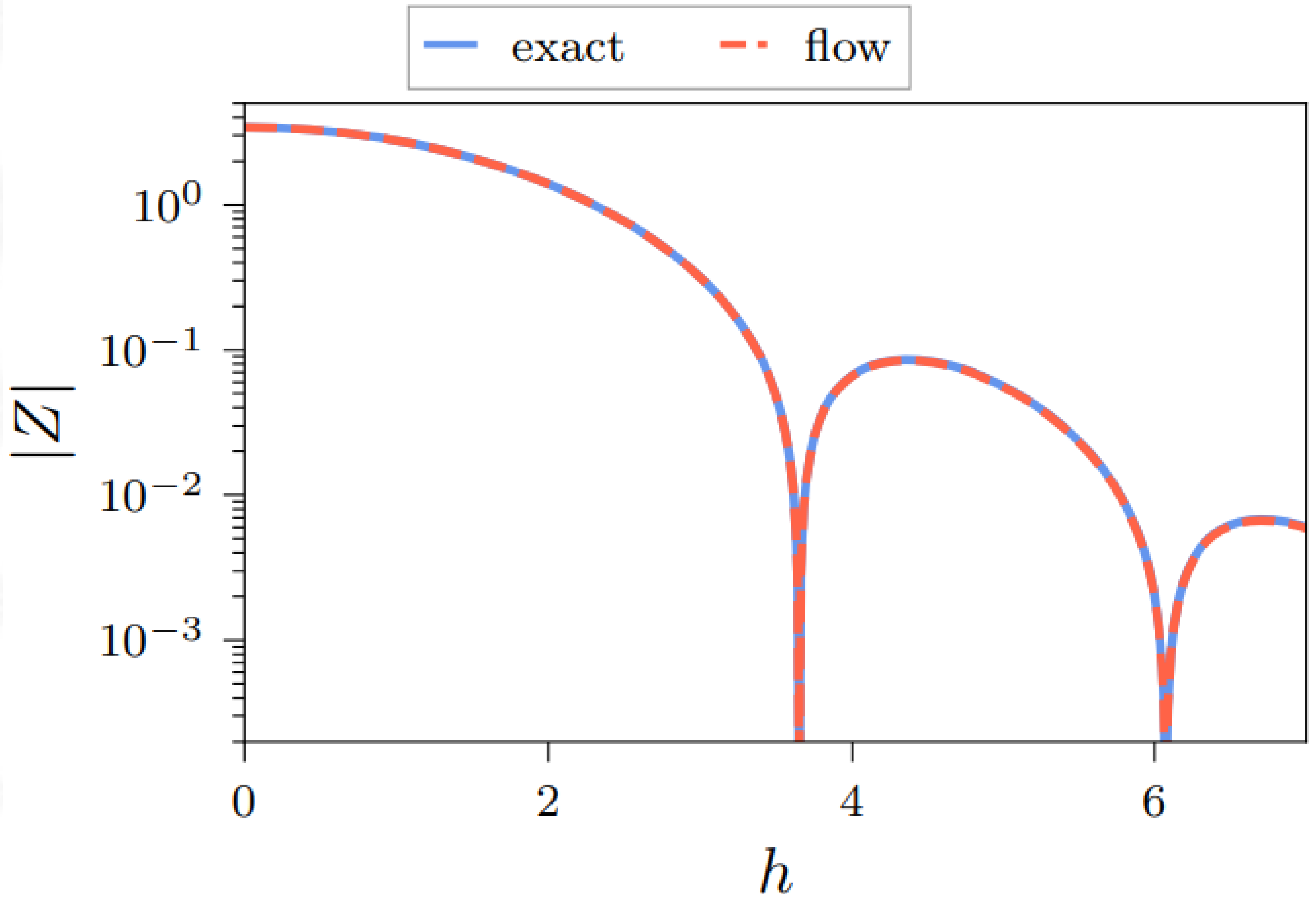
Several approaches use MCMC simulations at zero and/or imaginary chemical potential

Simulations at several values of imaginary chemical potential required in order to do extrapolation to real region

<u>After training Normalizing flow model gives access to "all" values of imaginary chemical potential</u>

Demonstration of flow-based Density of State

$$S(\phi) = \frac{m^2}{2}(\phi_1^2 + \phi_2^2) + \lambda(\phi_1^2 + \phi_2^2)^2 + ih\phi$$



Jan M. Pawlowski1 and Julian M. Urban, https://arxiv.org/pdf/2203.01243.pdf

Can we get larger chemical potential?

Increase signal to noise ratio via contour deformation

Variable transformation does not change integral

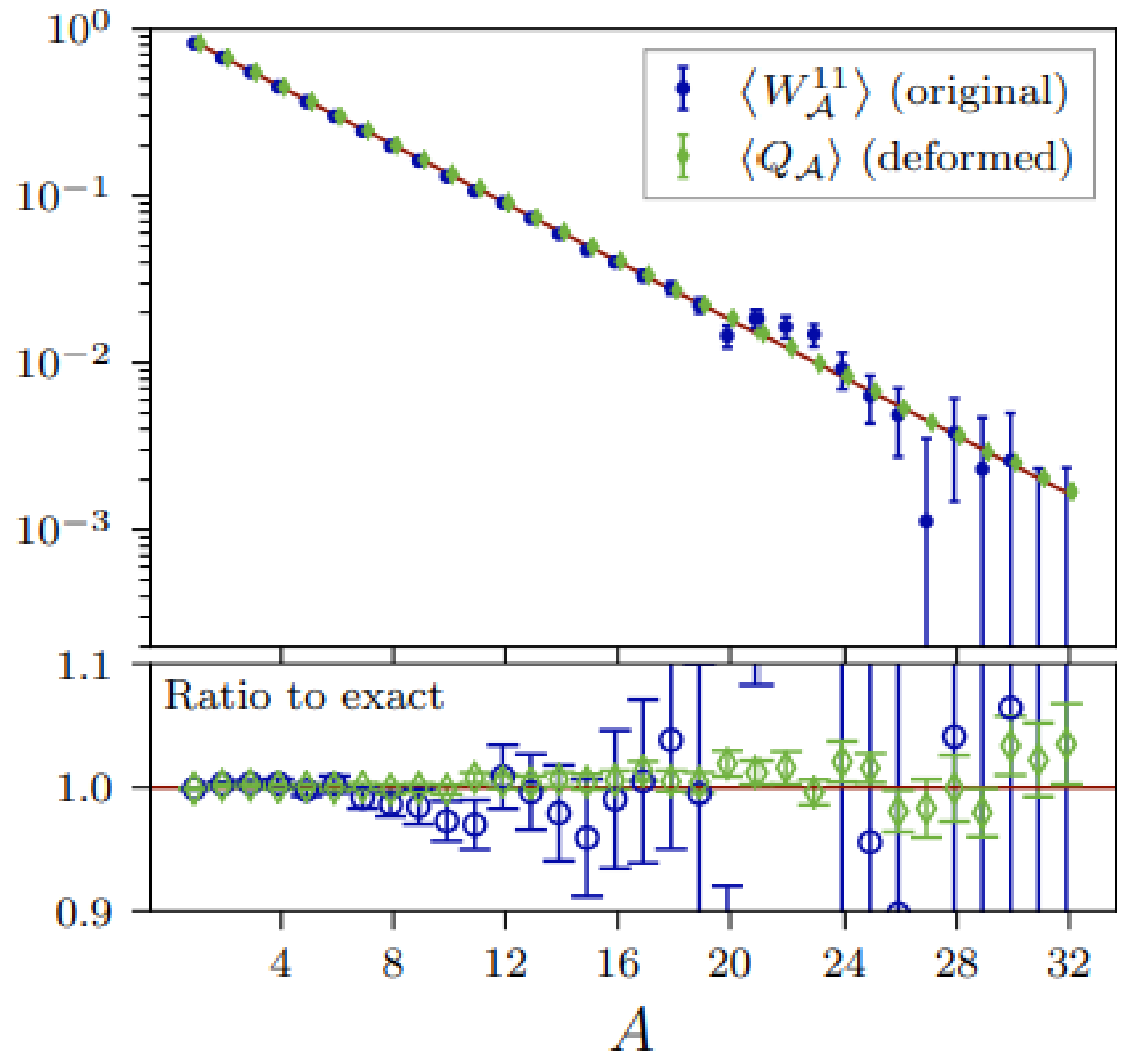
$$\langle O \rangle = \int D\,\tilde{U} e^{-S(\tilde{U})} O(\tilde{U}) = \int DU\, J(U) e^{-S(\tilde{U}(U))} O(\tilde{U}(U))$$

$$\langle O \rangle = \langle Q \rangle = \left\langle J(U) e^{-S(\tilde{U}(U)) + S(U)} \right\rangle$$

but changes uncertainties

transformation $\tilde{U} = f(U)$ is optimized such that $var(Q) \ll var\,(O)$

Demonstration in SU(3) gauge theory in 2D



W. Detmold, G. Kanwar, H. Lamm, M.L. Wagman, N. C. Warrington, Phys. Rev. D 103, 094517 (2021)

Can we apply it for viscosity computations in full QCD?

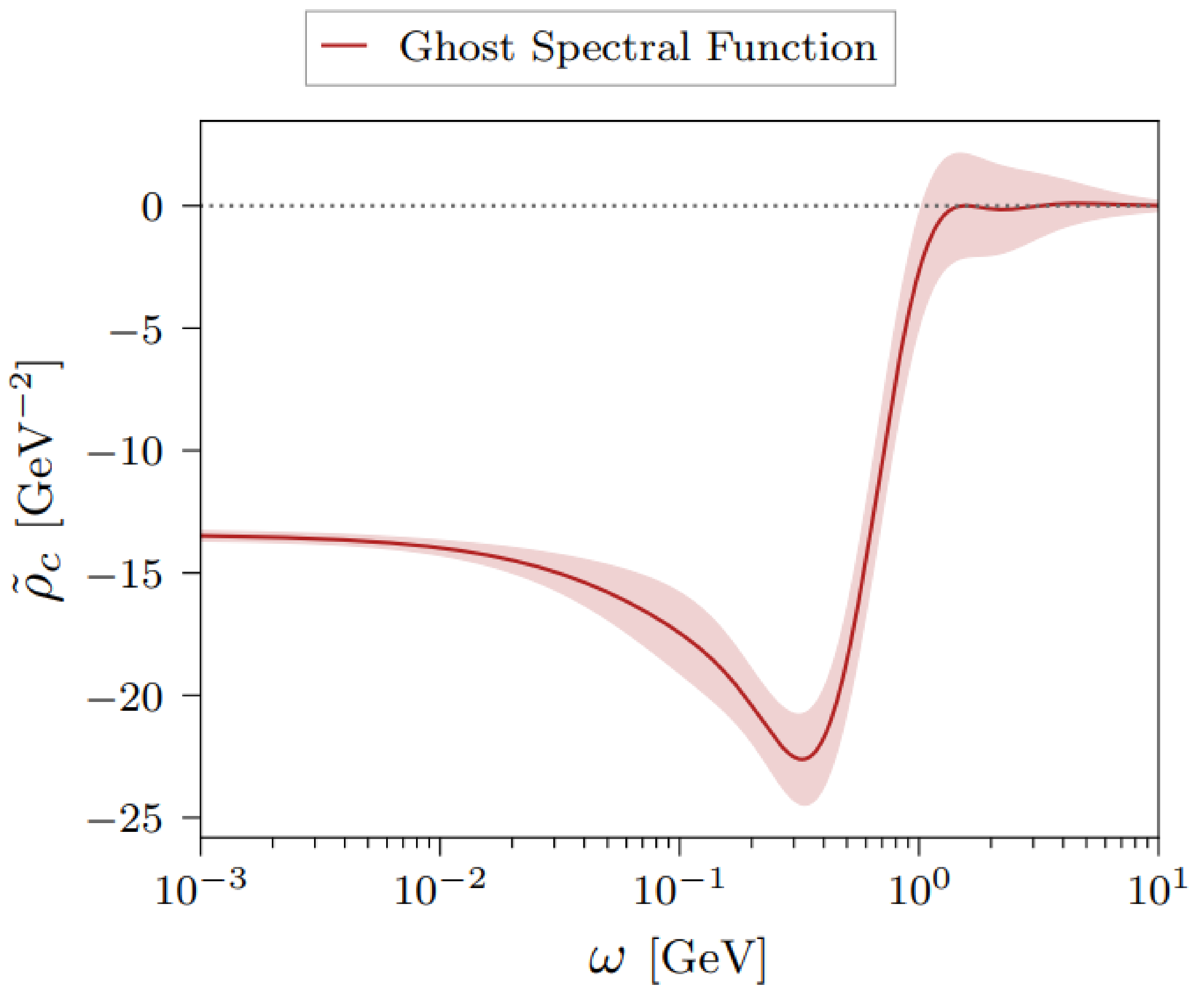
Reconstructing QCD Spectral Functions with Gaussian Processes

Spectral functions are extracted from lattice QCD correlator using inverse integral transformation which is ill-defined problem

Reconstruction using Gaussian Process Regression

what is most probably value and uncertainty of $\rho(\omega)$ given some observations $G(t_i)$ with uncertainties

Demonstration of extraction Ghost spectral function in 2 + 1 LQCD; band shows uncertainty.



J. Horak, J. M. Pawlowski, J. Rodríguez-Quintero, J. Turnwald, J. M. Urban, N. Wink, S. Zafeiropoulos, Phys.Rev.D 105, 036014 (2022)

Did we improve a solution of inverse problem?

Outlook

Some Machine learning techniques proved their usefulness for lattice QCD simulations.

They give a hope for solving RHIC challenges in near future.

However, majority of results were demonstrated in toy models requiring further development before providing useful data.

Acknowledgment

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