Flow-based Sampling for Effective String Theory

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Based on:

M.Caselle, **EC**, A.Nada, M. Panero

- JHEP 07 (2022) 015, arxiv:2201.08862

M. Caselle, **EC**, A. Nada

- arXiv: 2307.01107 (under review JHEP)
- arxiv: 2309.14983 (Lattice 2023 PoS)

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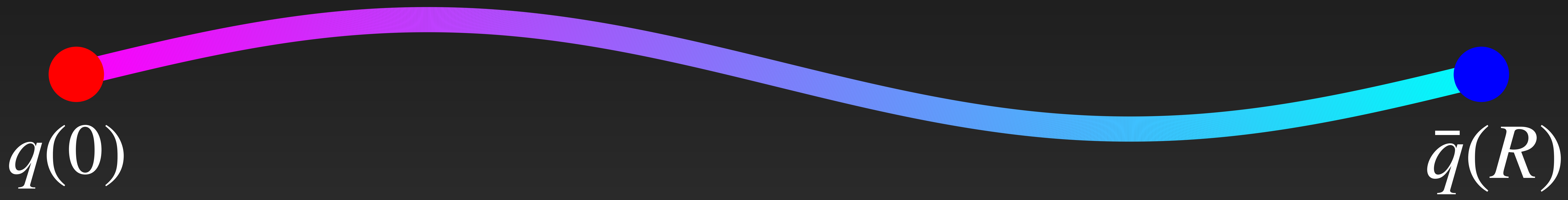
Outline

1. Effective String Theory
2. Normalizing Flows
3. Stochastic Normalizing Flows
4. Conclusion

Effective String Theory

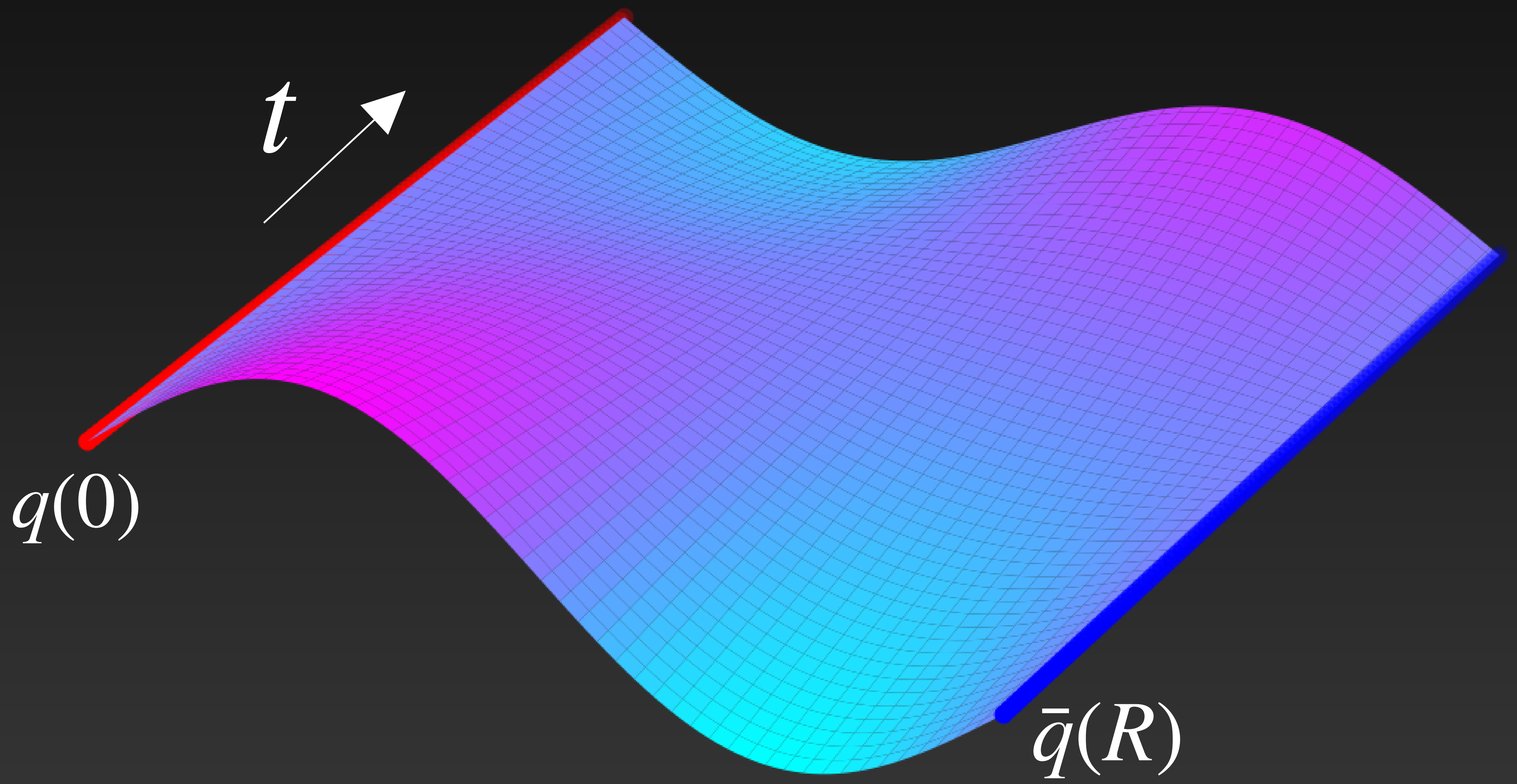
Effective String Theory

Effective String Theory (**EST**) is a powerful tool to study **confinement** in **Yang-Mills** theories



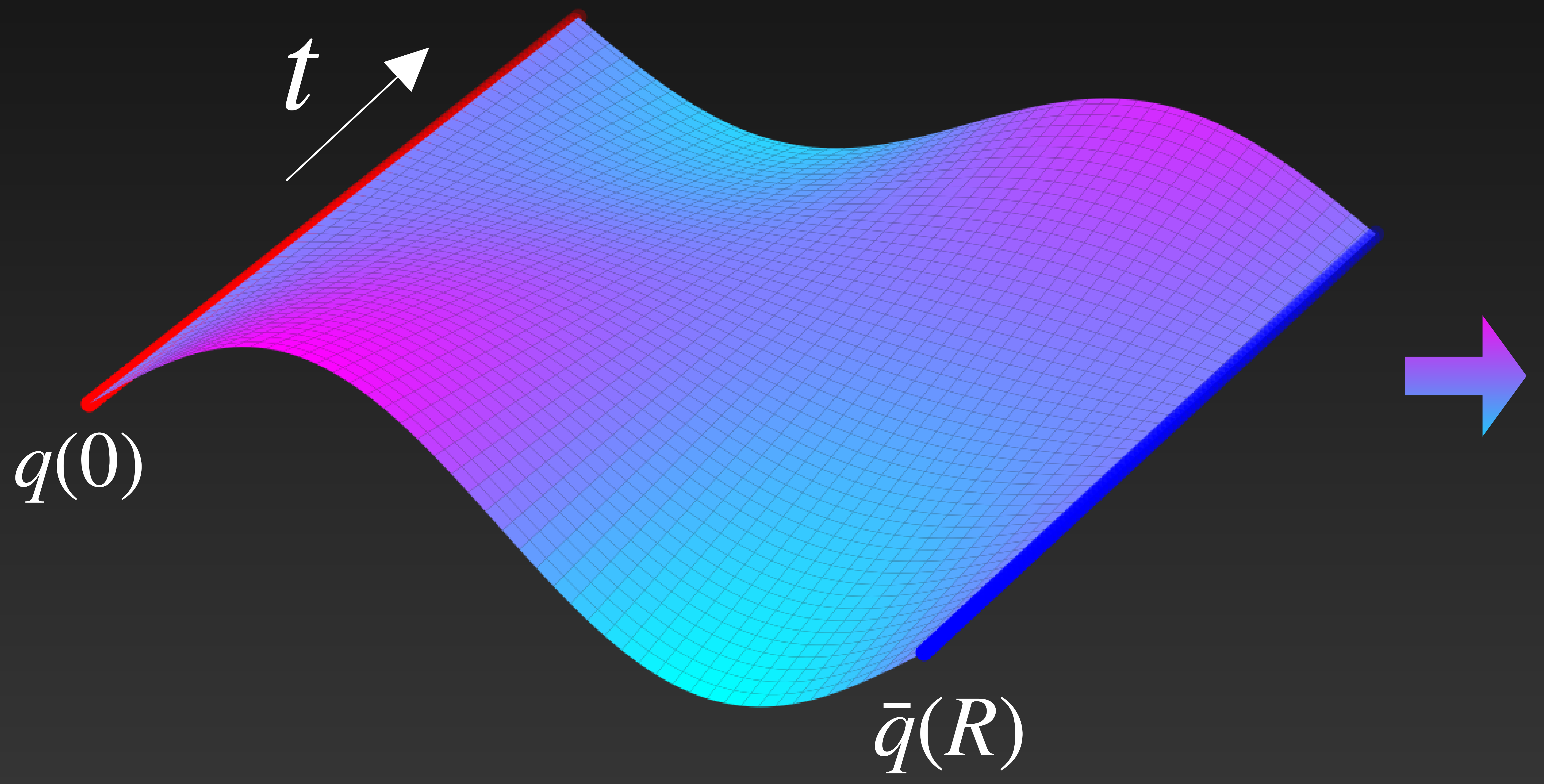
Effective String Theory

Effective String Theory (**EST**) is a powerful tool to study **confinement** in **Yang-Mills** theories



Effective String Theory

Effective String Theory (**EST**) is a powerful tool to study **confinement** in **Yang-Mills** theories



$$\langle P(0)P^{\dagger}(R)\rangle \sim \int DX e^{-S_{EST}[X]} \equiv Z_{EST}$$

Nambu-Goto Theory

The main choice for S_{EST} is the Nambu-Goto action:

$$S_{NG}[\phi] = \sigma \int d\xi^2 \sqrt{g}$$

- **Anomalous** at quantum level $\rightarrow$ **effective**, **large-distance** **description** of Yang-Mills theories.
  [Aharony and Komargodski; 1302.6257], [Brandt and Meineri; 1603.06969],[Caselle; 2104.10486]

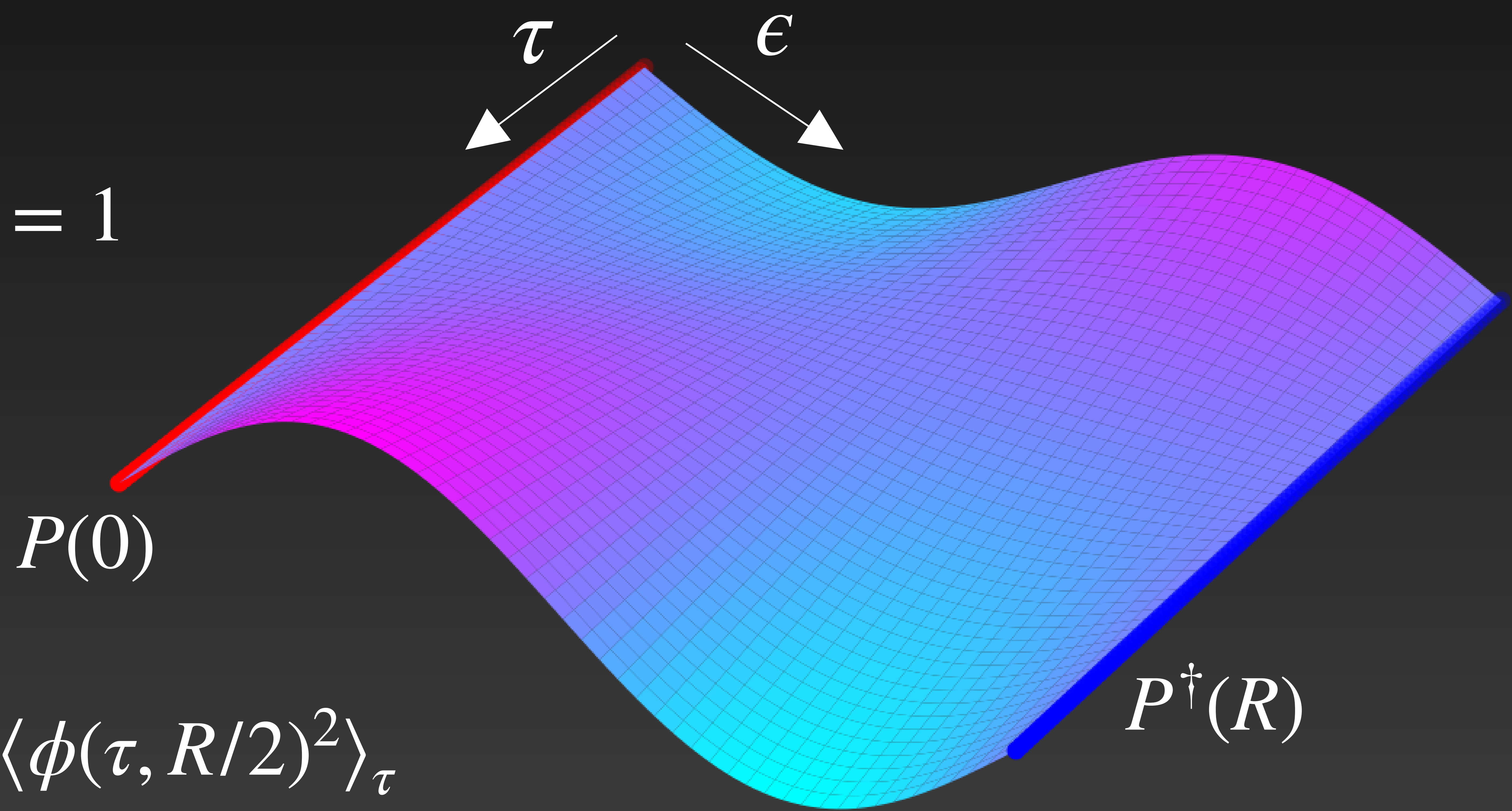
Analytical problems

- **Correlation functions** (e.g. width σw^2)
- **Partition functions** of higher order corrections

Lattice Nambu-Goto String

$$S_{NG}(\phi) = \sigma \sum_{x \in \Lambda} \left[\sqrt{1 + (\partial_\mu \phi(x))^2/\sigma} - 1 \right]$$

- d=2+1 target Yang-Mills
- σ string tension
- Λ : square lattice of size $L \times R$, $a = 1$
- $\phi(x) = \phi(\tau, \epsilon) \in \mathbb{R}$
- $\phi(\tau + L, \epsilon) = \phi(\tau, \epsilon)$
- $\phi(\tau, 0) = \phi(\tau, R) = 0$



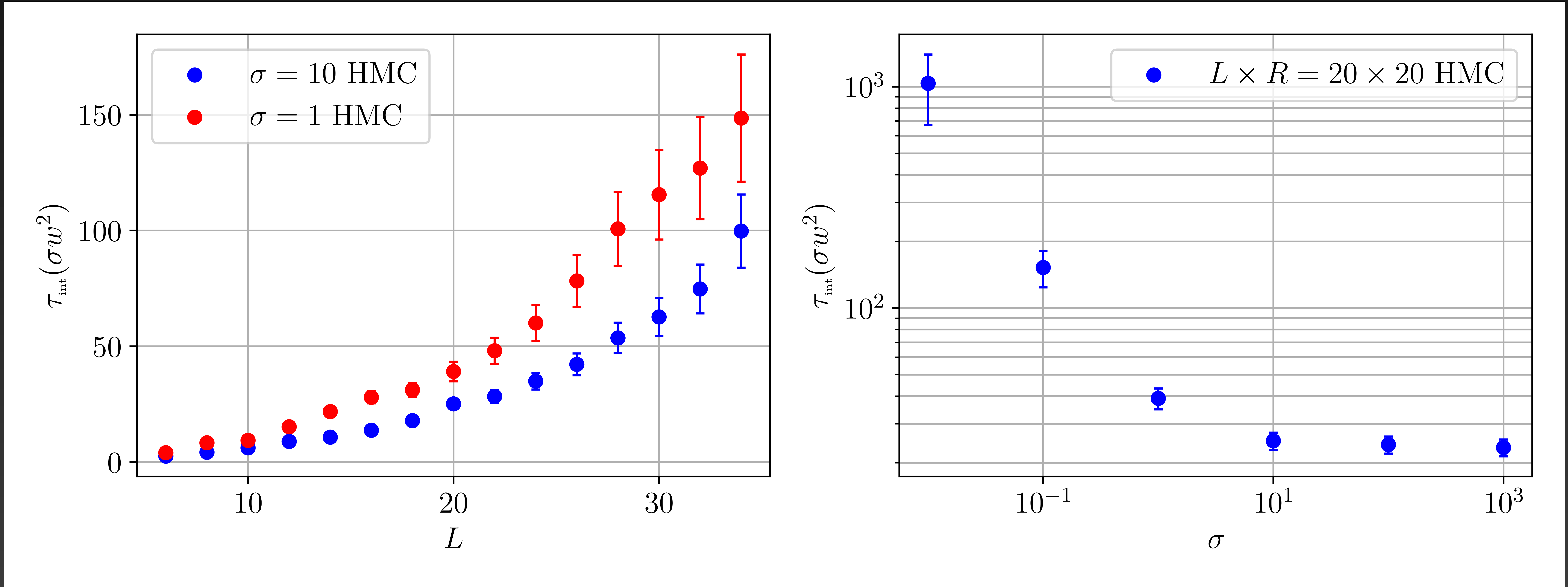
$$\sigma w^2 = \langle \phi(\tau, R/2)^2 \rangle_\tau$$

[Caselle, **EC**, Nada; 2307.01107]

Lacks of numerical methods

Numerical problems:

- Strong **non-linearity** → **critical** theory (**Critical Slowing Down**)
- Estimation of **partition functions**



Normalizing Flows

Normalizing Flows

A Normalizing Flow (**NF**) g_θ is a **parametric**, **invertible** and **differentiable** function:

[Rezende+; 1505.05770]

$$g_\theta: \; q_0 \to q_\theta \simeq p \qquad \phi = g_\theta(z) \qquad q_\theta(\phi) = q_0(g^{-1}(\phi))\,|J_g|^{-1}$$

Learning Boltzmann Distributions

NFs can be trained to $q_\theta \simeq p(\phi)$ with $p(\phi) = \exp(-S[\phi])/Z$ by minimizing the reverse **Kullback-Leibler divergence**:

[Albergo+; 1904.12072][Noé+; 1812.01729]

$$D_{KL}(q_\theta || p) = \int d\phi q_\theta(\phi) \log \frac{q_\theta(\phi)}{p(\phi)} \geq 0.$$

Sampling Boltzmann Distributions

Partition functions and **observables** can be computed using a re-weighting procedure also called **Importance Sampling**:

[Nicoli+; 2007.07115]

$$\langle \mathcal{O} \rangle_{\phi \sim p} = \frac{1}{Z} \langle \mathcal{O} \tilde{w} \rangle_{\phi \sim q_\theta} \qquad Z = \langle \tilde{w} \rangle_{\phi \sim q_\theta} \qquad \tilde{w} = \frac{e^{-S[\phi]}}{q_\theta(\phi)}$$

↓ Uncorrelated!

↓ Partition functions!

Continuous Normalizing Flows

Continuous NFs (CNFs) are NFs in which the flow g_θ is the solution of a Neural Ordinary Differential Equation (NODE):

$$\frac{d\phi(t)_x}{dt} = \sum_{y,f} W_{x,y,f} K(t)_f \phi(t)_y$$

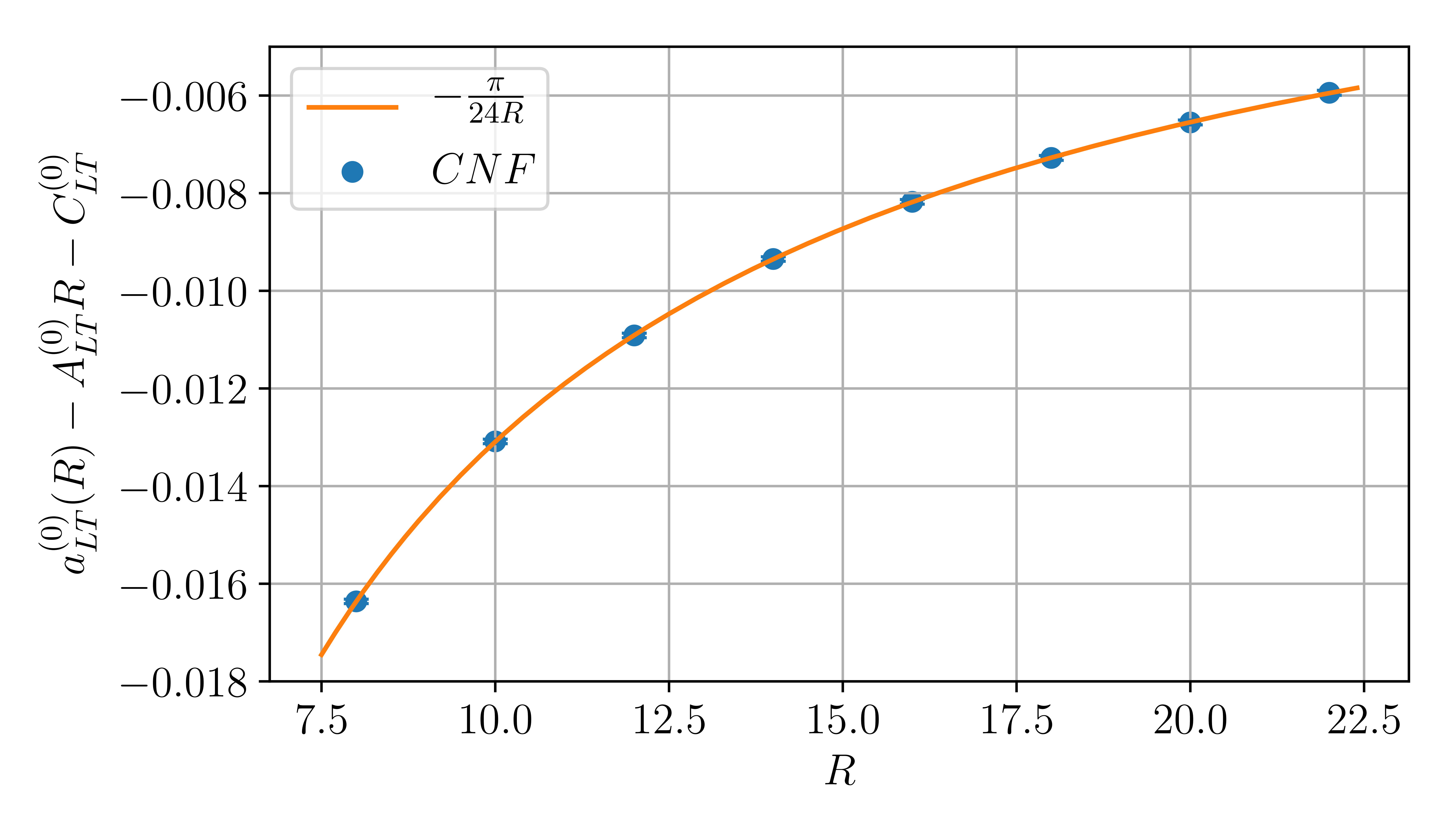
$$\frac{d \log q_\theta(\phi(t))}{dt} = -Tr\left[\sum_f W_f K(t)_f\right]$$

$K(t) \in \mathbb{R}^F$ temporal kernel of F Fourier coefficients

[Chen+;1806.07366],[Gerdes+,2207.00283] [Caselle, **EC**, Nada; 2307.01107]

Proof of Concept: Partition Function

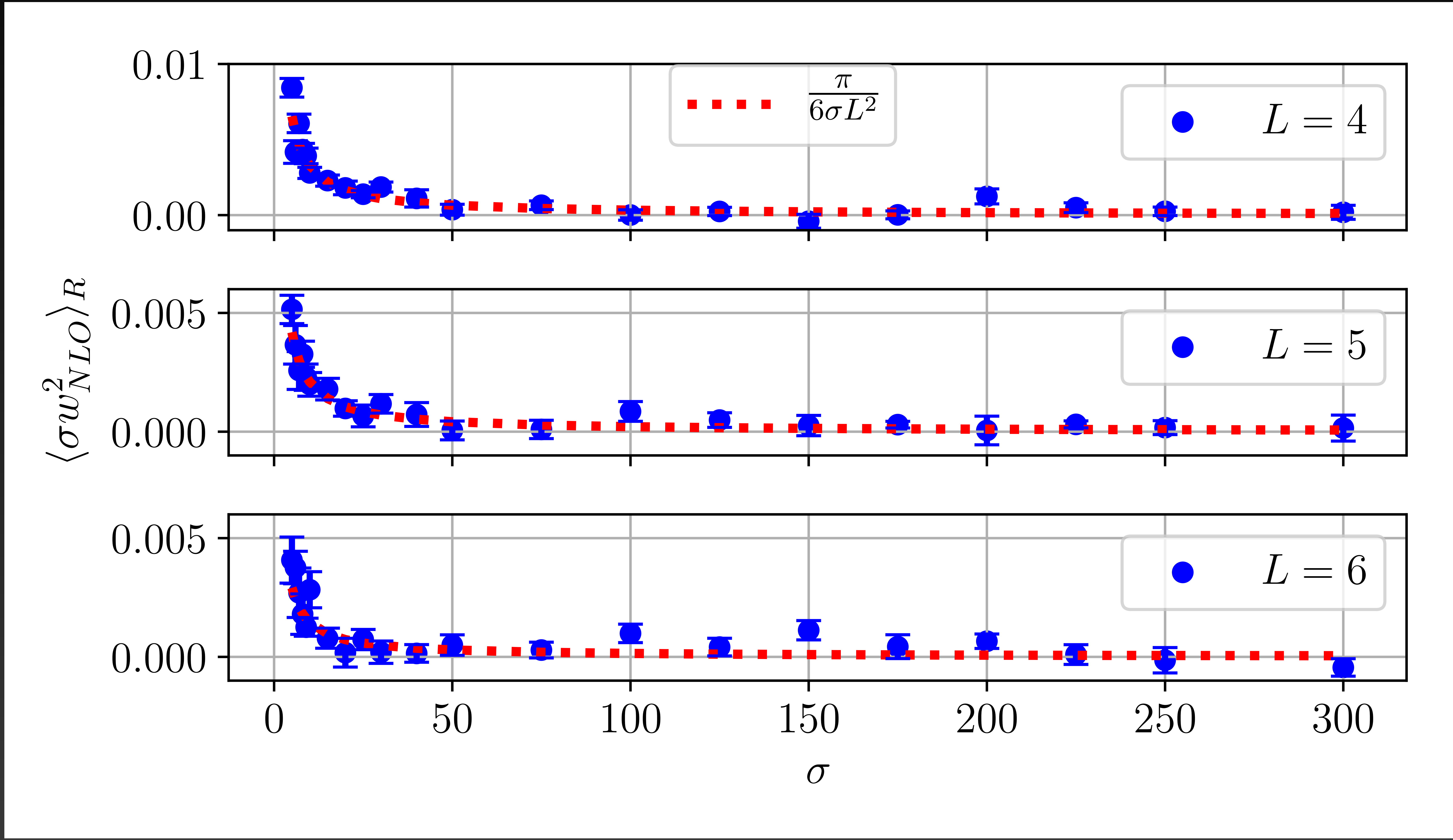
Large σ region ($\sigma \geq 40$), inferred coefficient: $-0.1309(2)$, target: $-0.1308996\ldots$



[Caselle, **EC**, Nada; 2307.01107]

Proof of Concept: Width

Large σ region ($\sigma \geq 5$), inferred coefficient: $0.55(5)$, target: $0.523598...$



[Caselle, **EC**, Nada; 2307.01107][Gliozzi+; 1002.4888]

Stochastic Normalizing Flows

Jarzynski's Equality

General equality that relates non-equilibrium experiments and equilibrium quantities:

[Jarzynski; cond-mat/9610209]

$$\langle e^{-W} \rangle_f = e^{-\Delta F}$$

We can prove (and exploit) this equality using as "physical" system a Markov Chain Monte Carlo (MCMC) algorithm!

Non-Equilibrium MCMC

$$q_0 \simeq e^{-S_0} \xrightarrow{P_1} e^{-S_1} \xrightarrow{P_2} \dots \xrightarrow{P_N} e^{-S_N} \simeq p$$

1. Thermalized q_0 "**prior**"
2. $P_i \propto \exp(-S_i)$ change along the processes and satisfy detailed balance.
3. $p = \exp(-S_N)/Z_N \rightarrow$ "**target**" distribution

Remark: no thermalization during the processes.

Non-Equilibrium MCMC

Forward probability density:

$$q_0(\phi_0)\prod_{n=0}^{N-1} P[\phi_i \rightarrow \phi_{i+1}] = q_0(\phi_0)P_f[\phi_0, \ldots, \phi_N]$$

Reverse probability density:

$$p(\phi_N)\prod_{n=0}^{N-1} P[\phi_{i+1} \rightarrow \phi_i] = p(\phi_N)P_r[\phi_N, \ldots, \phi_0]$$

Dissipated Work

Observe that:

$$\ln \frac{q_0(\phi_0)P_f[\phi_0, \ldots, \phi_N]}{p(\phi_N)P_r[\phi_N, \ldots, \phi_0]} = \underbrace{S_N(\phi_N) - S_0(\phi_0) - Q}_{\textbf{First Law}} - \Delta F = W(\phi_0, \ldots, \phi_N) - \Delta F = W_d$$

Where:

$$\underbrace{Q = \ln \frac{P_r[\phi_N, \ldots, \phi_0]}{P_f[\phi_0, \ldots, \phi_N]} = \sum_{n=0}^{N-1} \ln \frac{q_{n+1}(\phi_{n+1})}{q_{n+1}(\phi_n)}}_{\textbf{Detailed Balance}} = \sum_{n=0}^{N-1} \left(S_{n+1}(\phi_{n+1}) - S_{n+1}(\phi_n) \right)$$

Crooks Fluctuation Theorem

Thus:

$$\frac{q_0(\phi_0)P_f[\phi_0, \ldots, \phi_N]}{p(\phi_N)P_r[\phi_N, \ldots, \phi_0]} = \frac{\mathscr{P}_f(W_d)}{\mathscr{P}_r(-W_d)} = e^{W_d}$$

→ **Crooks Theorem**

[Crooks; cond-mat/9901352]

Observe also:

$$1 = \int \prod_{i=0}^{N} d\phi_i q_0(\phi_0)P_f[\phi_0, \ldots, \phi_N]\left(\frac{p(\phi_N)P_r[\phi_N, \ldots, \phi_0]}{q_0(\phi_0)P_f[\phi_0, \ldots, \phi_N]}\right) = \langle e^{-W_d}\rangle_f$$

Jarzynski's Equality

$$1 = \langle e^{-W_d} \rangle_f$$

$$\langle e^{-W} \rangle_f = e^{-\Delta F}$$

Jarzynski's equality

[Jarzynski; cond-mat/9610209]

$$\langle \mathcal{O} \rangle_{\phi \sim p} = \langle \mathcal{O} e^{-W_d} \rangle_f$$

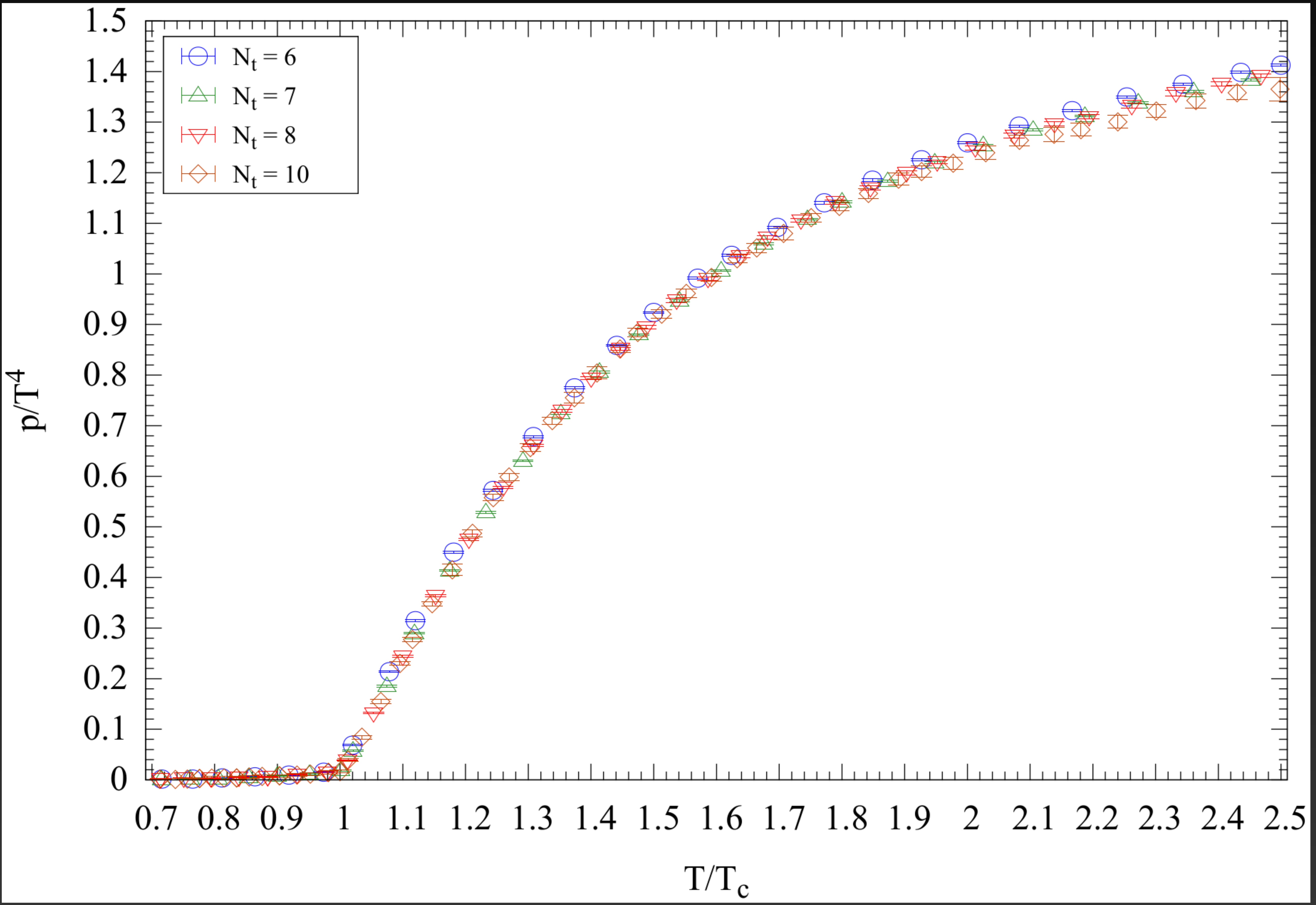
Non-Equilibrium Ensemble

Equilibrium Quantity

Jarzynksi for LFT

Jarzynksi's equality has been exploited to obtain **state-of-the-arts results** in LFT:

- Interface free energy.
  [Caselle+; 1604.05544]
- $SU(3)$ e.o.s.
  [Caselle+; 1801.03110]
- Running coupling
  [Francesconi+; 2003.13734]
- Entanglement entropy
  [Bulgarelli and Panero; 2304.03311]
- Topological freezing
  [Bonanno+; 2310.11979]



Equivalent to:

Annealed Importance Sampling
[Neal; physics/9803008]

Numerical Problem

The identities derived before are exact, however, the **exponential average** has an high **signal-to-noise** ratio.

$$\langle e^{-W_d} \rangle_f$$

In order to fight this problem, we want W_d to be "small"

Solution 1) Infinite MCMC steps → quasi-static transformations → "small" W_d

Stochastic Normalizing Flows (SNFs)

Solution 2) use Machine Learning to minimize W_d

$$\phi_0 \longrightarrow g_\theta^1(\phi_0) \xrightarrow{P_1} \phi_1 \longrightarrow g_\theta^2(\phi_1) \xrightarrow{P_2} \dots \xrightarrow{P_N} \phi_N = \phi$$

Where g_θ^i are NF layers with forward/reverse transition probability:

$$P[\phi_n \to \phi_{n+1}] = \delta(\phi_{n+1} - g_\theta^n(\phi_n))$$

$$P[\phi_{n+1} \to \phi_n] = \delta(\phi_n - (g_\theta^n)^{-1}(\phi_{n+1}))$$

[Wu+; 2002.06707],[Caselle, **EC**, Nada, Panero; 2201.08862]

SNFs: Dissipated Work

We have now:

$$W_d^\theta = W_\theta(\phi_0, \ldots, \phi_N) - \Delta F = S_N(\phi_N) - S_0(\phi_0) - Q_\theta - \Delta F$$

Where:

$$Q_\theta = \sum_{n=0}^{N-1} \left(S_{n+1}(\phi_{n+1}) - S_{n+1}(\phi_n) + \ln|\det J_{g_\theta^i}| \right)$$

SNFs: Training

We can now train a SNF to minimize W_d^θ

$$\mathscr{L}(\theta) = \langle W_d^\theta \rangle_f = D_{KL}(q_0 P_f || p P_r) \geq 0$$

$$\langle W^\theta \rangle_f \geq \Delta F$$

Second Law!

Measure how reversible the process is.

SNFs: Physics-Informed Design

In the $\sigma \to \infty$ region:

$$S_{NG}(\phi) \sim S_{FB}(\phi) + \dots \qquad S_{FB}(\phi) = \frac{1}{2}\sum_x (\partial_\mu \phi(x))^2$$

Prior:

$$q_0(\phi_0) = \frac{1}{Z} e^{S_{FB}(\phi_0)}$$

MCMC update i:

$$S_i(\phi) = S_{NG}(\phi_i, \sigma_i); \qquad \sigma_i > \sigma_{i+1}$$

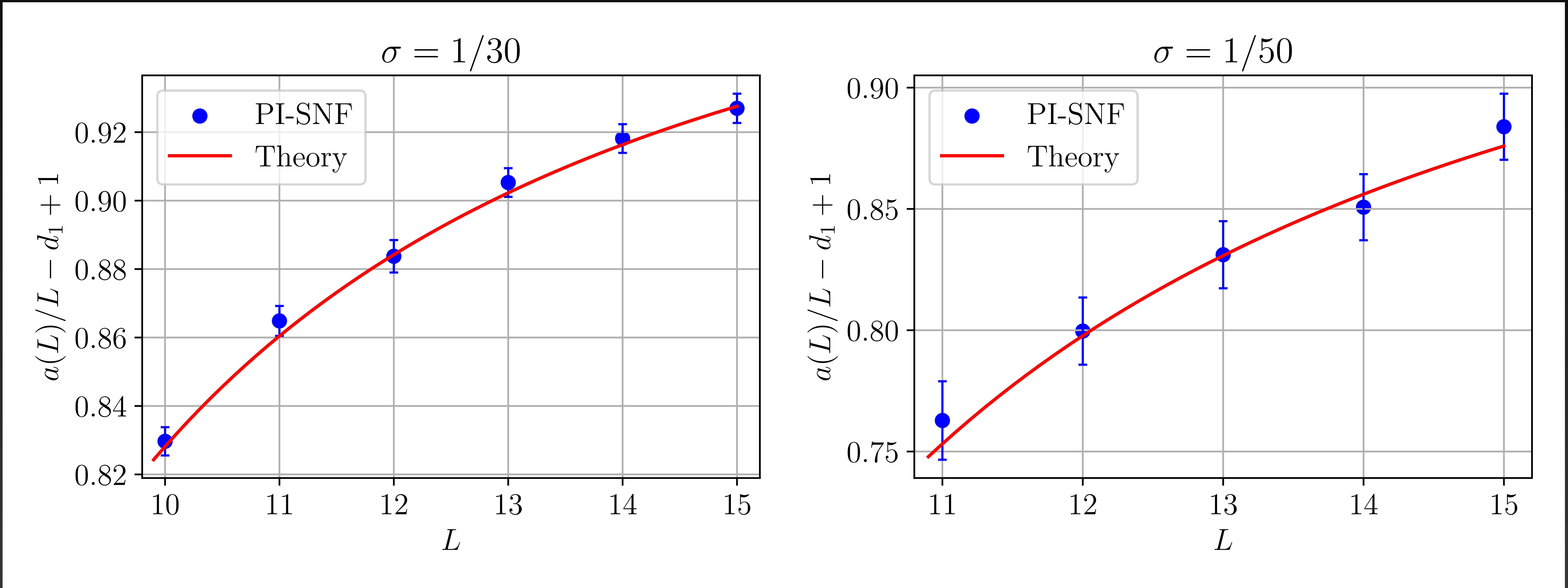
- Design inspired by the $T\bar{T}$ integrable irrelevant perturbation.

  [Cavaglià+; 1608.05534],[Smirnov and Zamolodchikov; 1608.05499]

SNFs: NG Partition Functions

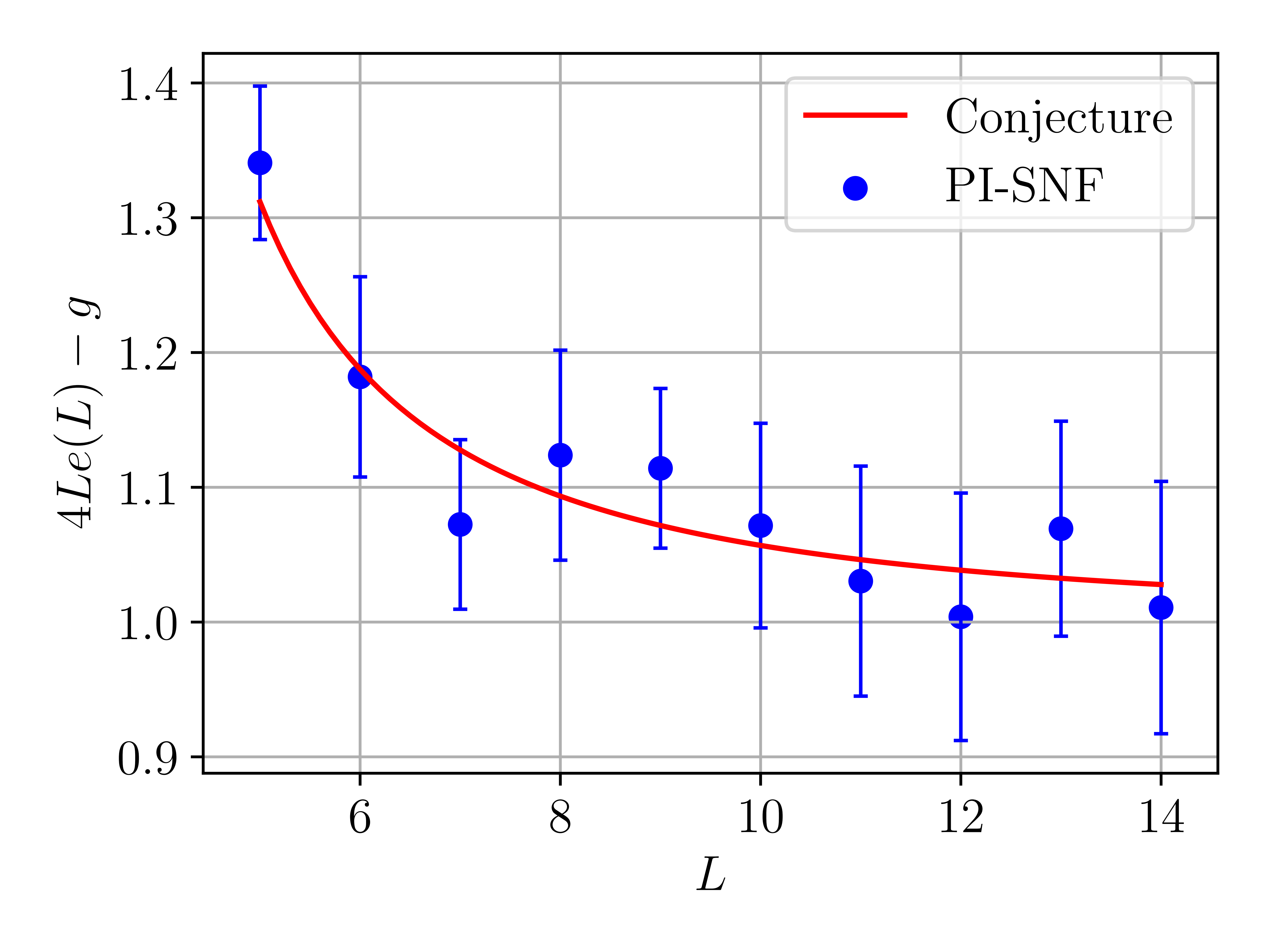
inferred: $-1.03(2)$, target: $-1.047...$

inferred: $-1.04(7)$, target: $-1.047...$



SNFs: NG Width

$\sigma = 1/10$, inferred: $1.09(8)$, target: $1.047...$



[Caselle, E.C., Nada; 2309.14983][Caselle;1004.3875]

Conclusion

We showed that (S)NFs can be successful applied to sample from the EST probability distribution!

1. Flow-based application to Lattice Field Theory which is not a toy-model.
2. State-of-the-art results for Effective String Theory.
3. Toward the study of the “rigid” string:

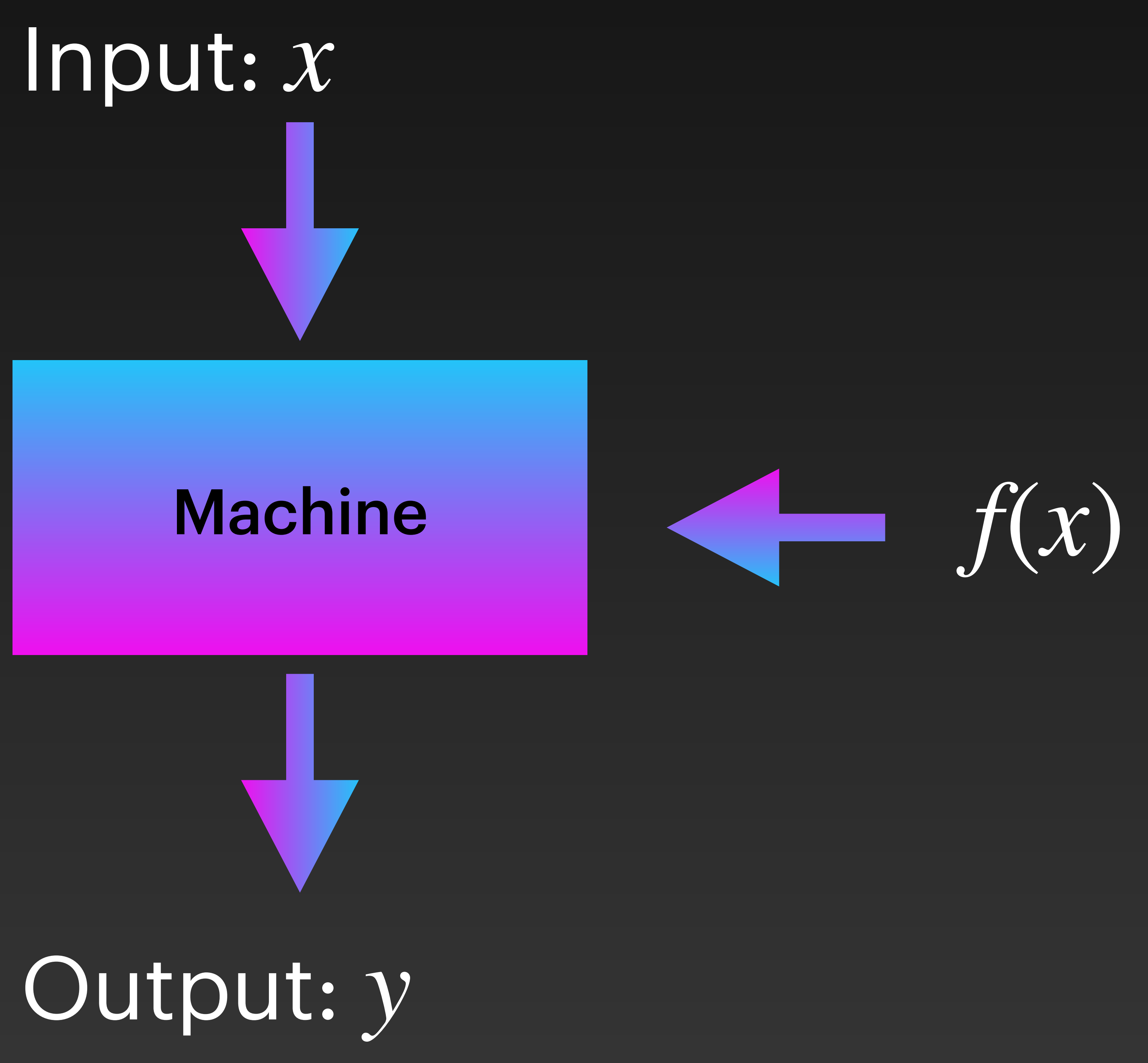
$$S_{BNG} = S_{NG} + \gamma \mathcal{K}^4$$

Thank you for your attention!

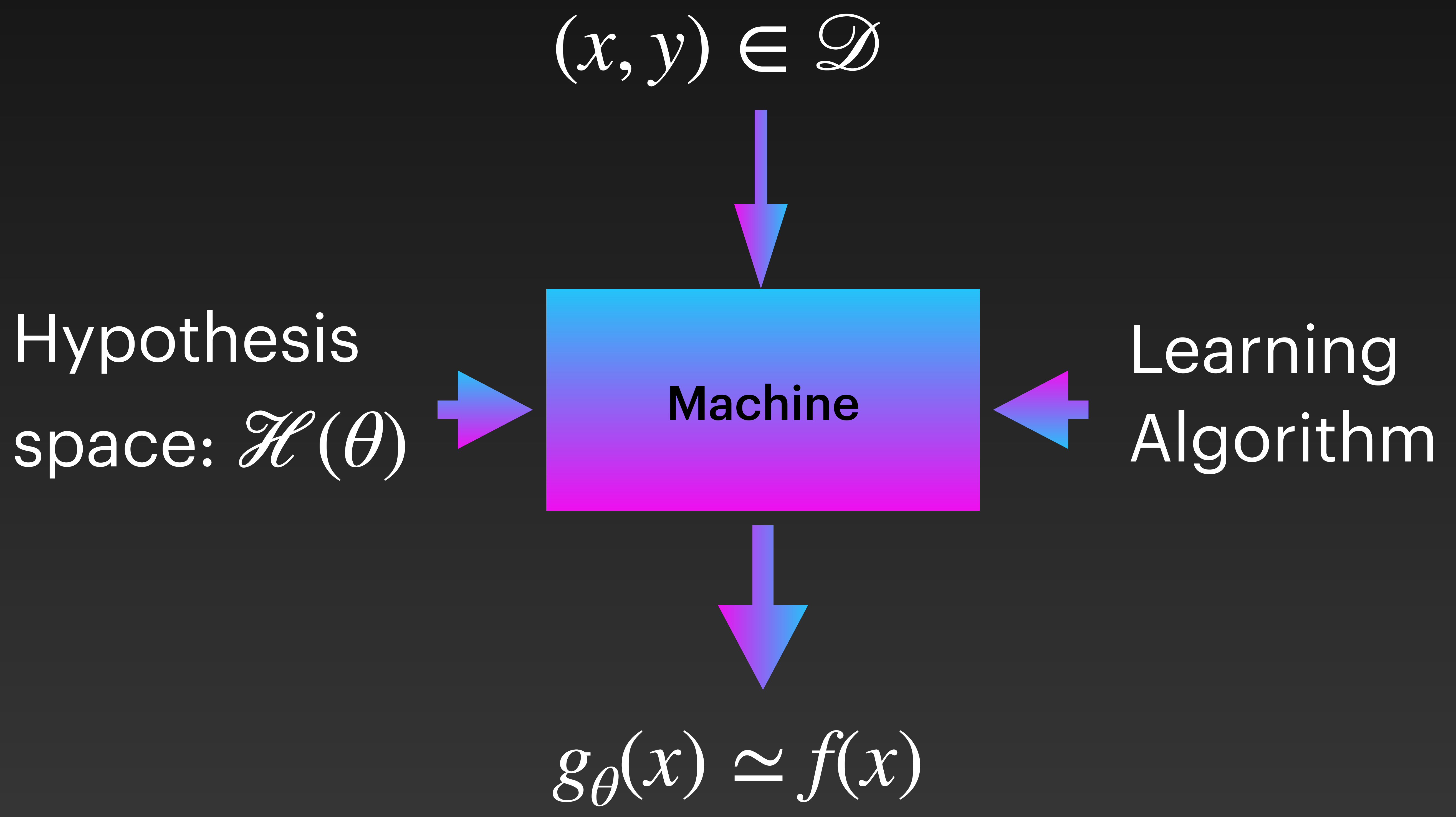
Machine Learning

We want a program ables to compute: $f(x) = y$ for a given input x

Classical programming:



Machine Learning:



SNFs: Technical details

- Prior massless free boson and linear protocol in $t = 1/\sigma \rightarrow$ Inspired by Irrelevant Perturbations
- HMC for stochastic updates
- Affine coupling layers, 3 convolutional layers with $3 \times 3 \times 16$ kernels and a two channels output layer. Each blocks (even-odd) share the same network

SNFs: Related Works

- Annealed Importance Sampling: Equivalent to Jarzynski's equality. Used in the original SNF paper

  [Neal; physics/9803008]

- Sequential Monte Carlo: Generalization of AIS.

  [Dai+; 2007.11936]

- SNF idea reworked in CRAFT

  [Matthews+; 2201.13117]

- An hybrid (deterministic/stochastic) approach with no neural networks has been proposed also by Jarzynksi in 2011

  [Vaikuntanathan and Jazynski; 1101.2612]

- FAB: combination of NFs and AIS.

  [Midgley+; 2208.01893]