Quantum Next Generation Reservoir Computing:

An efficient quantum algorithm for forecasting quantum dynamics

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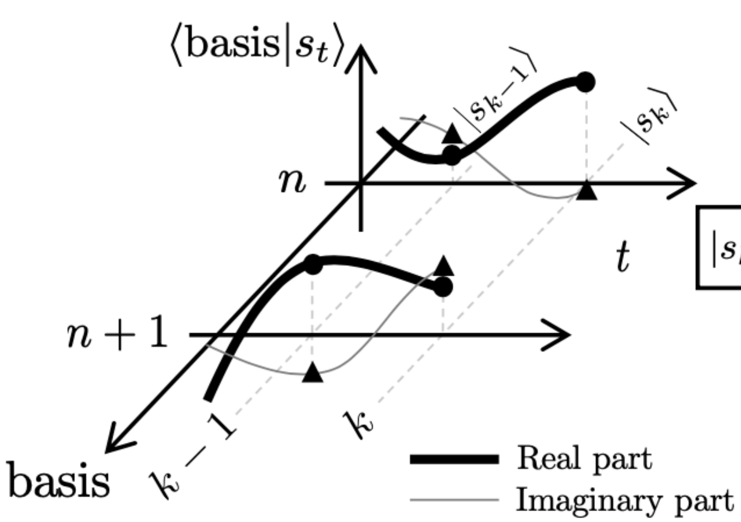
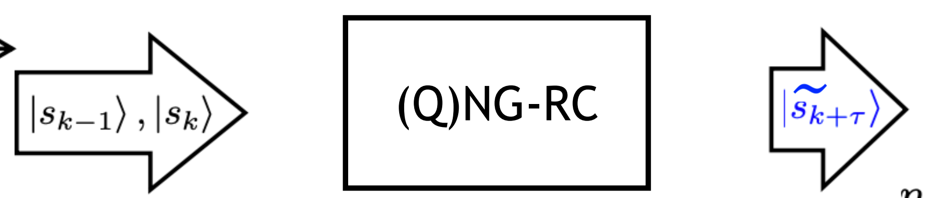
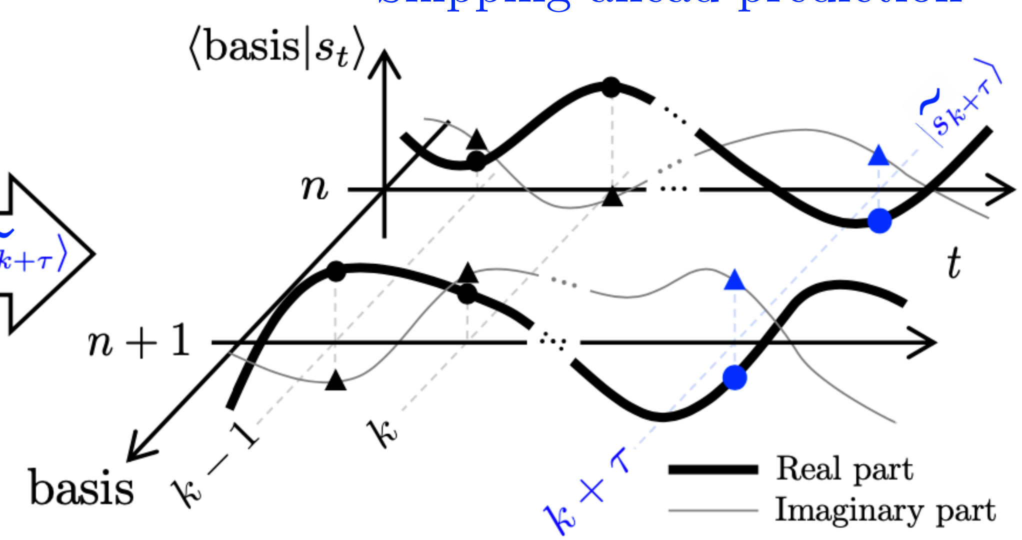
CERN, Geneva
November 24, 2023

$|s_t\rangle = e^{iHt}|s_0\rangle$

Quantum dynamics



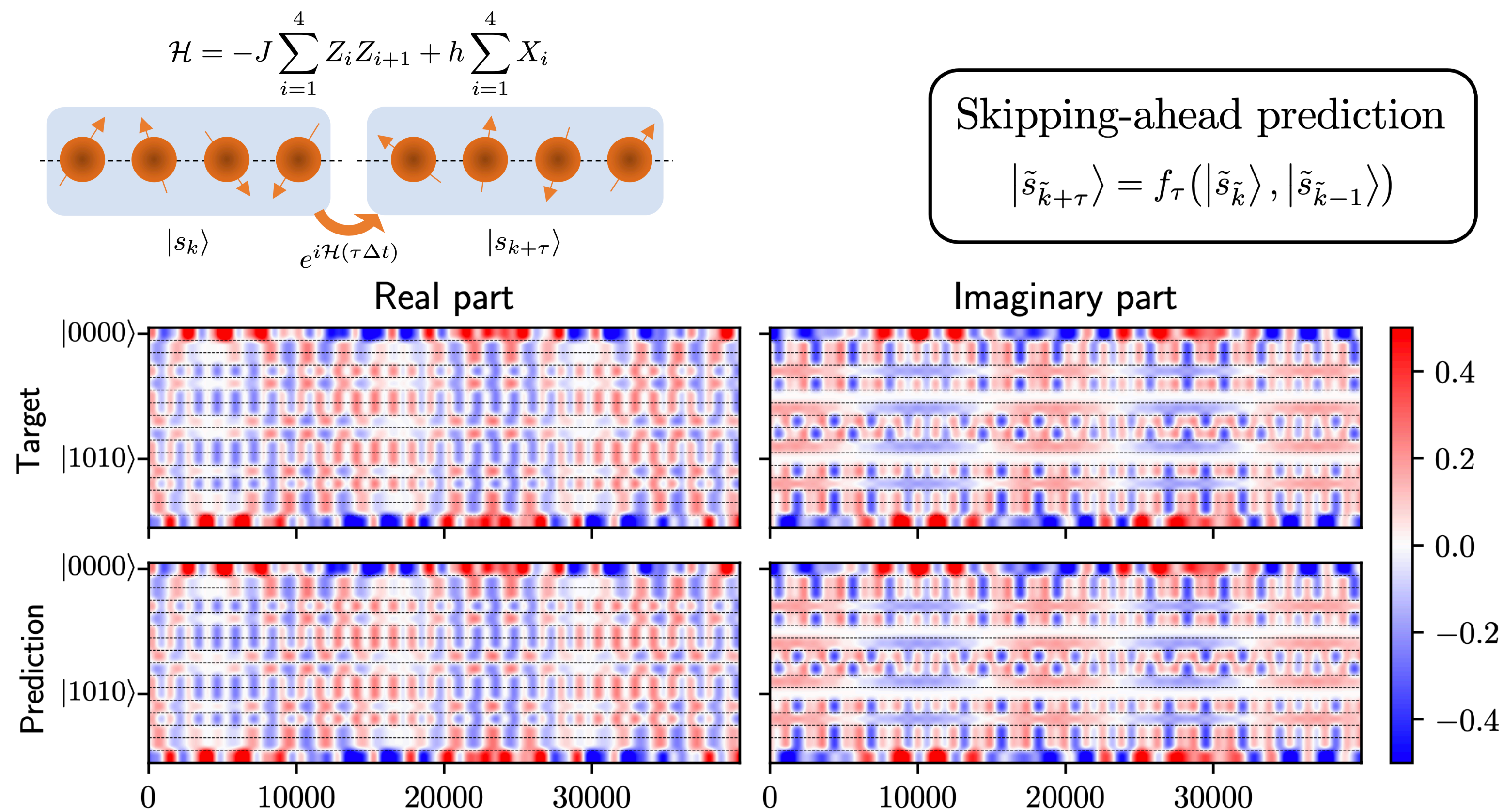




A. Sornsaeng, N. Dangniam, **T. Chotibut** arXiv: 2308.14239

Outline

Part 1: NG-RC for Many-body Quantum Dynamics Prediction



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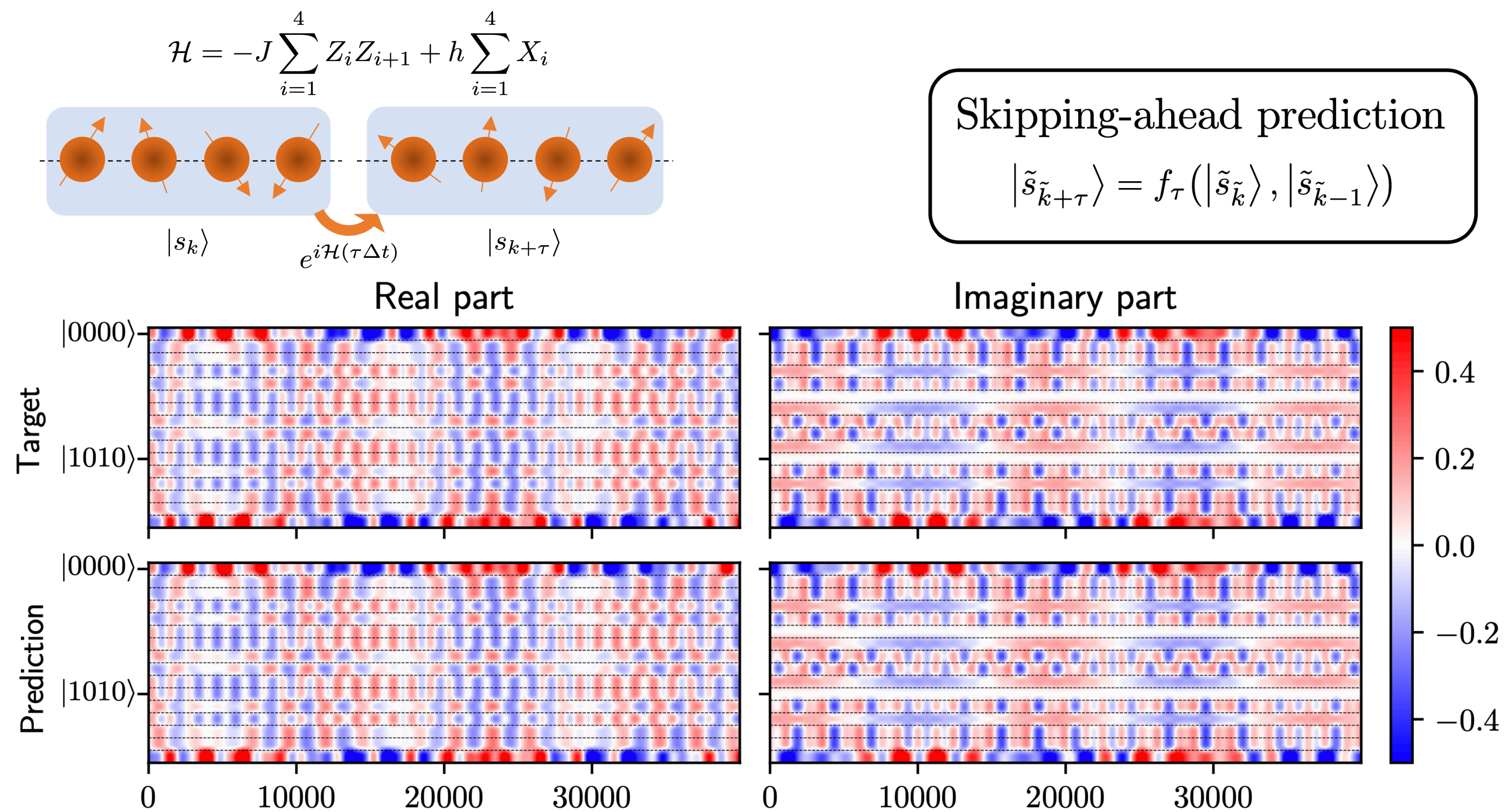
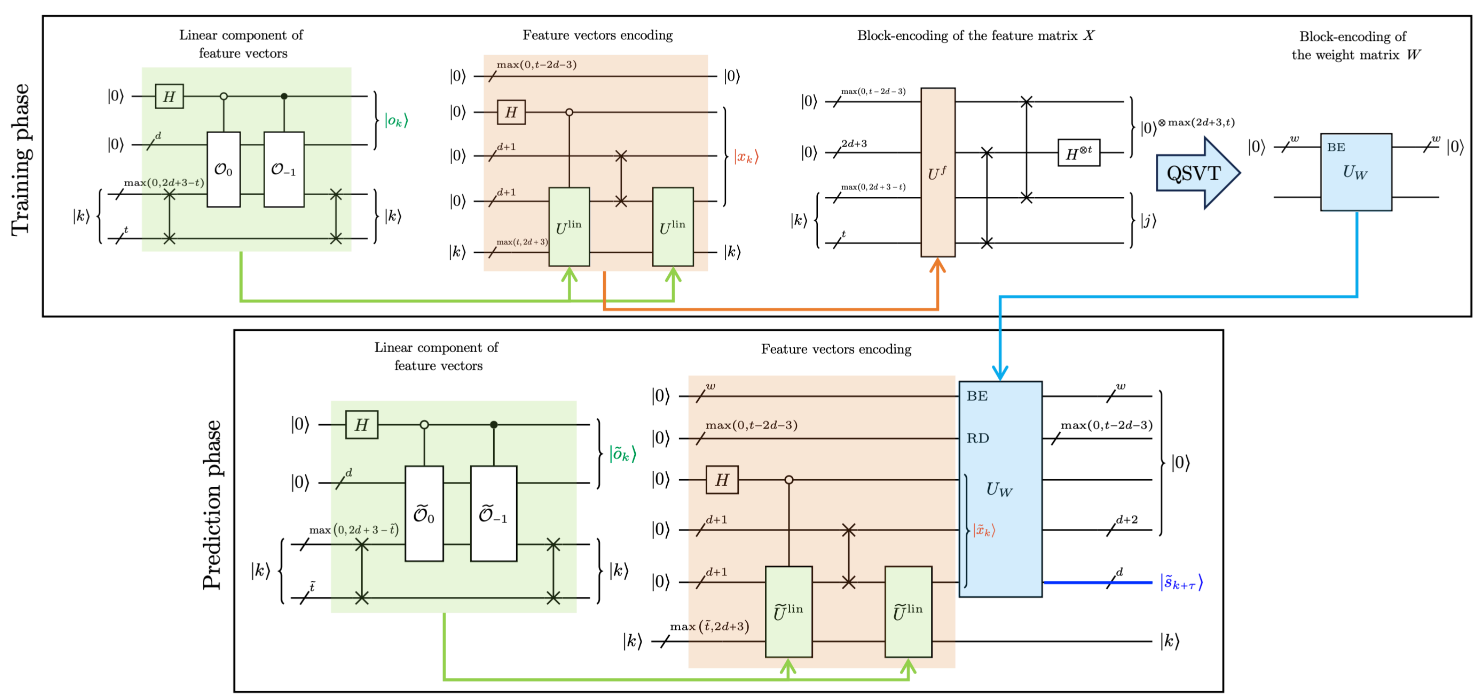


Part 2: Quantum Algorithm for NG-RC (QNG-RC)



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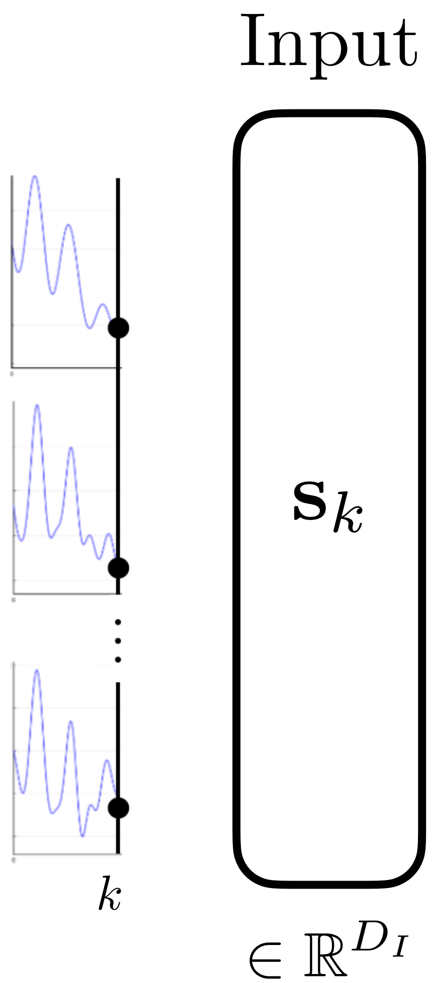
Reservoir Computing (RC) in a nutshell



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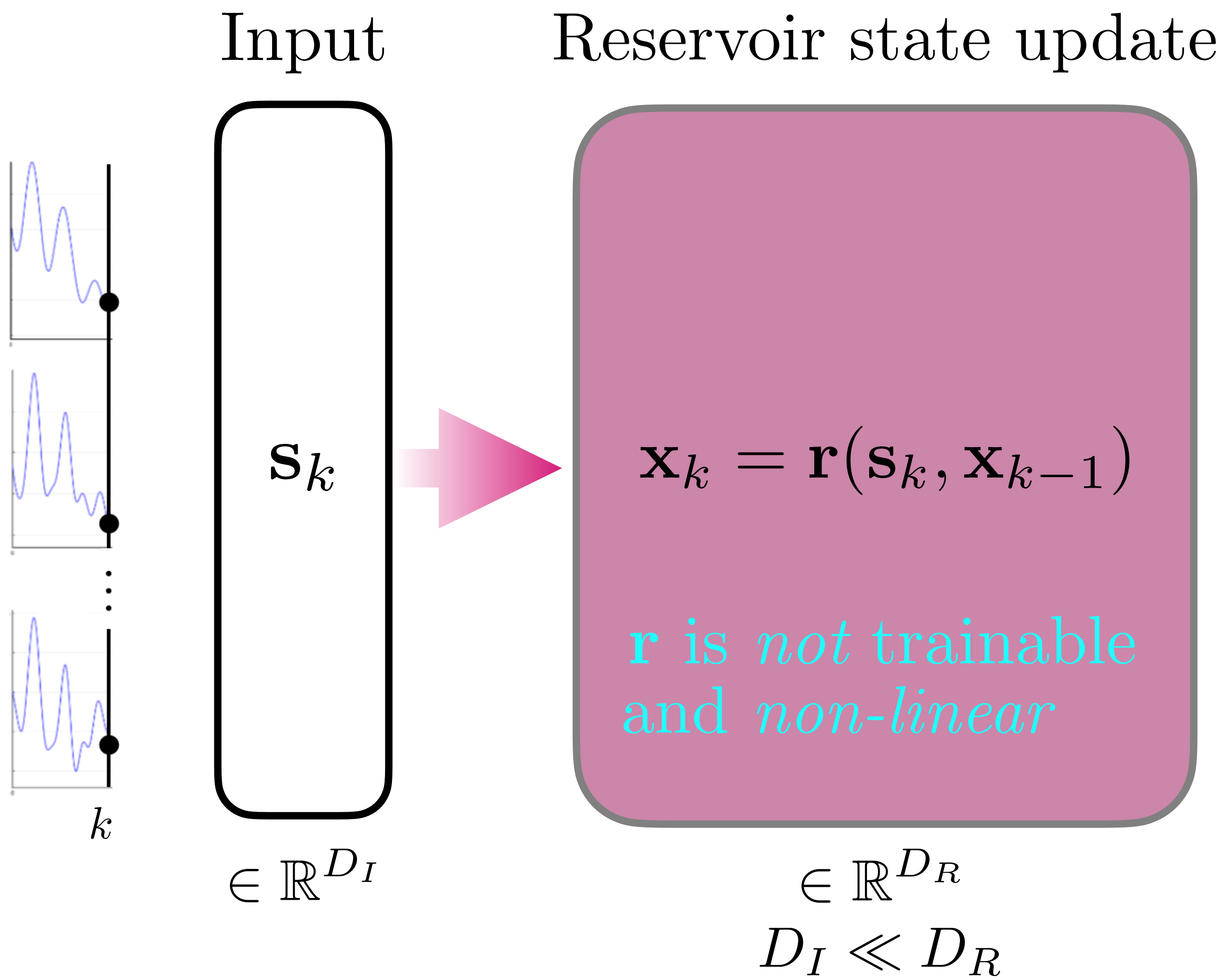

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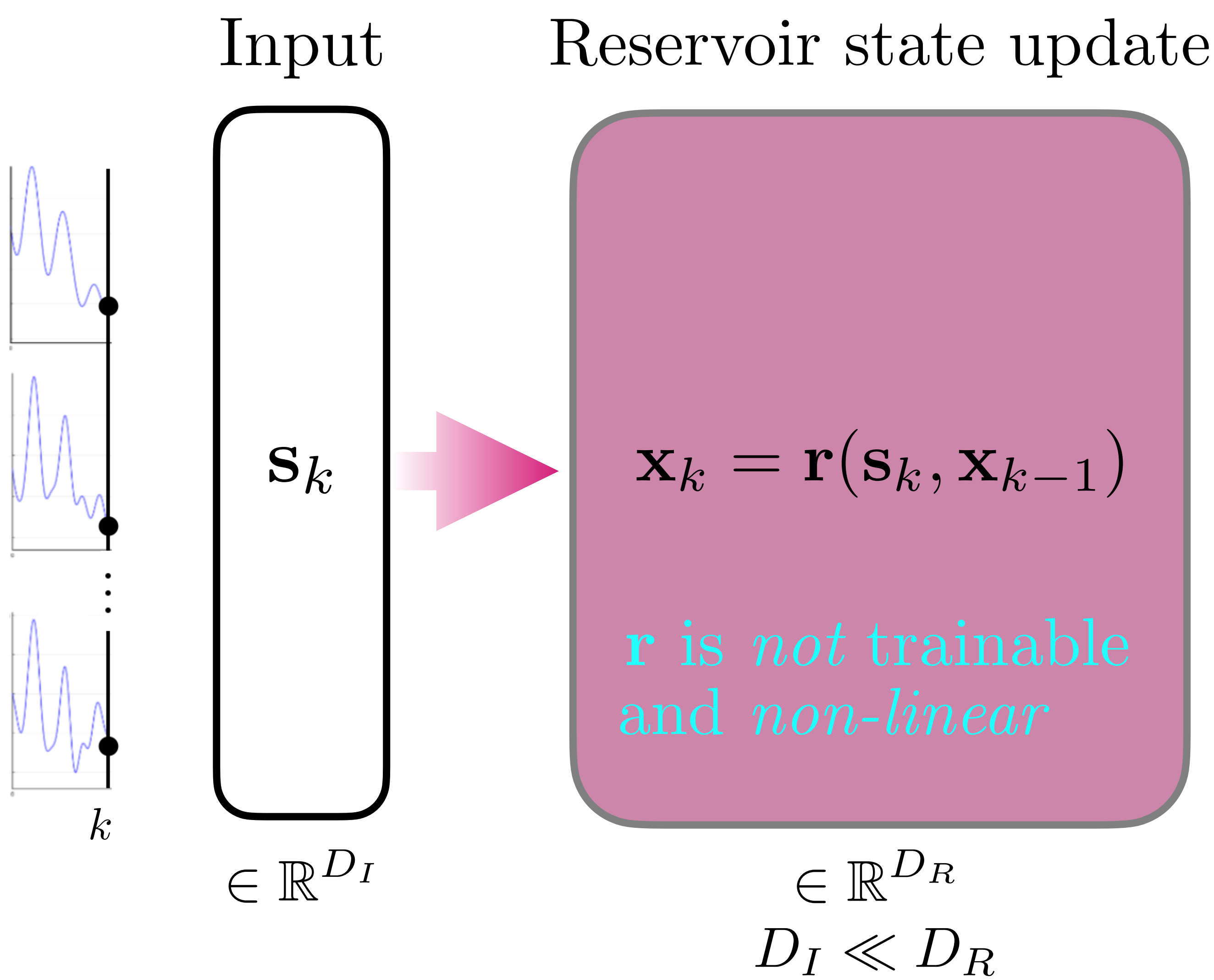
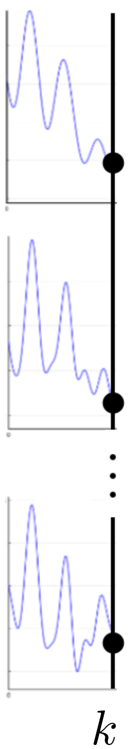


The current state of the reservoir is influenced by the past inputs

$$\mathbf{x}_k = \mathbf{r}(\mathbf{s}_k, \mathbf{r}(\mathbf{s}_{k-1}, \ldots, \mathbf{r}(\mathbf{s}_1, \mathbf{x}_0 \underbrace{) \ldots))}_{k}$$

Reservoir Computing (RC) in a nutshell



Input

$\mathbf{s}_k$

$\in \mathbb{R}^{D_I}$

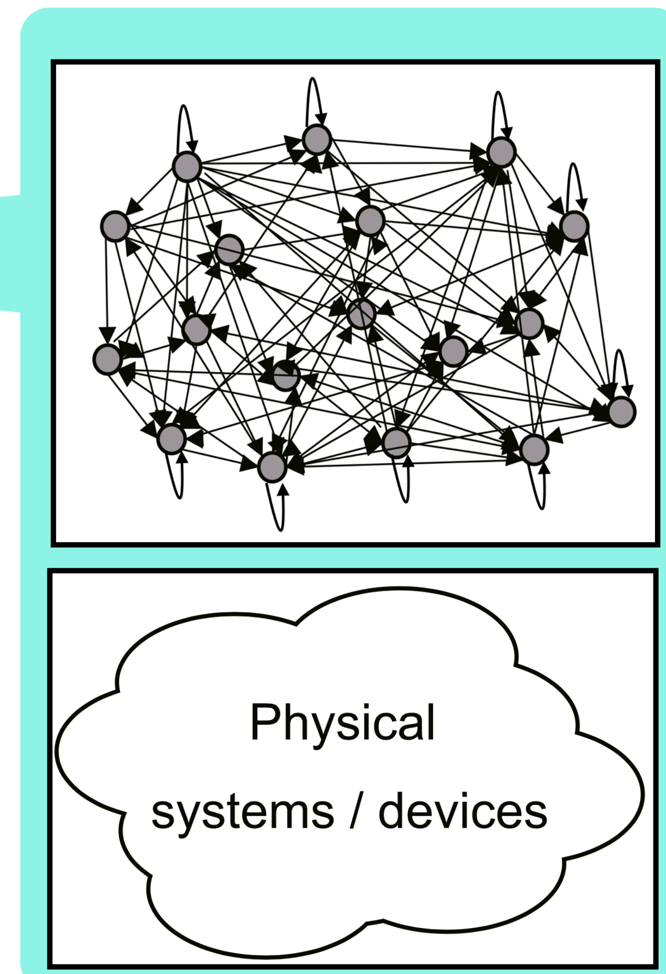
Reservoir state update

$$\mathbf{x}_k = \mathbf{r}(\mathbf{s}_k, \mathbf{x}_{k-1})$$

$\mathbf{r}$ is *not* trainable and *non-linear*

$\in \mathbb{R}^{D_R}$

$D_I \ll D_R$



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G. Tanaka et. al. Recent advances in physical reservoir computing: a review, *Neural Networks*, (**115**) 100-123, 2019

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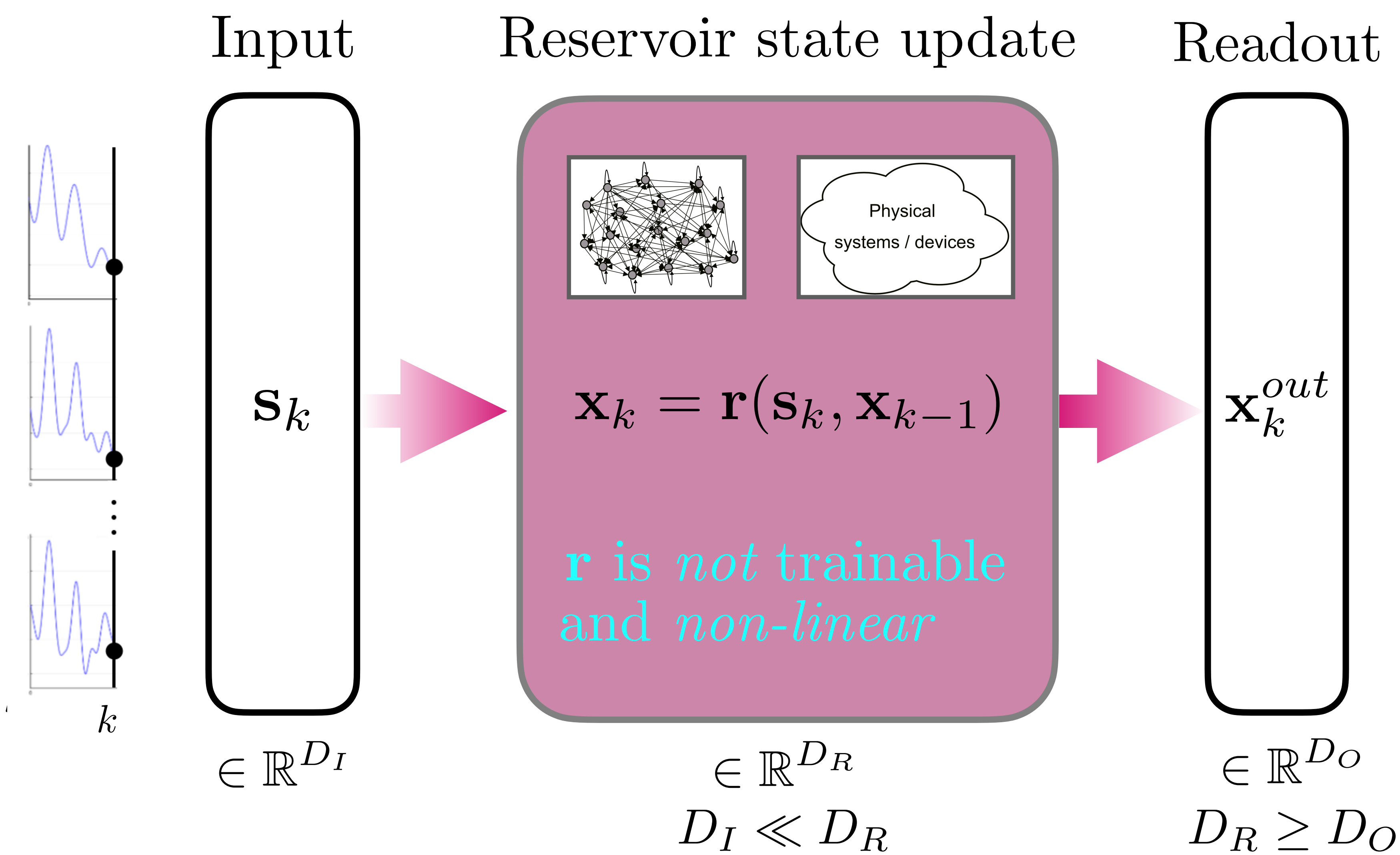

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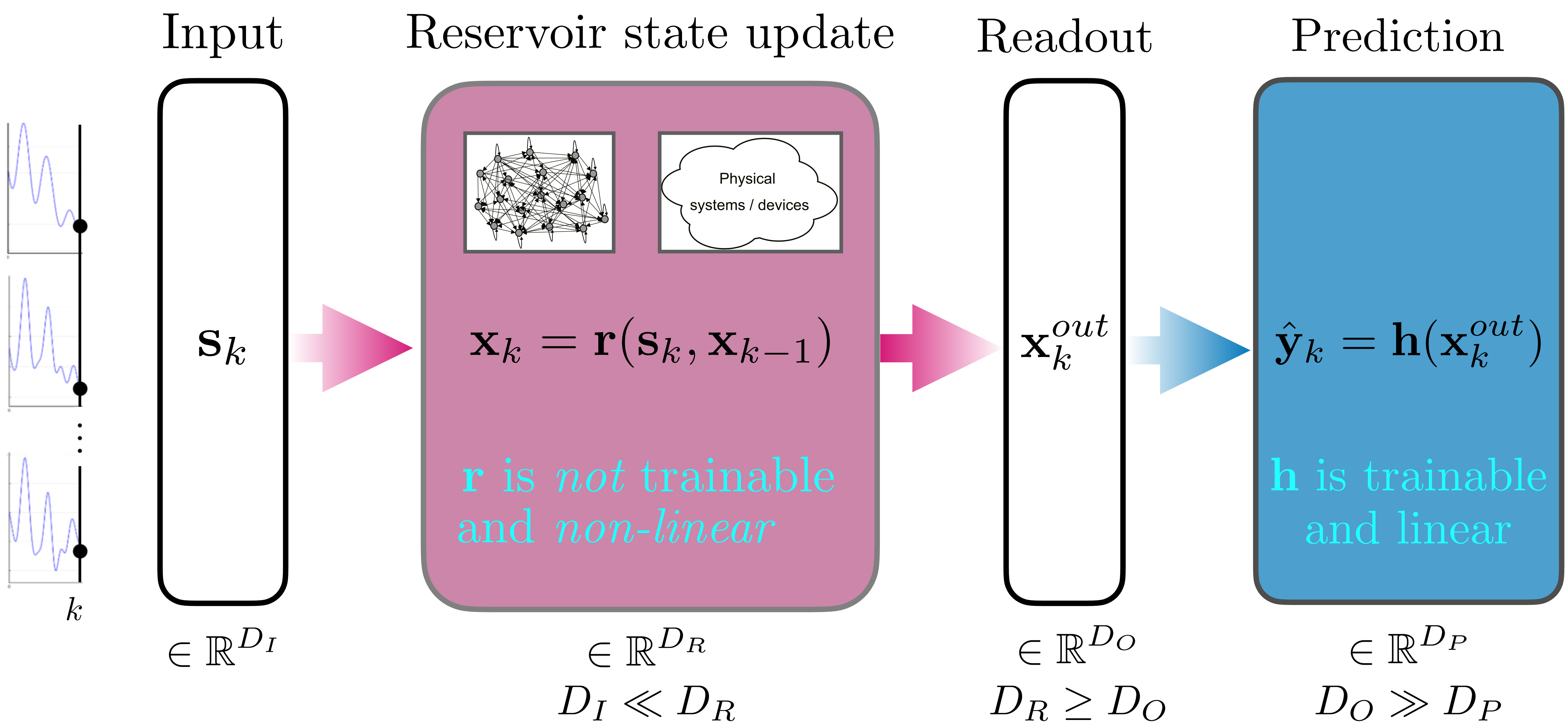

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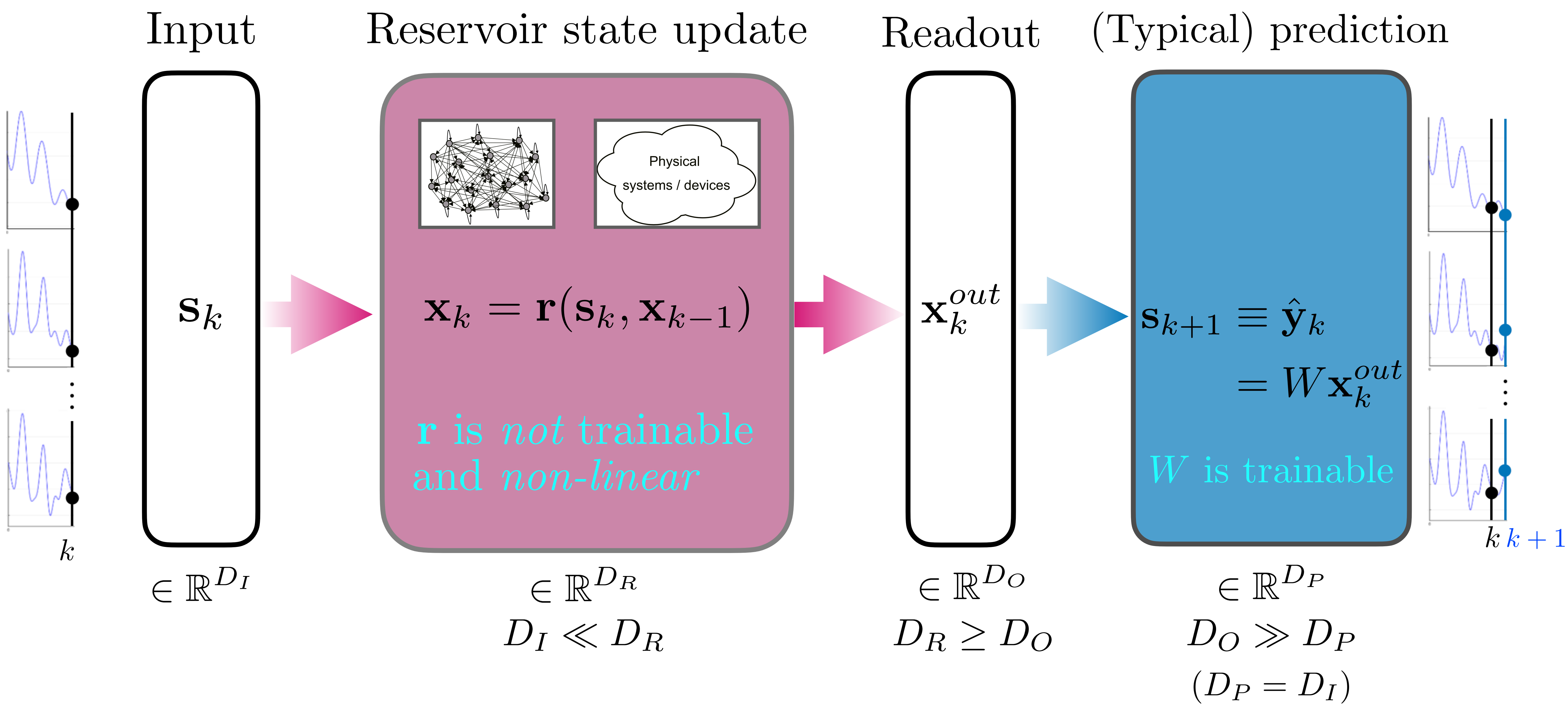

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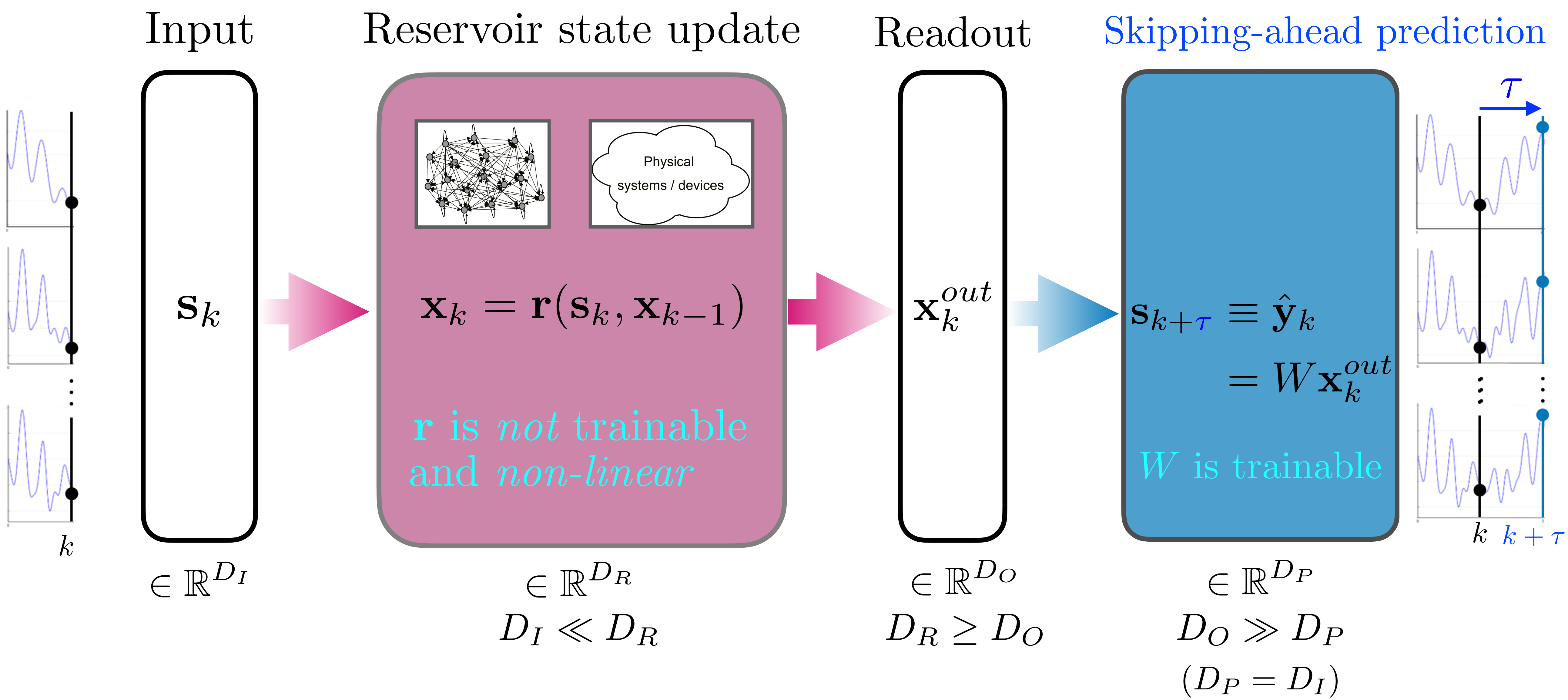

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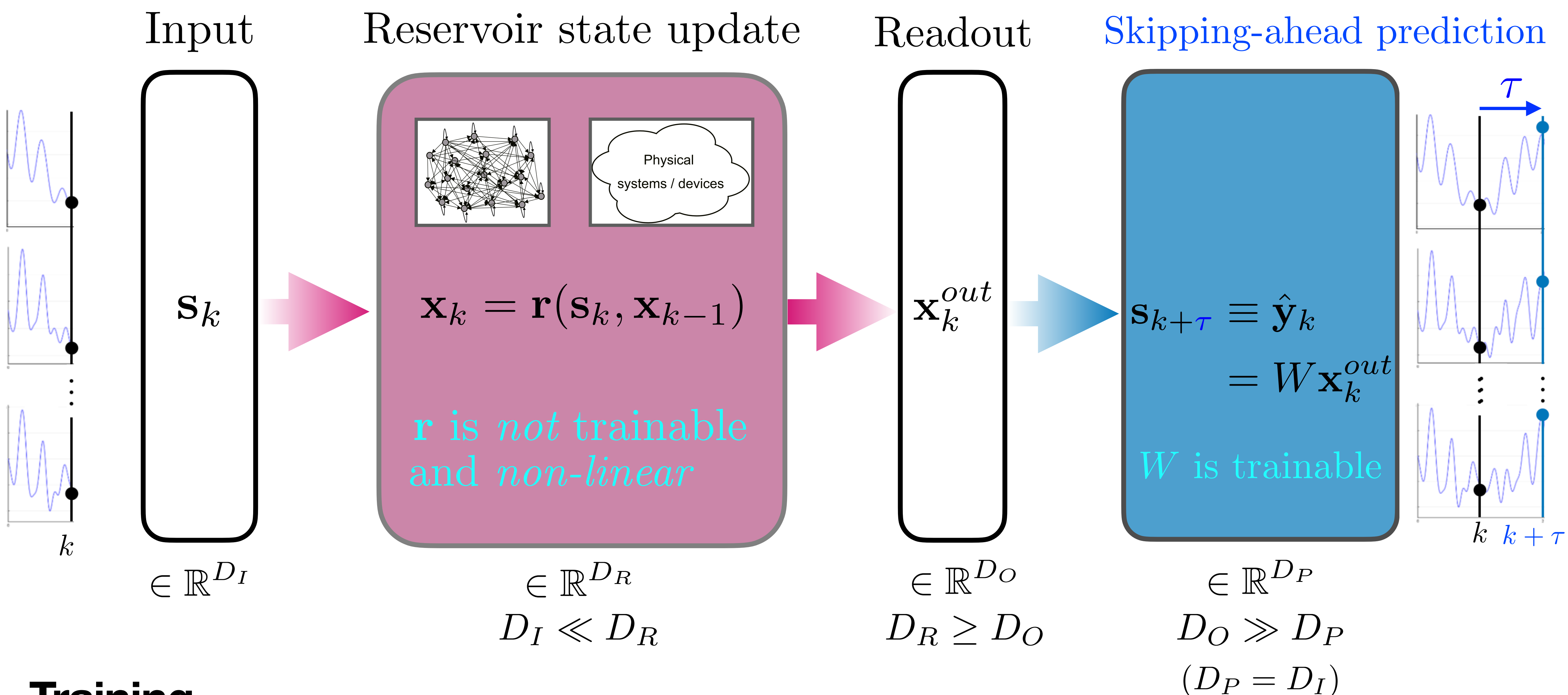

Training

W is “trained” by minimizing

$$\frac{1}{T}\sum_{k=0}^{T-1} ||\hat{\mathbf{y}}_k - W\mathbf{x}_k^{out}||_2^2 + \lambda||W||^2$$

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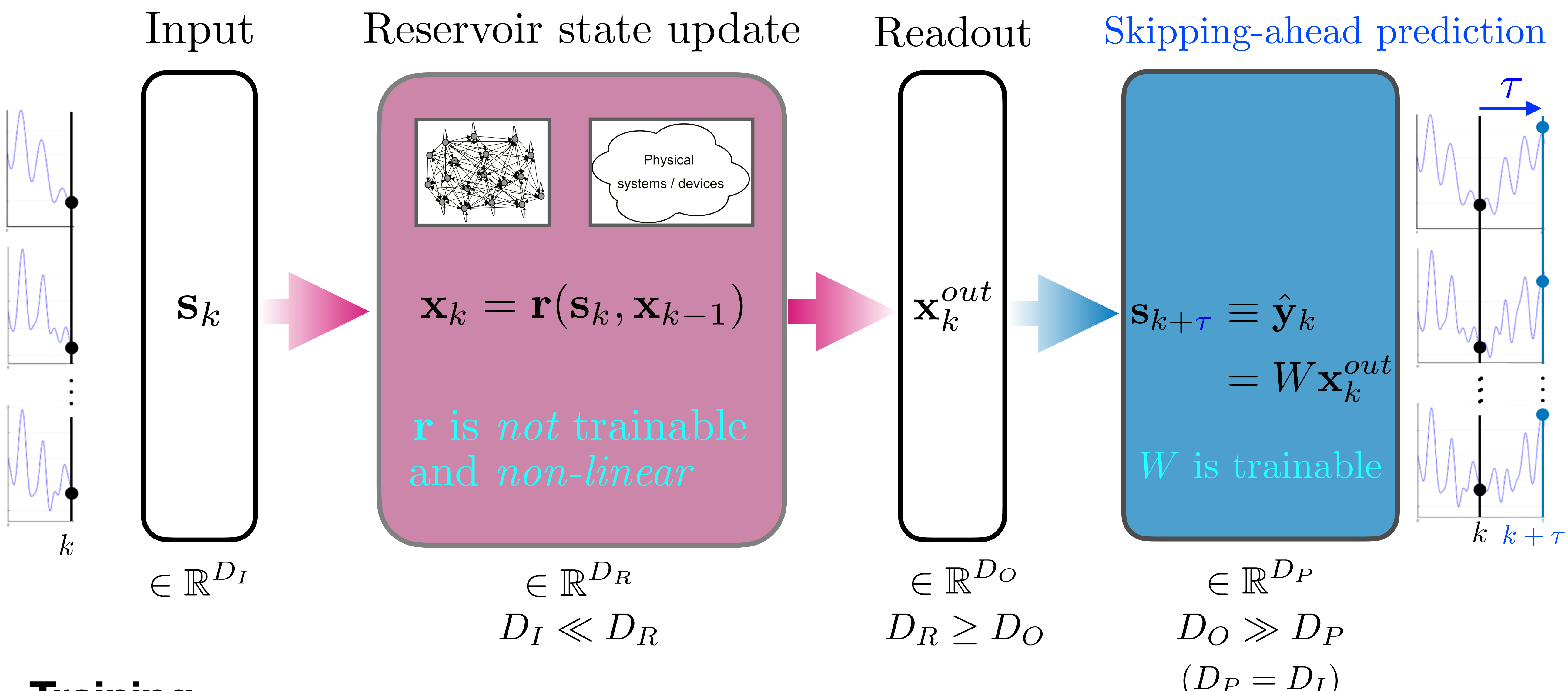


Training

W is "trained" by minimizing

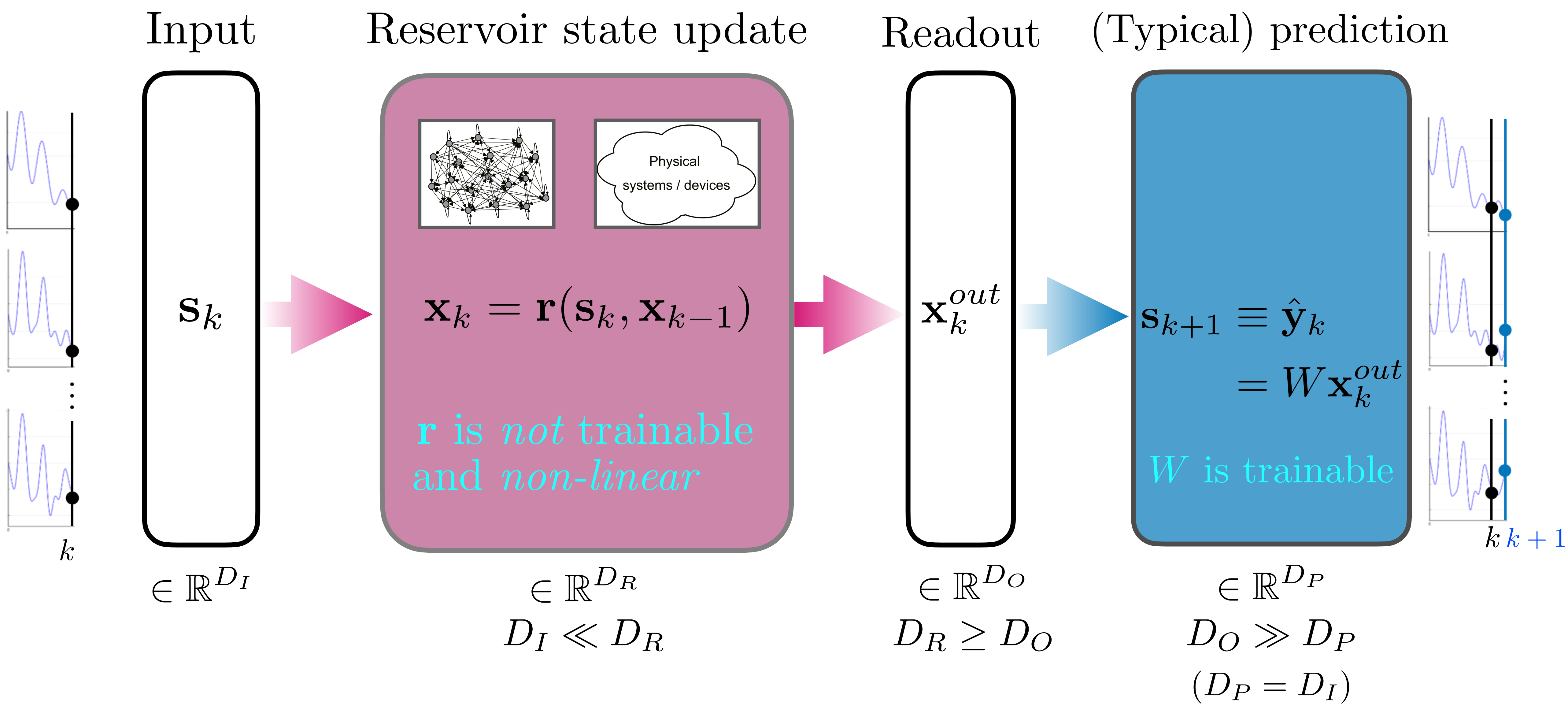
$$\frac{1}{T}\sum_{k=0}^{T-1} ||\hat{\mathbf{y}}_k - W\mathbf{x}_k^{out}||_2^2 + \lambda||W||^2$$

$$\boxed{W = YX^\dagger(XX^\dagger + \lambda I)^{-1}}$$

$Y = (\hat{\mathbf{y}}_0, \ldots, \hat{\mathbf{y}}_{T-1}) \in \mathbb{R}^{D_P \times T}$ target matrix

$X = (\mathbf{x}_0^{out}, \ldots, \mathbf{x}_{T-1}^{out}) \in \mathbb{R}^{D_O \times T}$ feature matrix

Reservoir Computing (RC) in a nutshell



Typical Prediction

$$(\mathbf{x}_k^{out} = \mathbf{x}_k)$$

$$\mathbf{s}'_{k+1} = W\mathbf{x}_k = W\mathbf{r}(\mathbf{s}'_k, \mathbf{x}_{k-1})$$

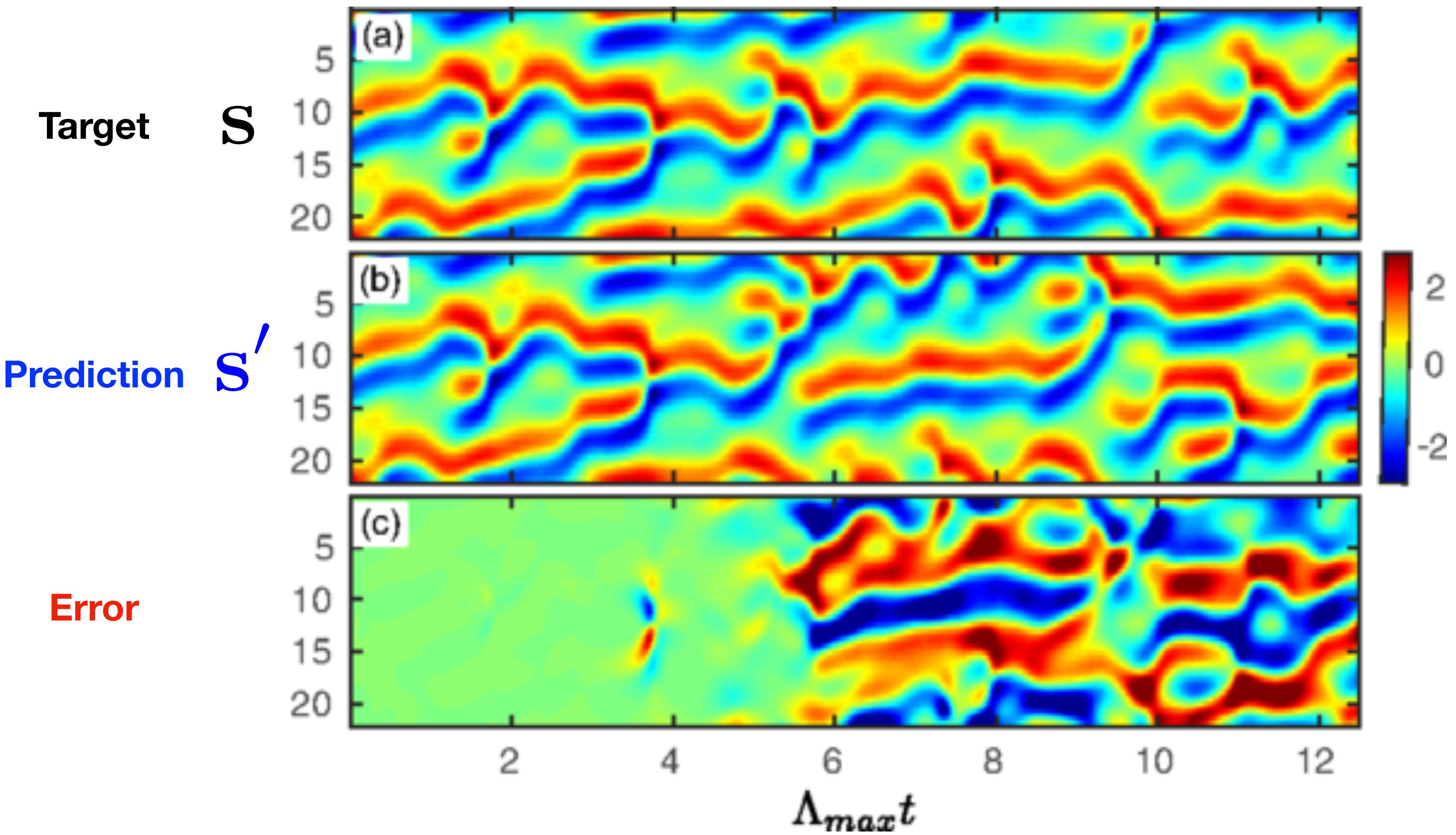
$$\mathbf{s}'_{k+2} = W\mathbf{r}(\mathbf{s}'_{k+1}, \mathbf{x}_k) = W\mathbf{r}(W\mathbf{r}(\mathbf{s}'_k, \mathbf{x}_{k-1}), \mathbf{x}_k)$$

$$\vdots$$

kuramoto-sivashinsky spatiotemporal chaos

reservoir

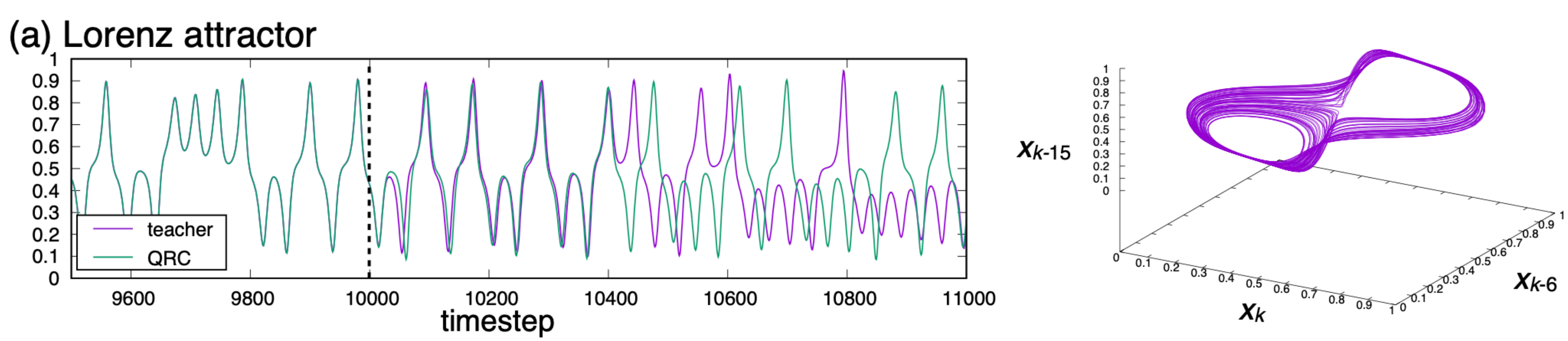
RNN



J. Pathak et. al. Model-Free Prediction of Large Spatiotemporally Chaotic Systems from Data: A Reservoir Computing Approach, *Phys. Rev. Lett.* **120**, 024102, 2018

reservoir

quantum Ising



K. Fujii, K. Navajoma Quantum Reservoir Computing: A Reservoir Approach Toward Quantum Machine Learning Near-Term Devices, *Reservoir Computing* 423-450, 2021

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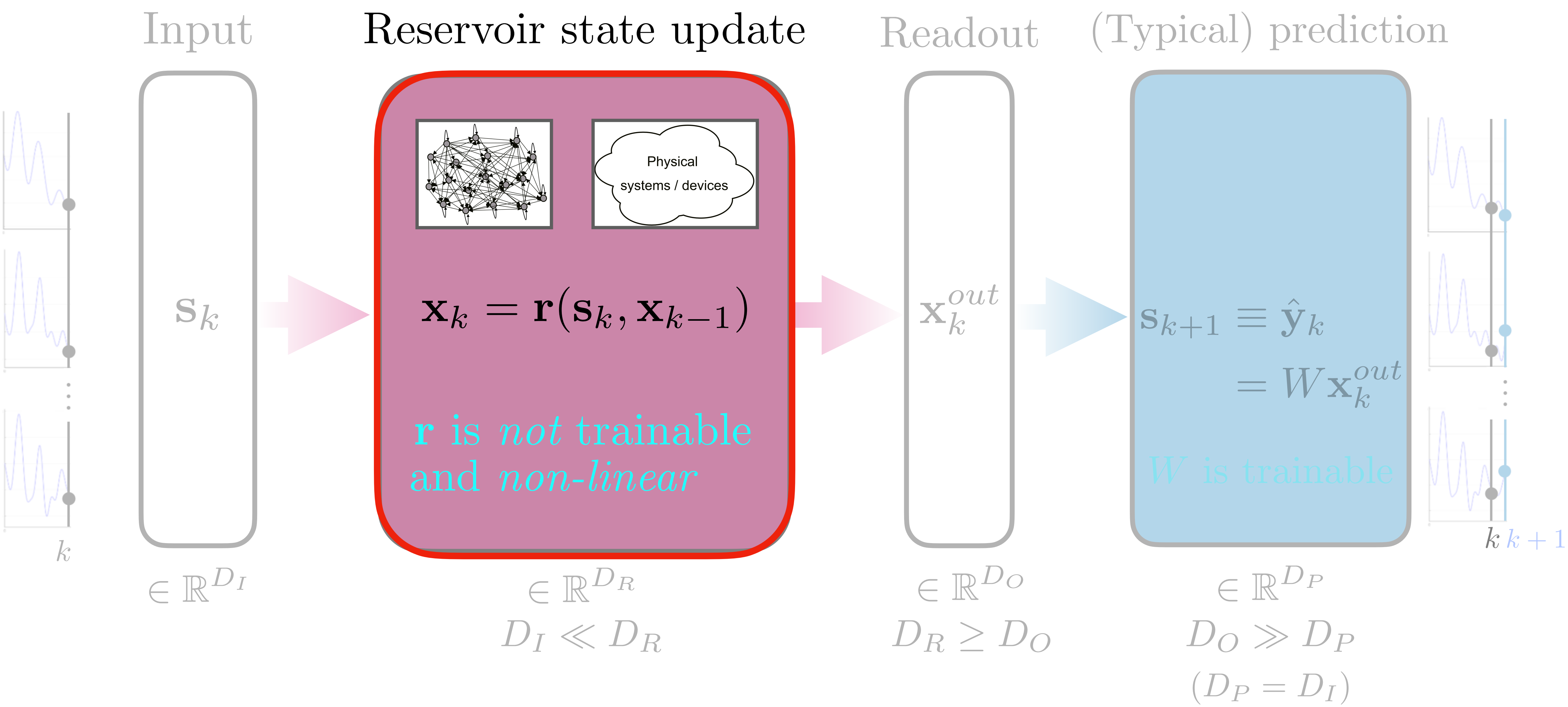
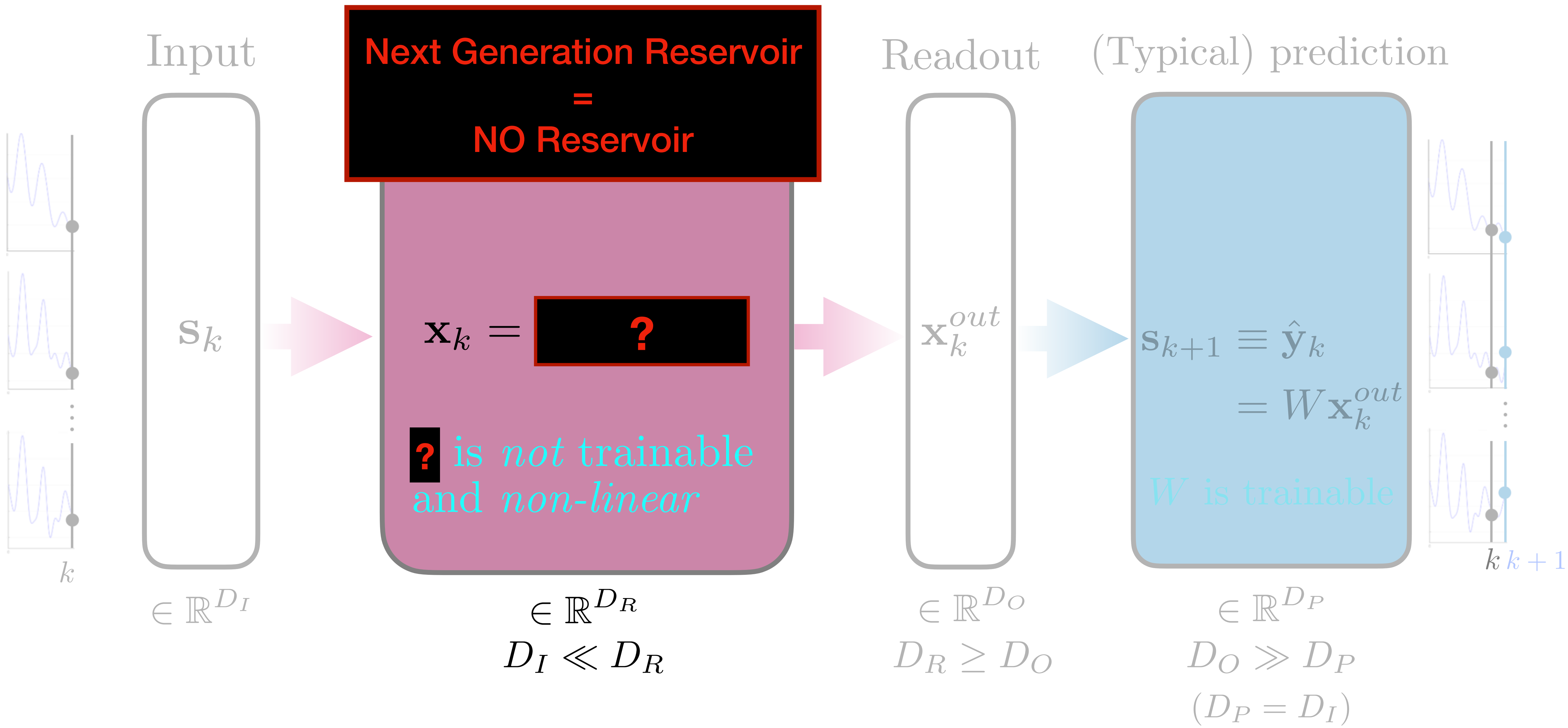
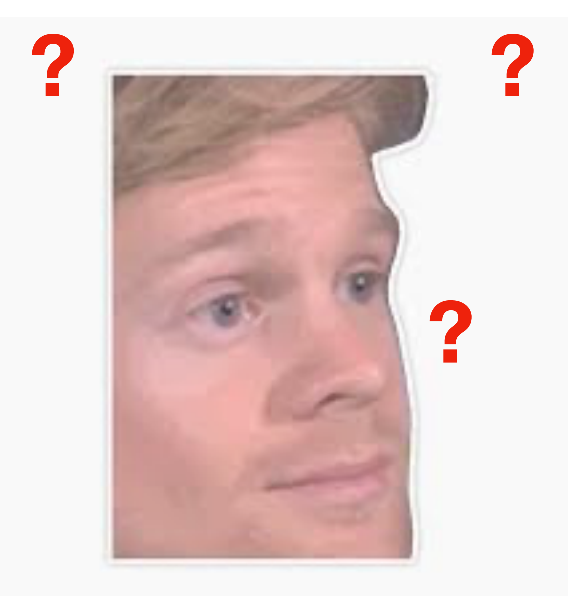


! No clear strategy on how to initialize different types of reservoir !

Next Generation Reservoir Computing (NG-RC) in a nutshell





D. J. Gauthier et. al. Next generation reservoir computing *Nature Communications* 12:5564 (2021)

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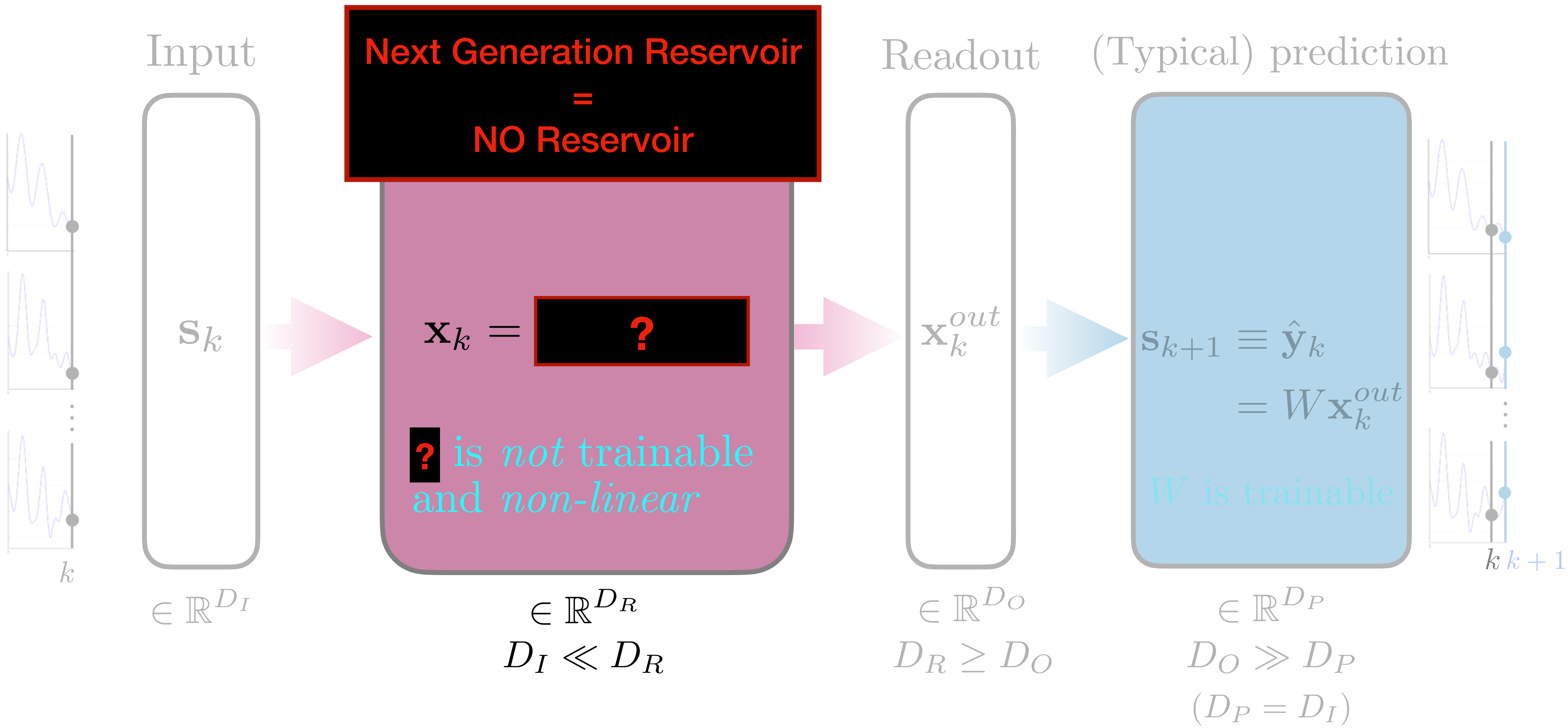

Non-linear feature map with "memory" of the past data

$$\boldsymbol{o}_k = \mathbf{s}_k \oplus \mathbf{s}_{k-\Delta} \oplus \mathbf{s}_{k-2\Delta} \oplus \ldots \oplus \mathbf{s}_{k-(m-1)\Delta}$$

$$\mathbf{x}_k = \boldsymbol{o}_k \oplus (\boldsymbol{o}_k)^{\otimes p}$$ (non-linear for $p > 1$)

In some limit, equivalent to nonlinear vector autoregression (NVAR) with universal approximation property for dynamical systems

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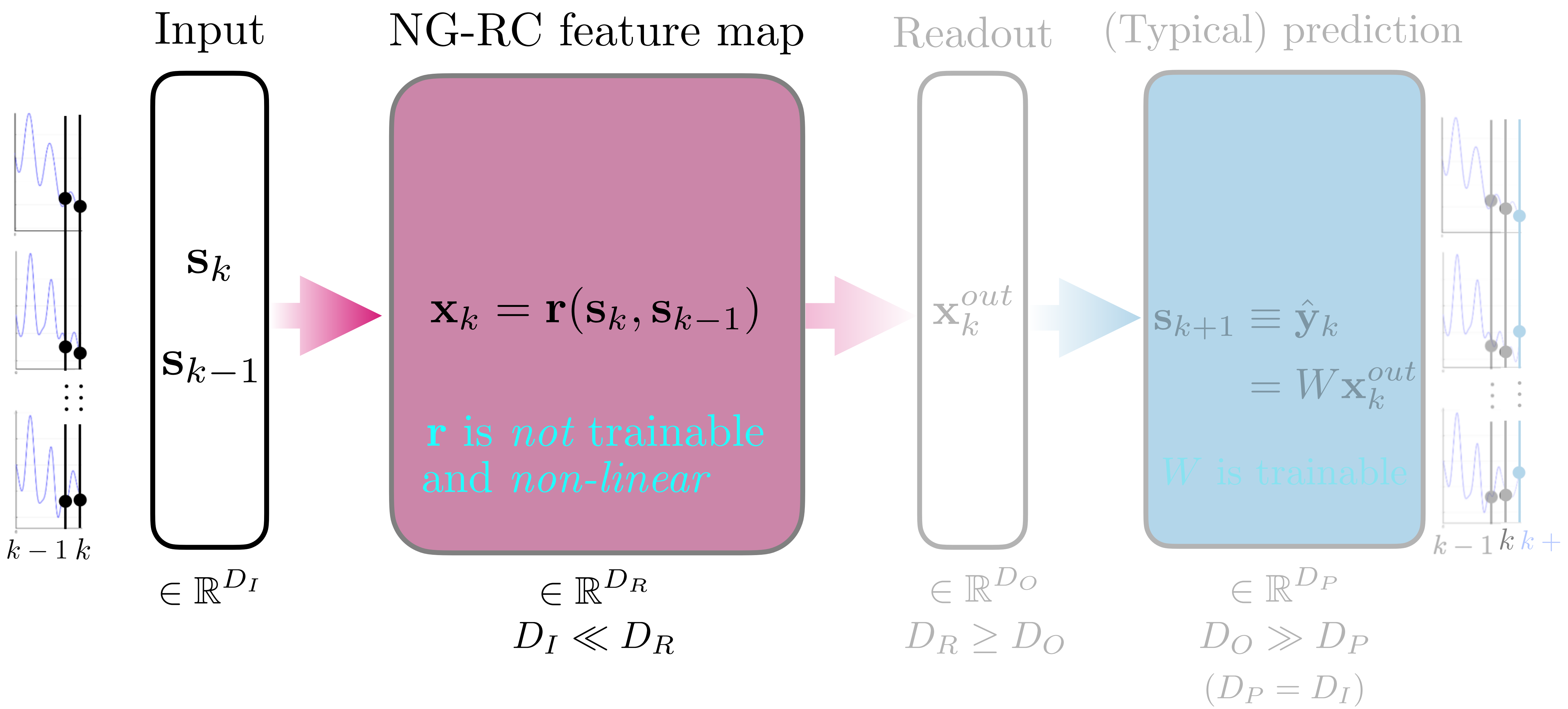

For example $\Delta = 1, m = 2, p = 2$

$$\mathbf{x}_k = \mathbf{s}_k \oplus \mathbf{s}_{k-1} \oplus \left[\left(\mathbf{s}_k \oplus \mathbf{s}_{k-1} \right) \otimes \left(\mathbf{s}_k \oplus \mathbf{s}_{k-1} \right) \right]$$
$$\equiv \mathbf{r}\left(\mathbf{s}_k, \mathbf{s}_{k-1} \right)$$

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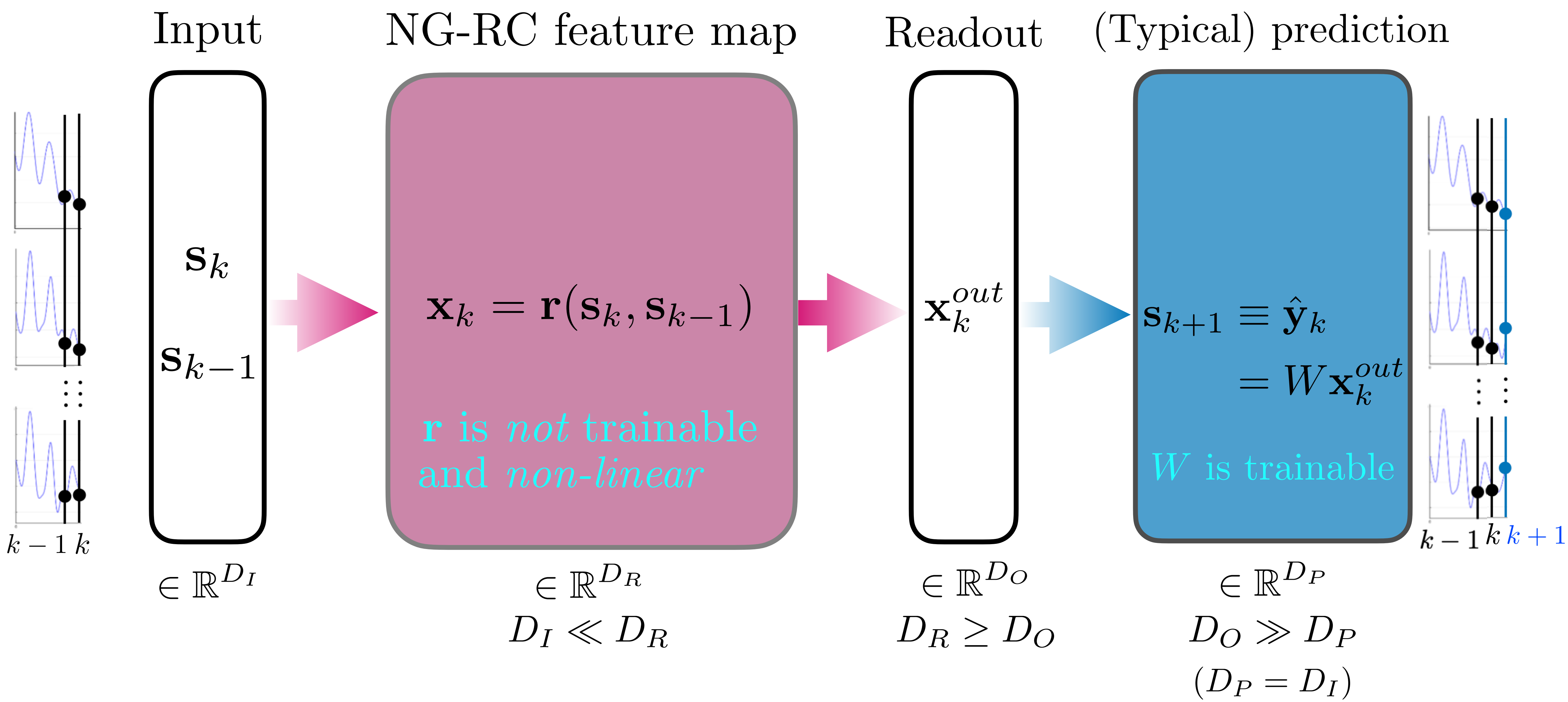
Next Generation Reservoir Computing (NG-RC) in a nutshell



Training $$W = YX^{\dagger}(XX^{\dagger} + \lambda I)^{-1}$$

Typical prediction $$\mathbf{s}'_{k+1} = W\mathbf{x}_k = W\mathbf{r}(\mathbf{s}'_k, \mathbf{s}'_{k-1}) \qquad (\mathbf{x}_k^{out} = \mathbf{x}_k)$$

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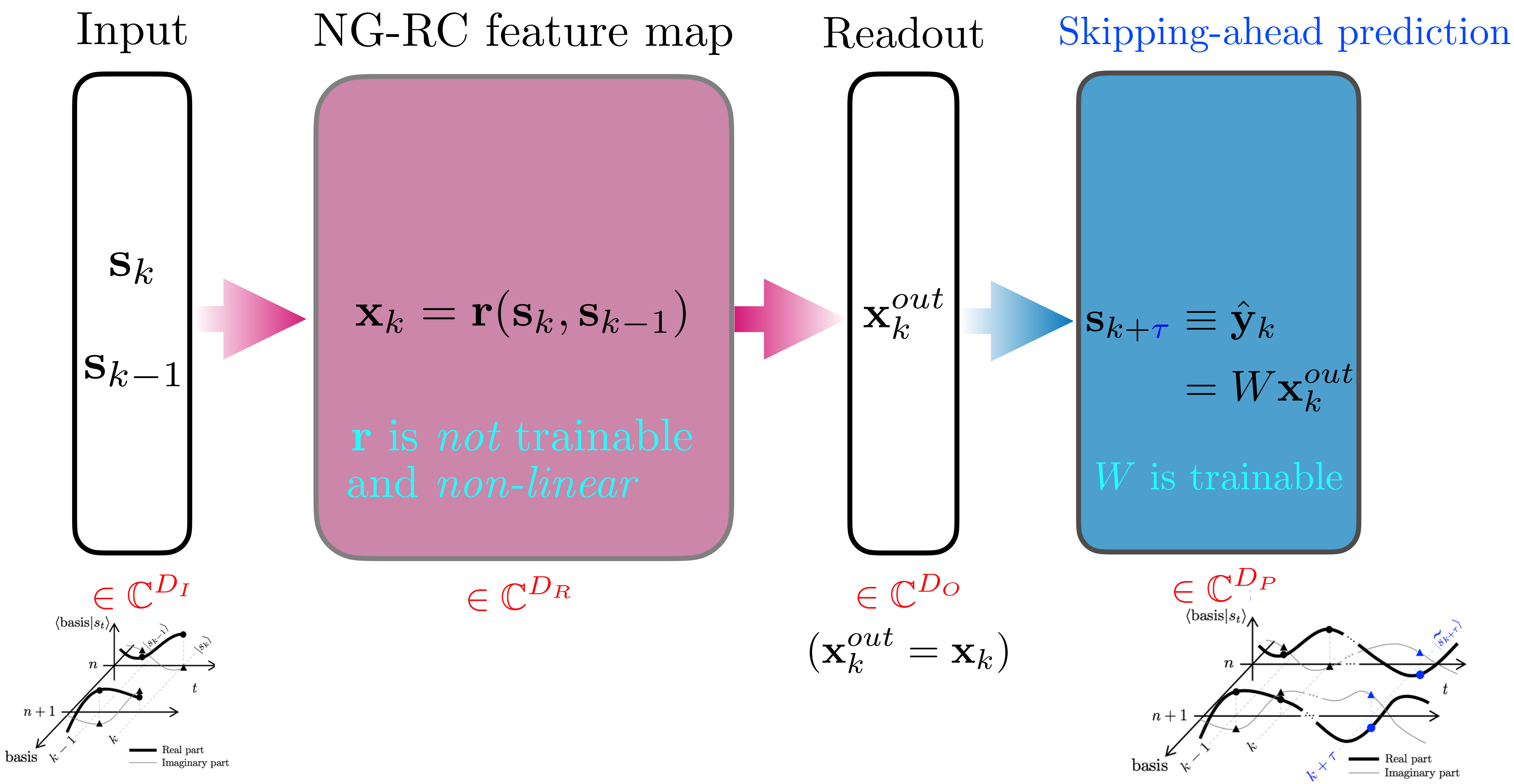
NG-RC for forecasting quantum dynamics

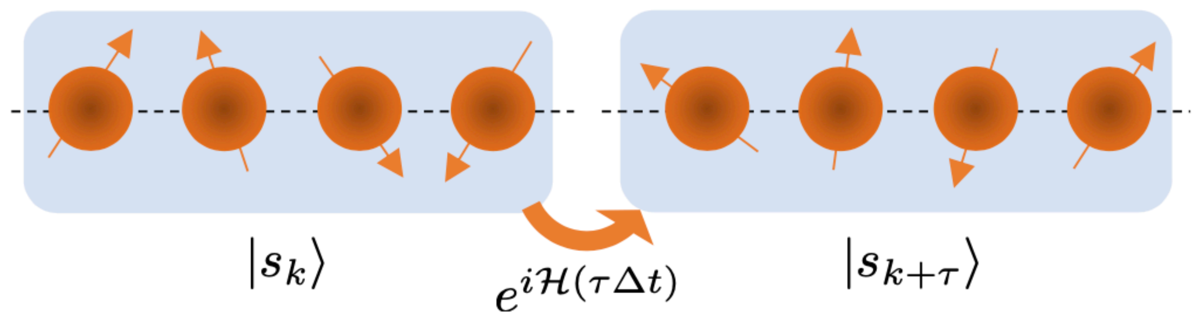


Training $$W = YX^\dagger(XX^\dagger + \lambda I)^{-1}$$

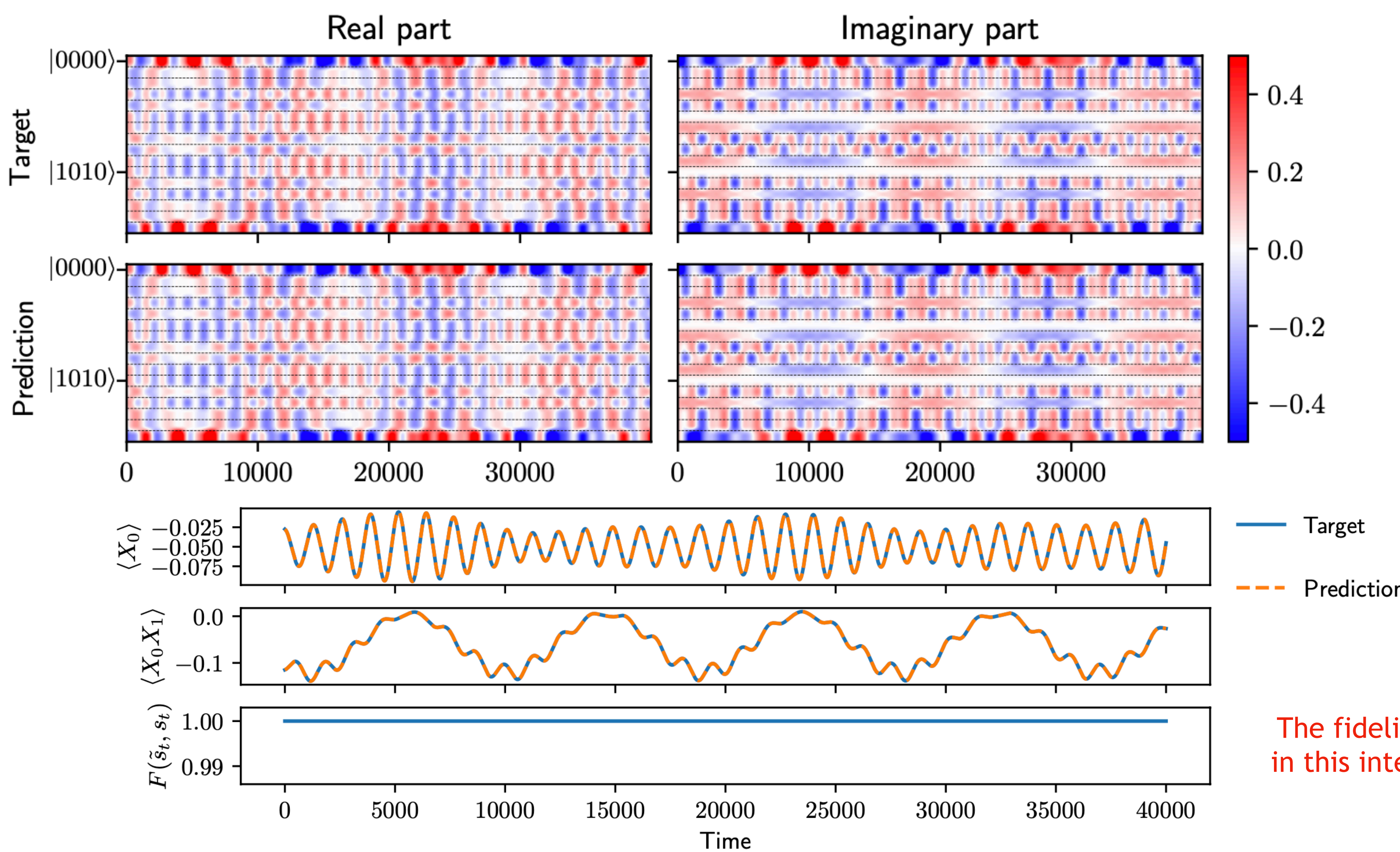
Skipping-ahead prediction $$\mathbf{s}'_{k+\tau} = W\mathbf{x}_k = W\mathbf{r}(\mathbf{s}'_k, \mathbf{s}'_{k-1})$$

NG-RC for forecasting integrable quantum dynamics

$$\mathcal{H} = -J \sum_{i=1}^{4} Z_i Z_{i+1} + h \sum_{i=1}^{4} X_i$$



skipping-ahead with $\tau = 10^6$



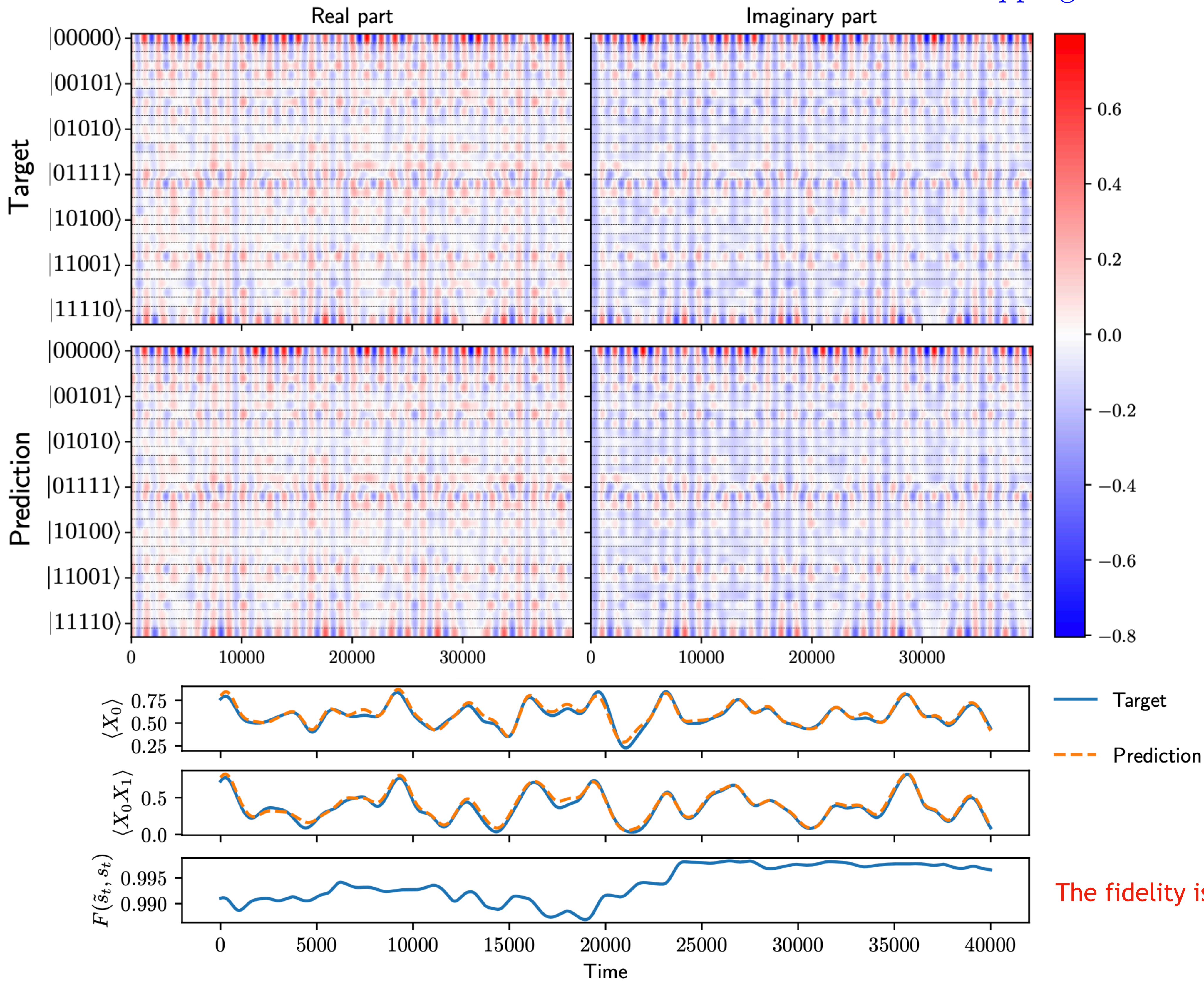
The fidelity is almost 1
in this integrable model

NG-RC for forecasting *chaotic* quantum dynamics

$$\mathcal{H}_{\text{tilted}} = J \sum_{i=1}^{d-1} Z_i Z_{i+1} + h \sum_{i=1}^{d} (X_i \sin\theta + Z_i \cos\theta)$$

$d = 5, \theta = 15\pi/32$

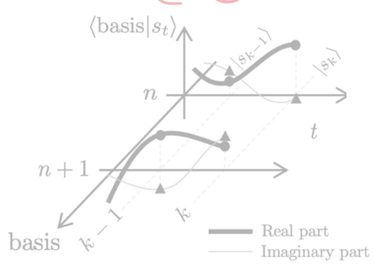
skipping-ahead with $\tau = 10^6$

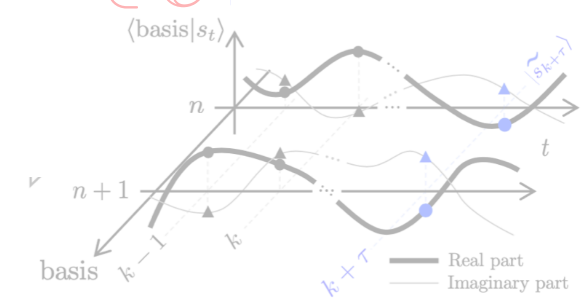


The fidelity is above 0.99

Scalability issue of classical NG-RC for many-body systems

Input	NG-RC feature map	Readout	Skipping-ahead prediction
$\mathbf{s}_k$ $\mathbf{s}_{k-1}$	$\mathbf{x}_k = \mathbf{r}(\mathbf{s}_k, \mathbf{s}_{k-1})$ $\mathbf{r}$ is *not* trainable and *non-linear*	$\mathbf{x}_k^{out}$	$\mathbf{s}_{k+\tau} \equiv \hat{\mathbf{y}}_k$ $= W\mathbf{x}_k^{out}$ W is trainable
$\in \mathbb{C}^{D_I}$	$\in \mathbb{C}^{D_R}$	$\in \mathbb{C}^{D_O}$ $(\mathbf{x}_k^{out} = \mathbf{x}_k)$	$\in \mathbb{C}^{D_P}$





Training

$$W = YX^{\dagger}(XX^{\dagger} + \lambda I)^{-1}$$

$O(2^{2d}T)$

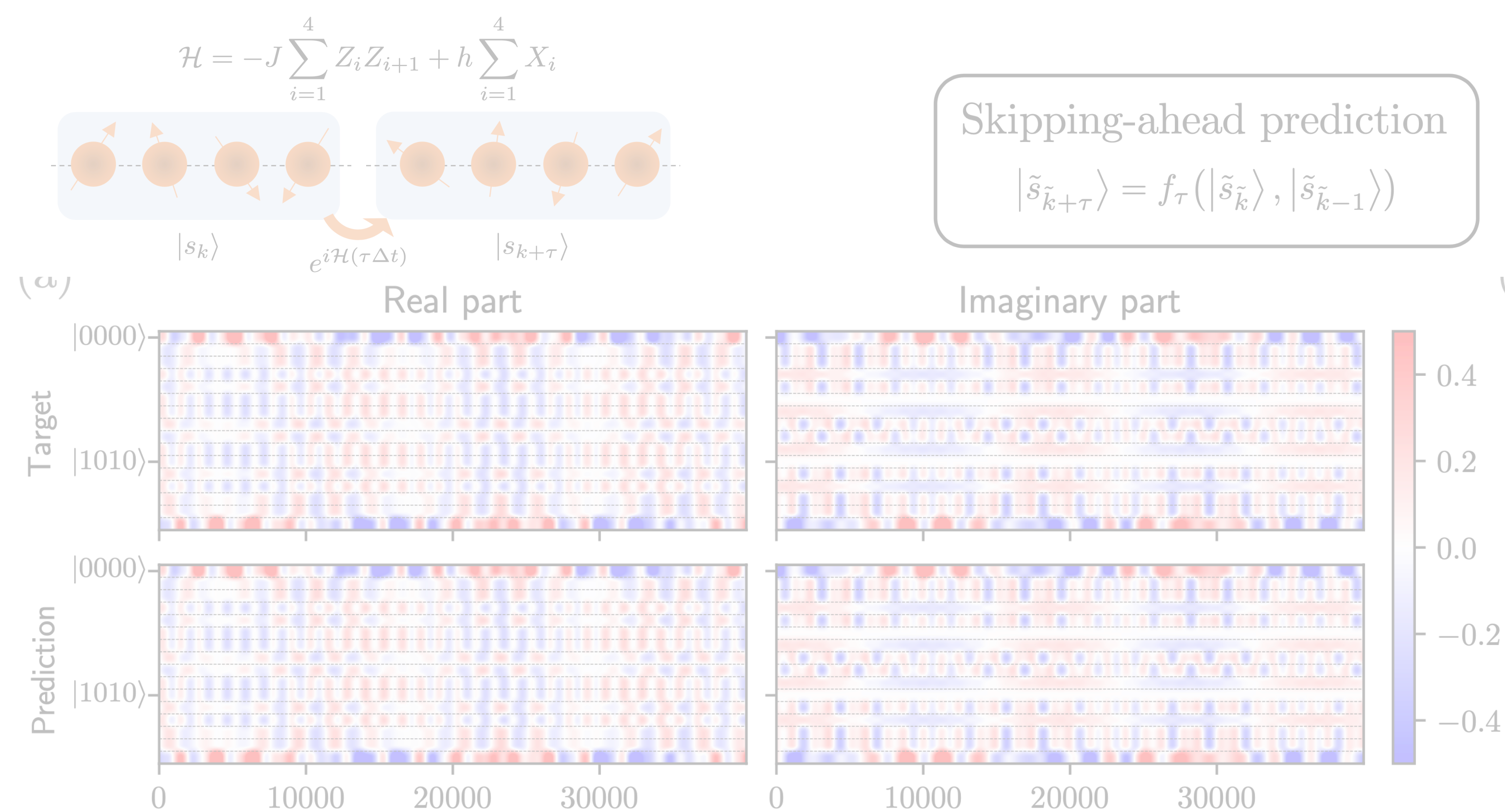
Pseudoinverse Computation
d = # of qubits

Skipping-ahead prediction

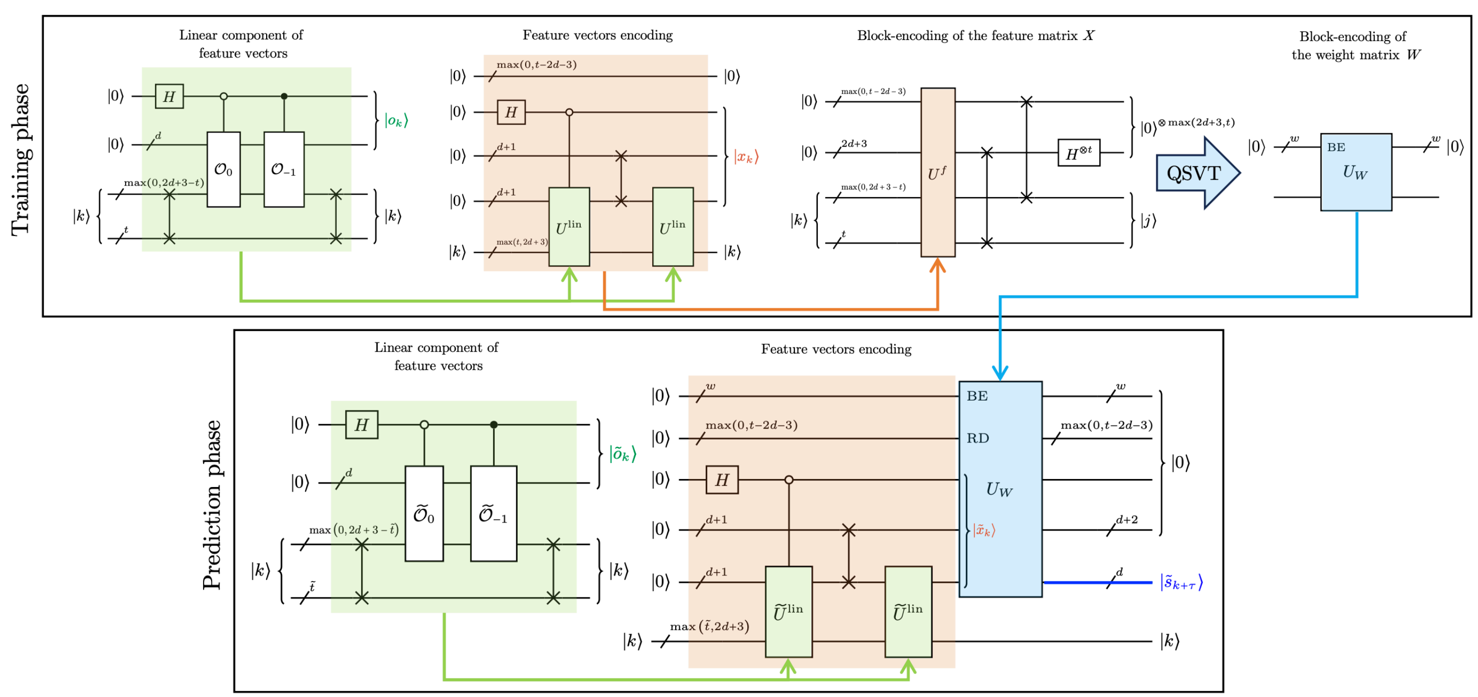
$$\mathbf{s}'_{k+\tau} = W\mathbf{x}_k = W\mathbf{r}(\mathbf{s}'_k, \mathbf{s}'_{k-1})$$

Outline

Part 1: NG-RC for Many-body Quantum Dynamics Prediction



Part 2: Quantum Algorithm for NG-RC (QNG-RC)



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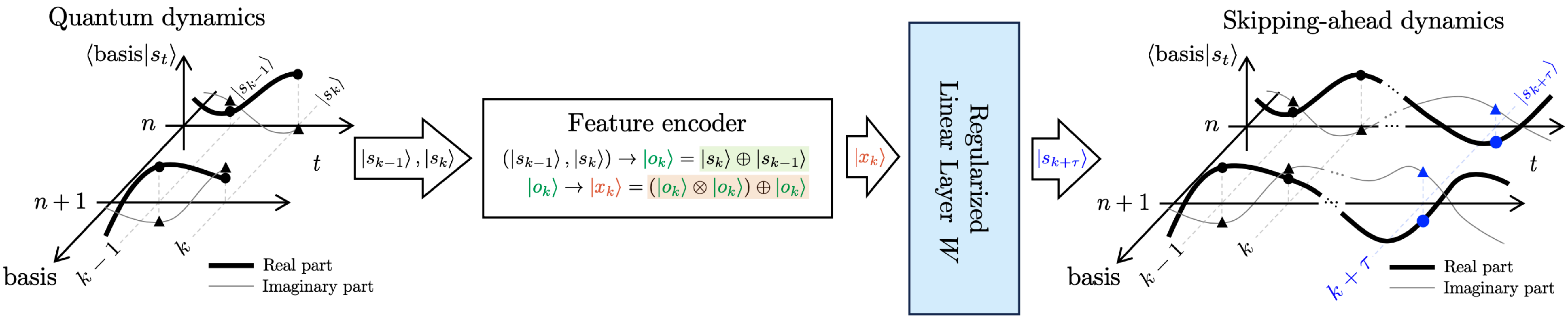
Quantum Algorithm for NG-RC (QNG-RC)



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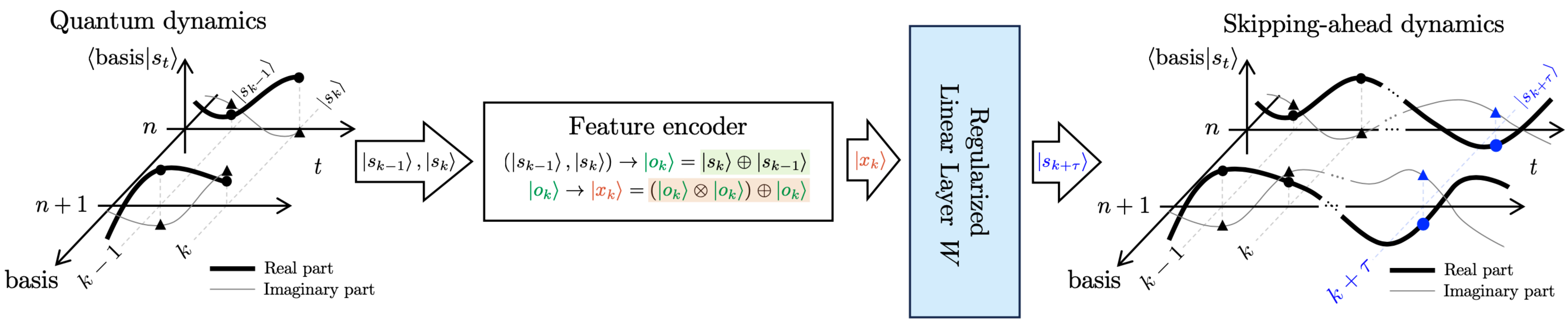
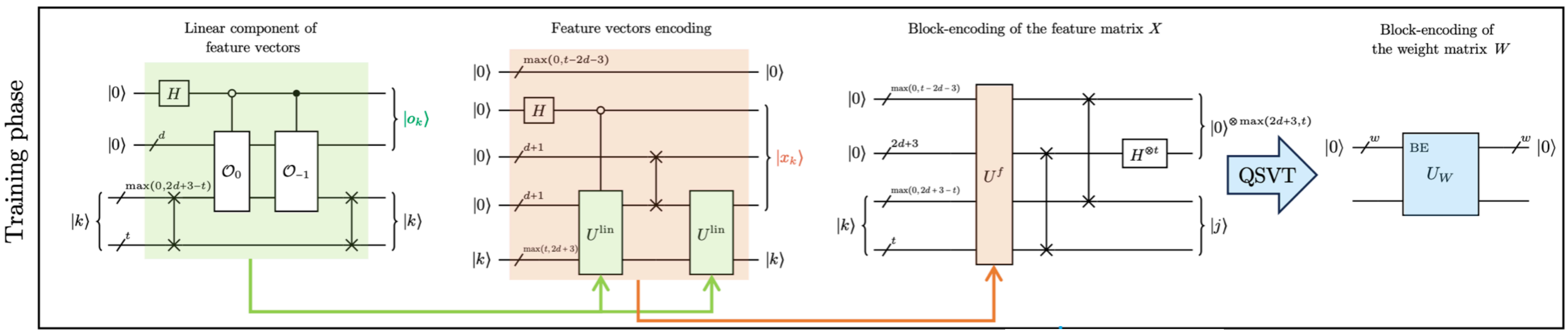


Training

$$W = Y X^{\dagger} \left(X X^{\dagger} + \lambda I \right)^{-1}$$



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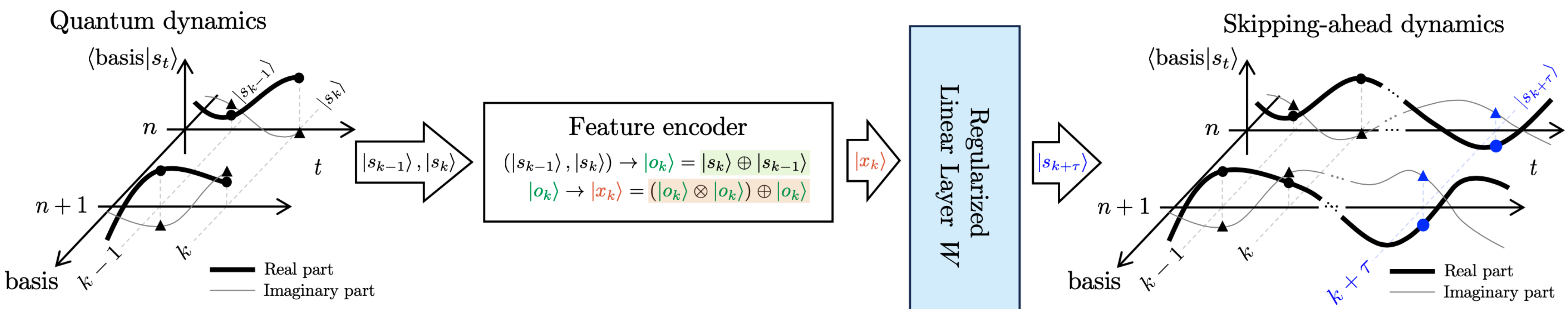
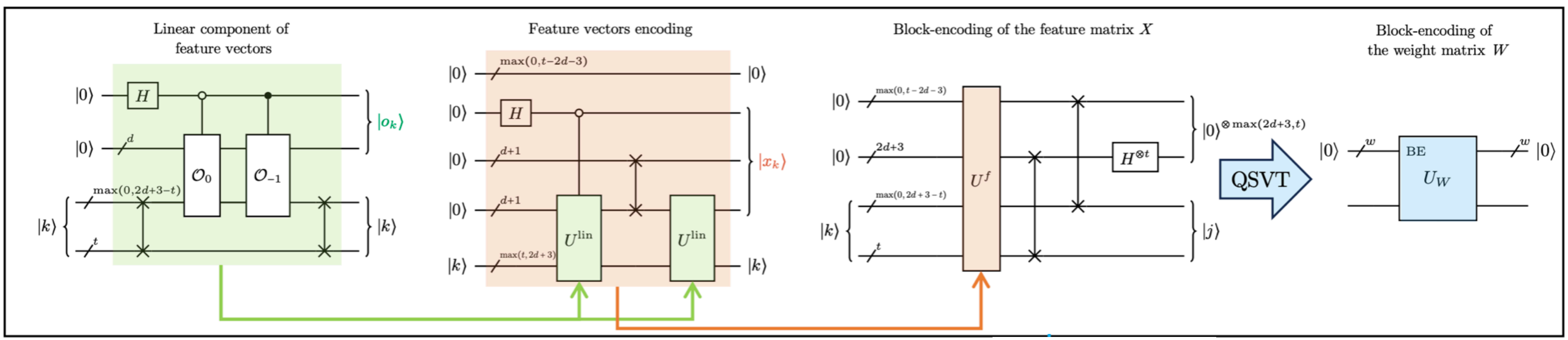


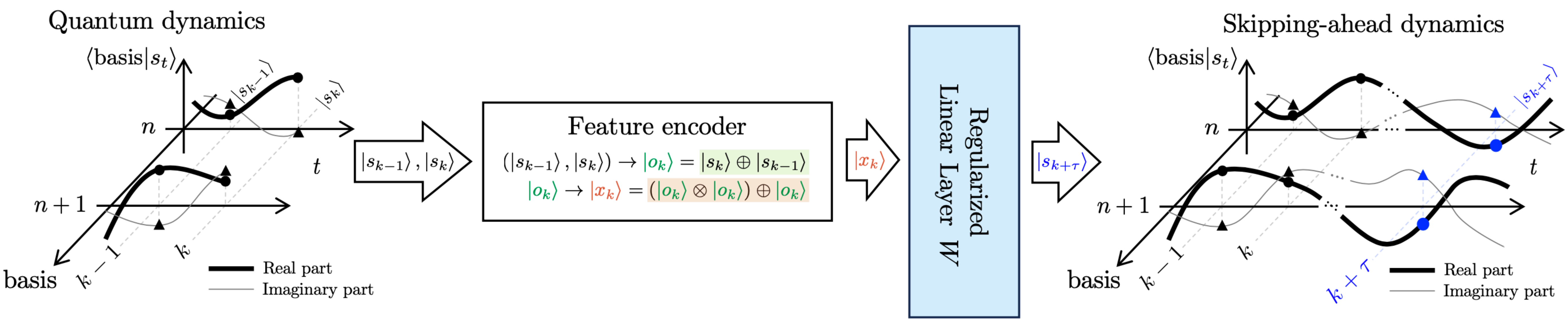
Training

$$W = Y X^{\dagger}\left(X X^{\dagger} + \lambda I\right)^{-1}$$



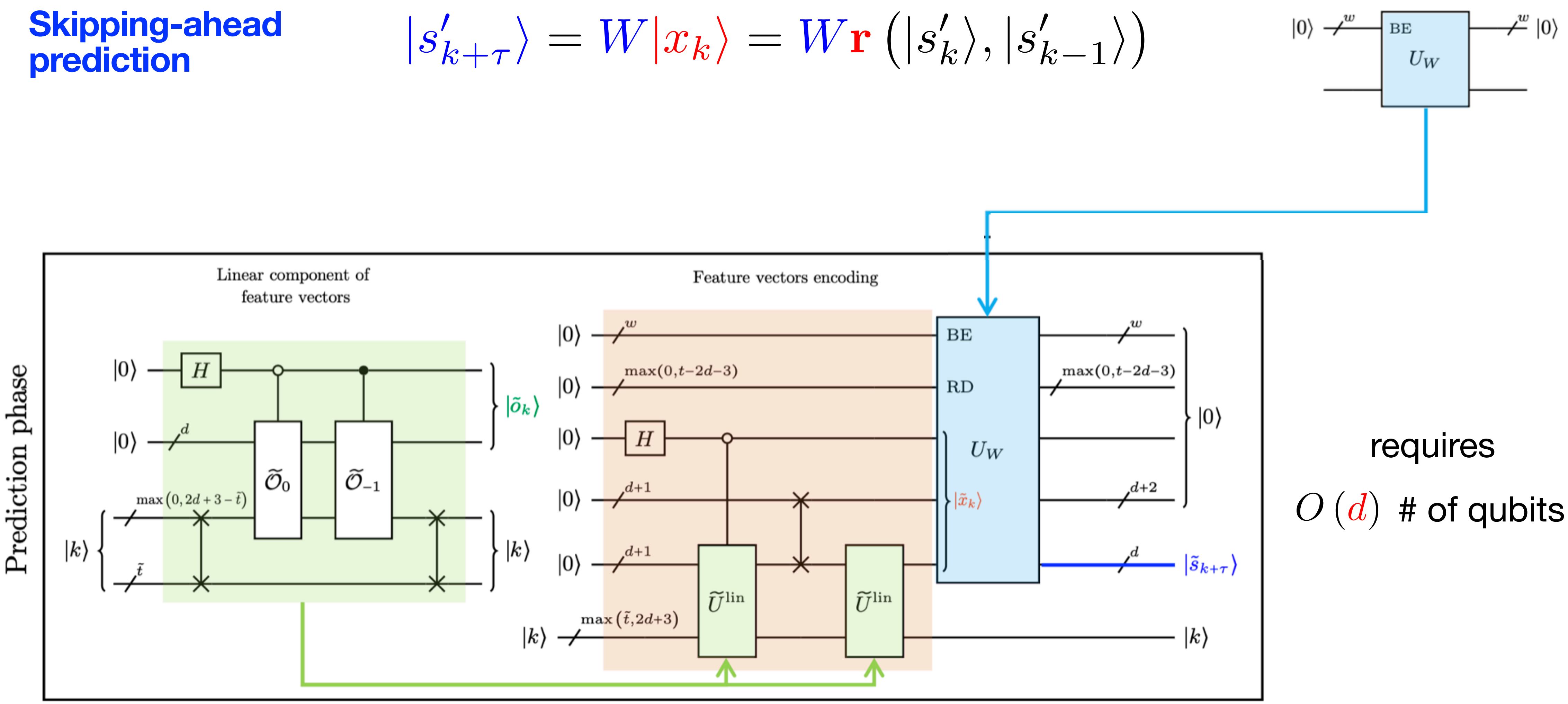
Theorem Given the block-encoded feature matrix X and target matrix Y, constructed in time T_O , and κ being a condition number of the Tikhonov-regularized feature matrix $\begin{pmatrix} X & \sqrt{\lambda} I \\ 0 & 0 \end{pmatrix}$, then the block-encoding of W, with error $\delta_W \in (0,1)$, can be constructed in time $T_W = O\left(d\kappa T \log\left(\frac{\kappa T}{\delta_W}\right) T_O\right)$ with $O(d)$ number of qubits.

Quantum Algorithm for NG-RC (QNG-RC)



Skipping-ahead prediction

$$|s'_{k+\tau}\rangle = W|x_k\rangle = W\mathbf{r}\left(|s'_k\rangle, |s'_{k-1}\rangle\right)$$

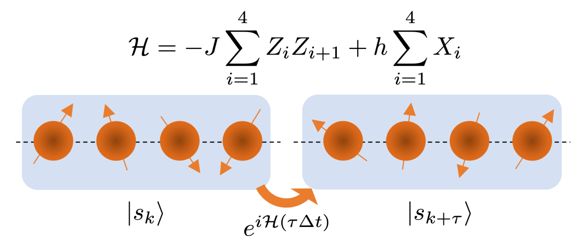


requires

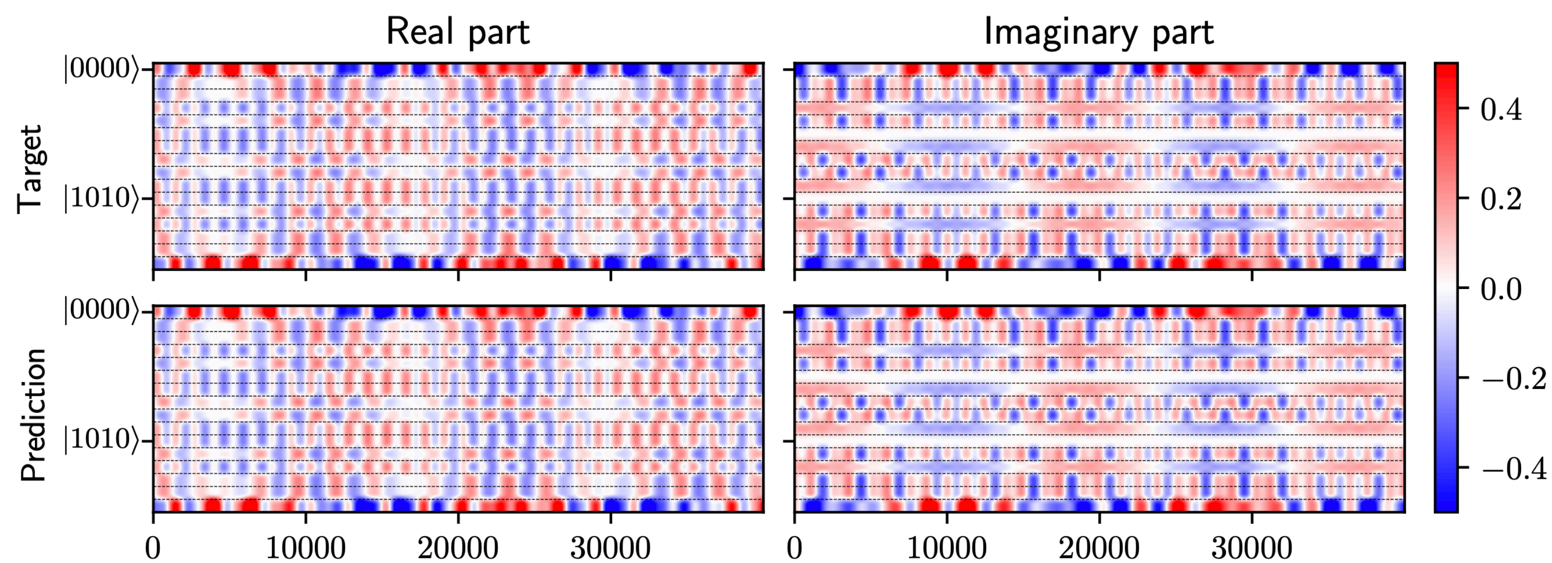
$O(d)$ # of qubits

Summary

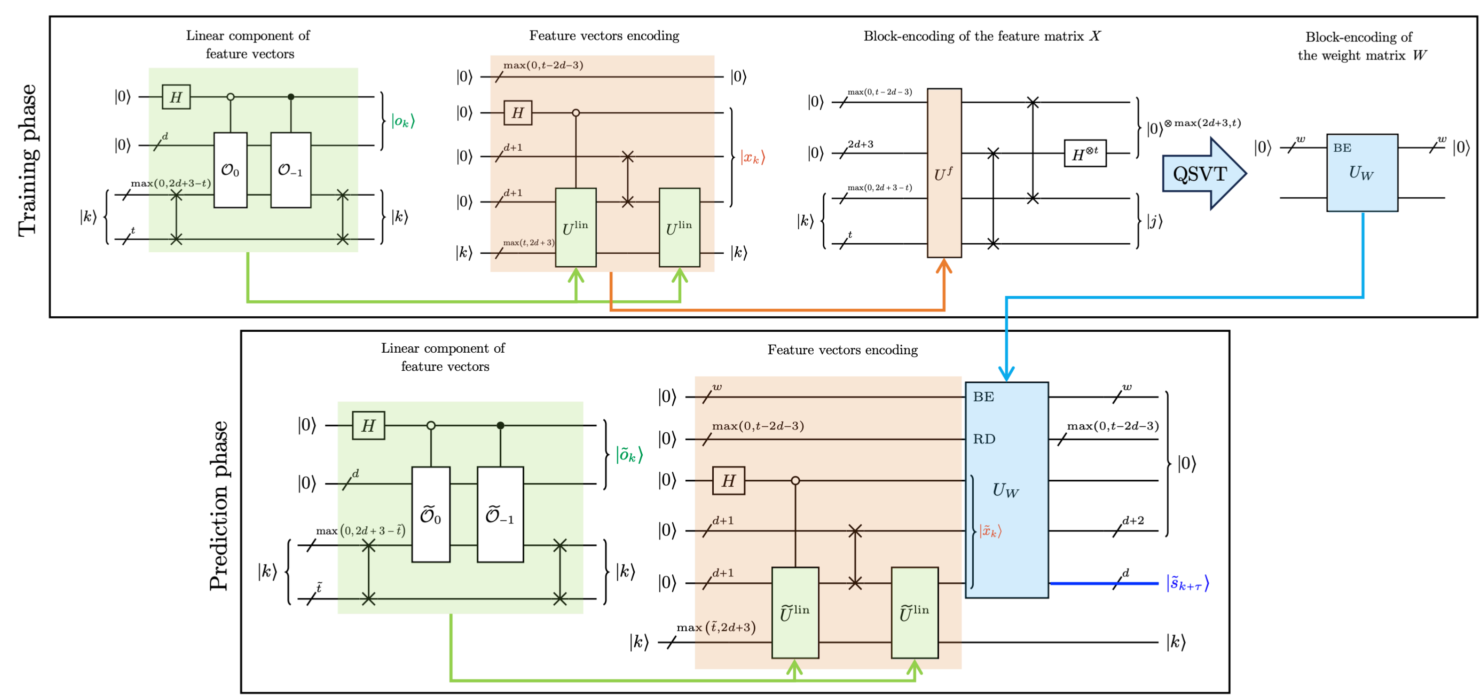
1. NG-RC can be applied to forecast *full* many-body dynamics far into the future, but with the time cost that scales as $O\left(2^{2d}\right)$



Skipping-ahead prediction
$|\tilde{s}_{\tilde{k}+\tau}\rangle = f_\tau\left(|\tilde{s}_{\tilde{k}}\rangle, |\tilde{s}_{\tilde{k}-1}\rangle\right)$



2. There is a quantum algorithm that performs skipping-ahead prediction coherently with the time cost and resource that scales as $O\left(d\right)$



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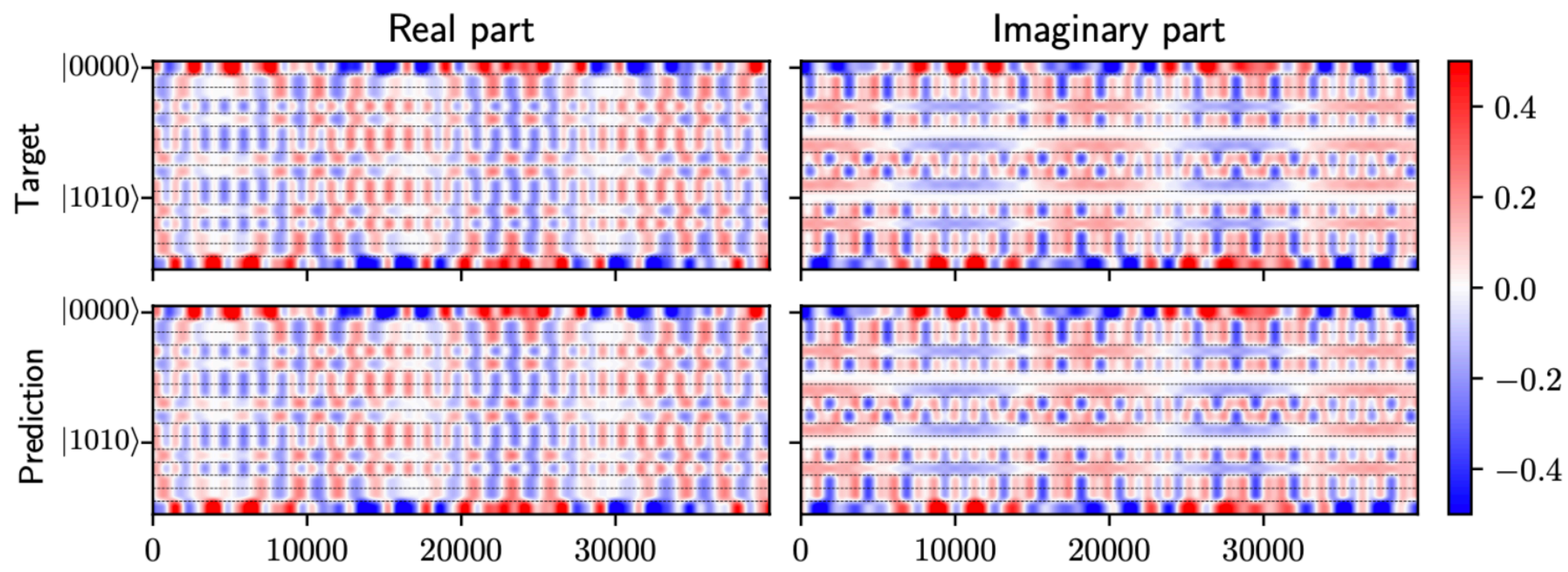
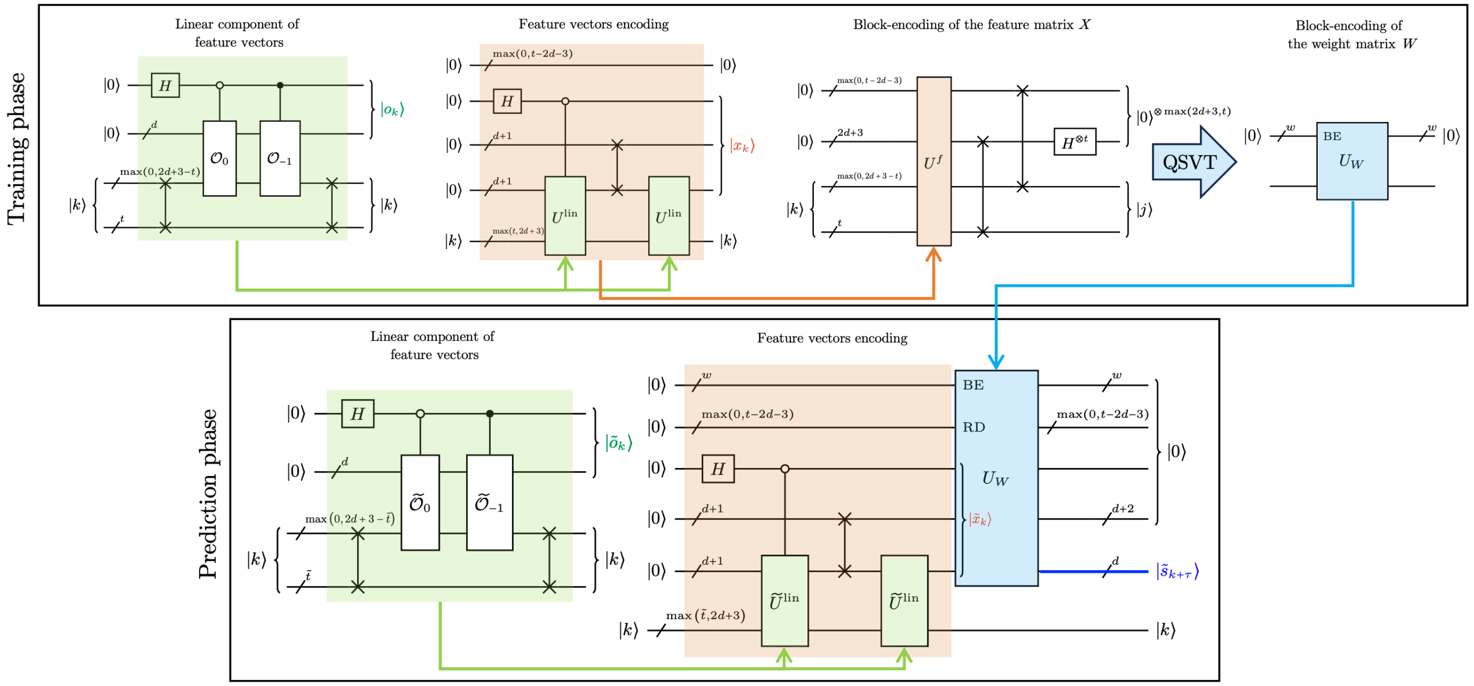
Outlook

- Theoretical understanding of classical NG-RC expressivity



- Quantum circuit implementation of block-encoding formalism



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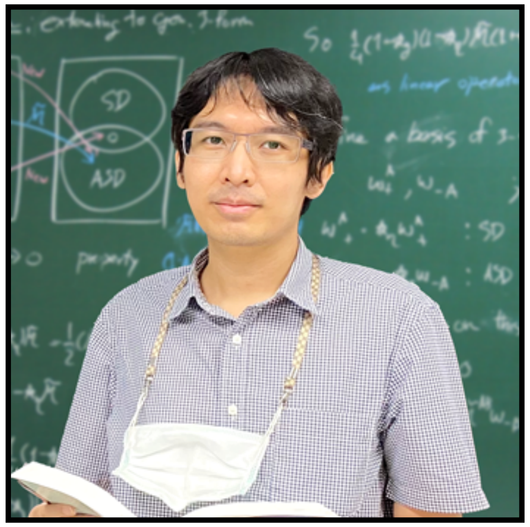

Institute for Fundamental Study
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