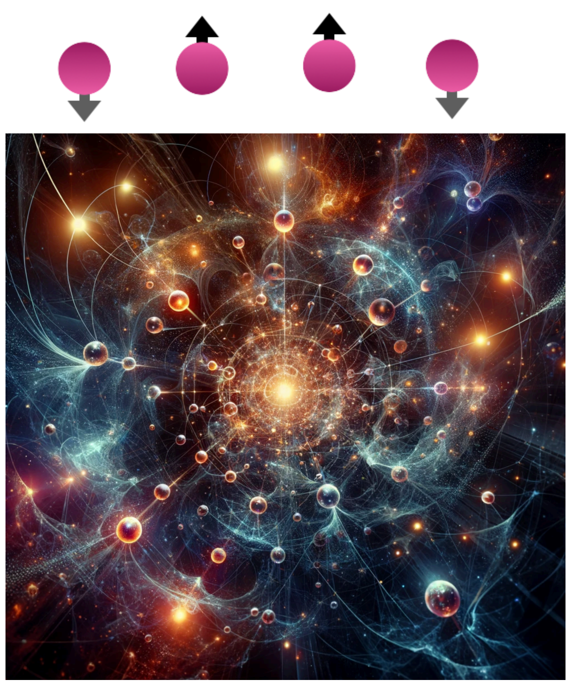
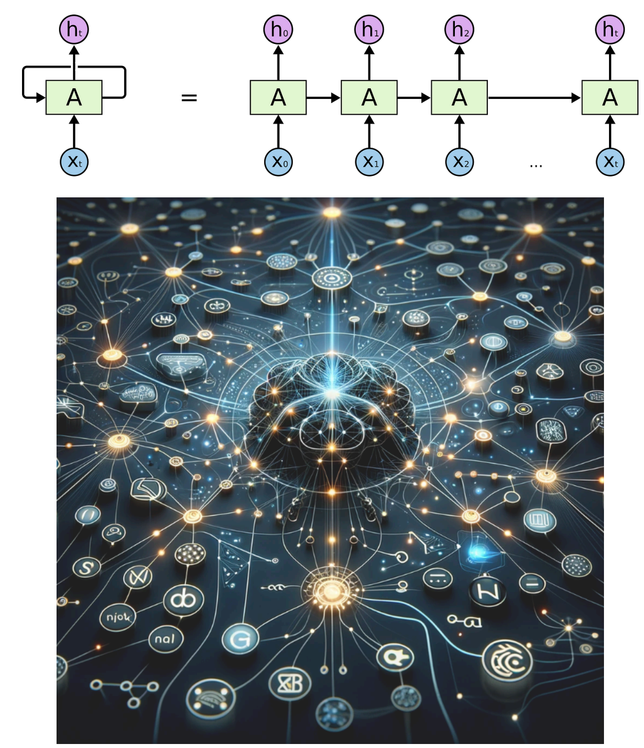
From explainable NLP to quantum dynamics prediction:

A two-way synergy between many-body quantum physics and temporal machine learning models

Thiparat Chotibut (Thip)
Chula Intelligent and Complex Systems Research Unit,
Chulalongkorn University, Bangkok, Thailand

April 18, 2024
CS Katha Barta





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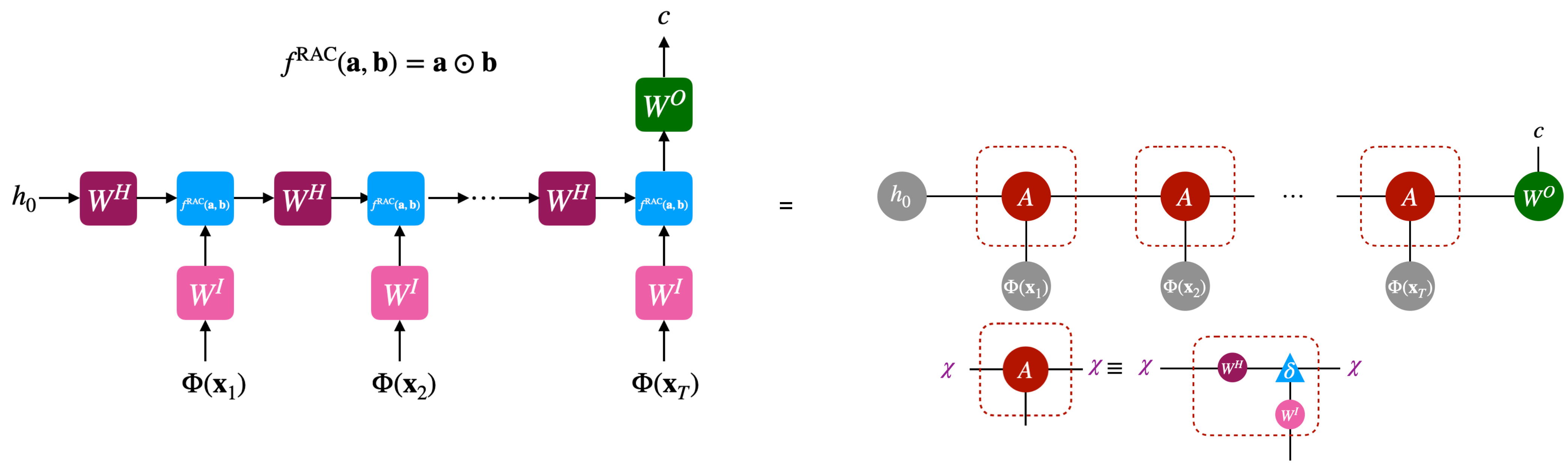
Outline

Part 1: Quantum Meets Language



J. Tangpanitanon, ...,**T. Chotibut**

NJP 2022

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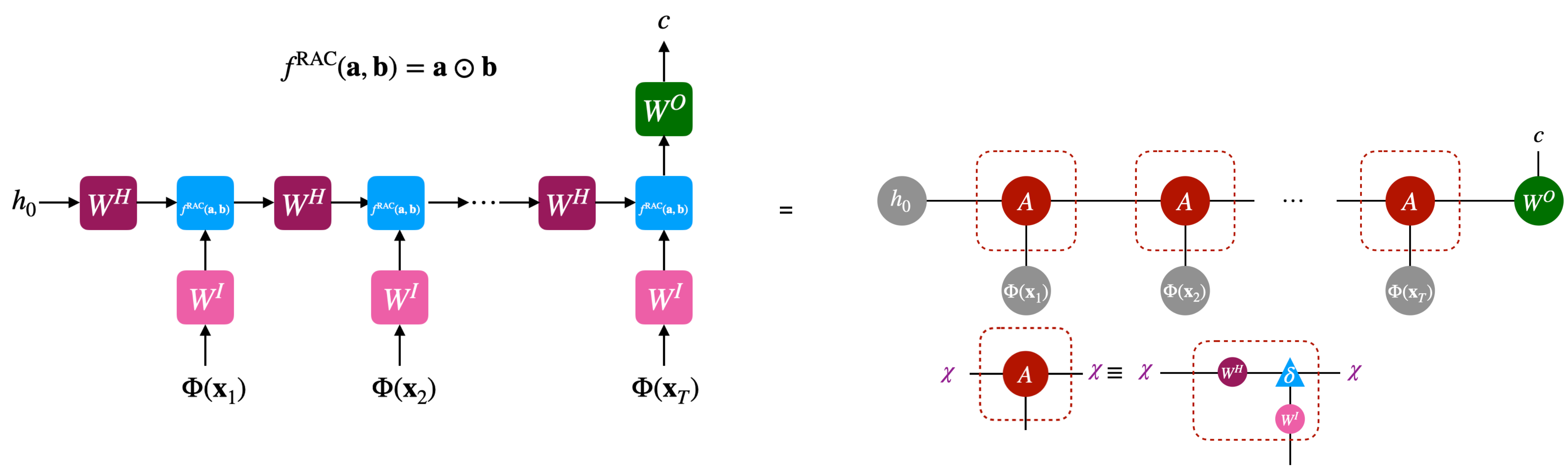

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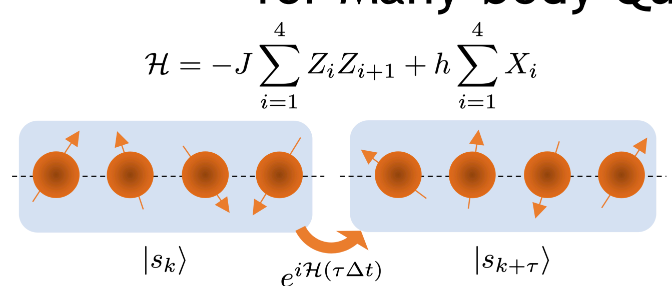
Part 2: Next Generation Reservoir Computing (NG-RC) for Many-body Quantum Dynamics Prediction



Skipping-ahead prediction

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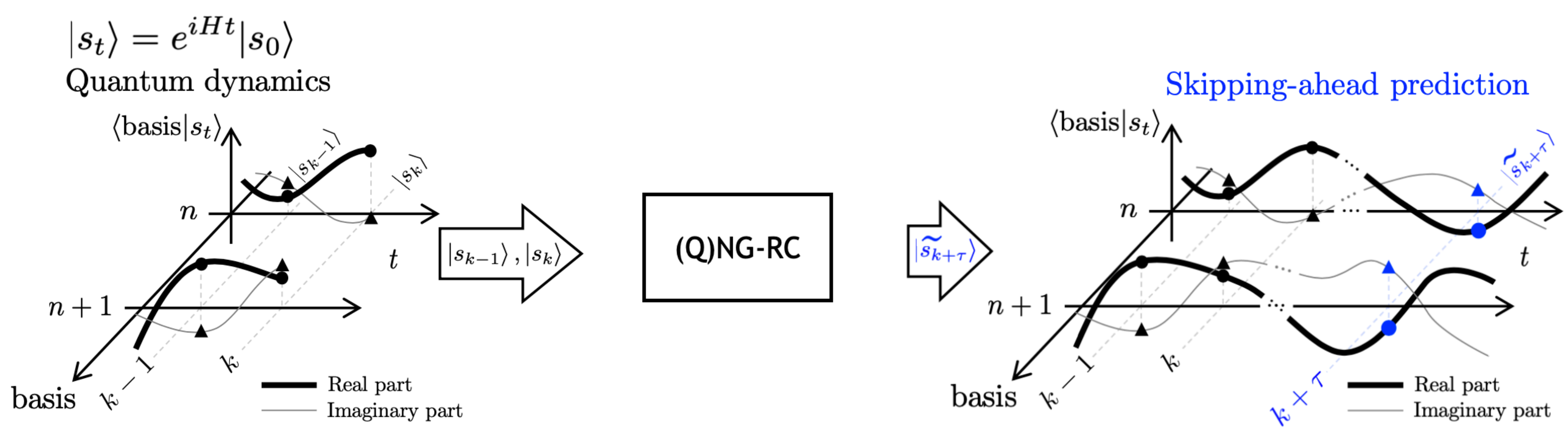

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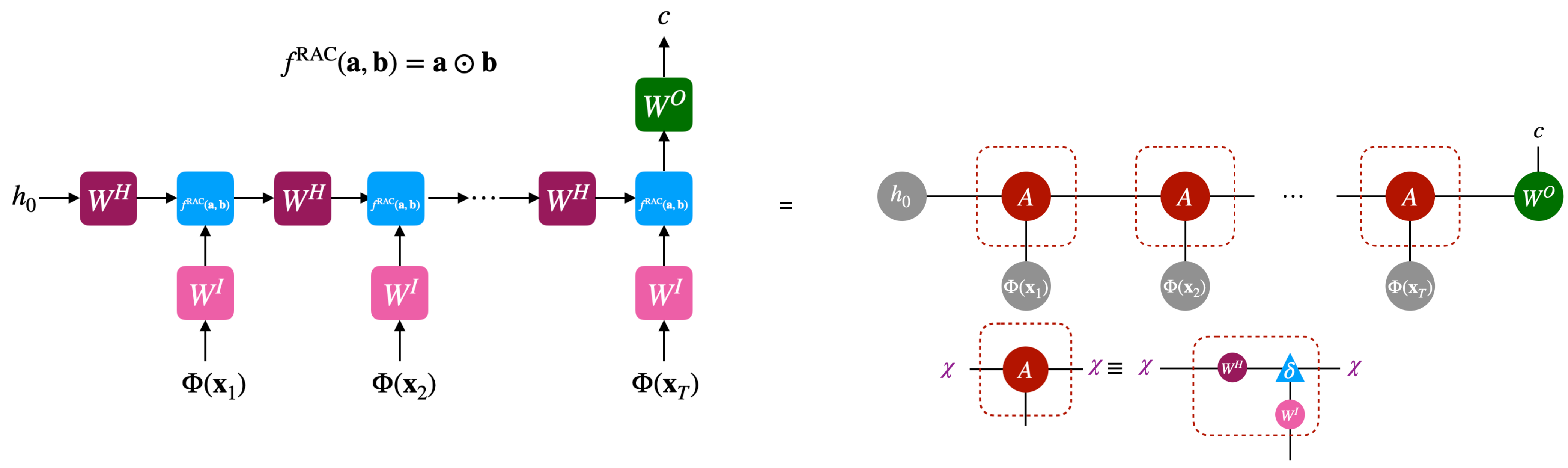

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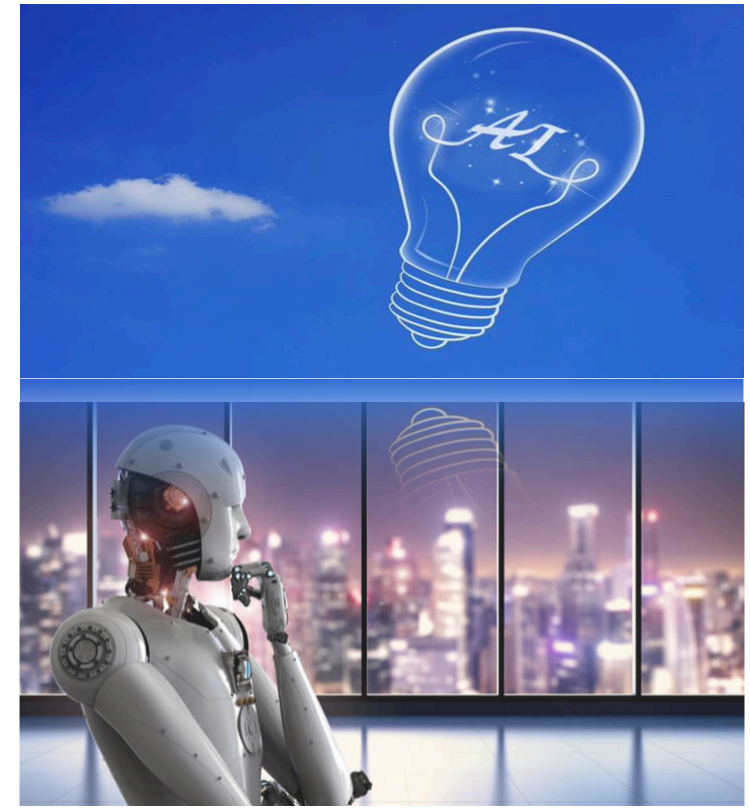

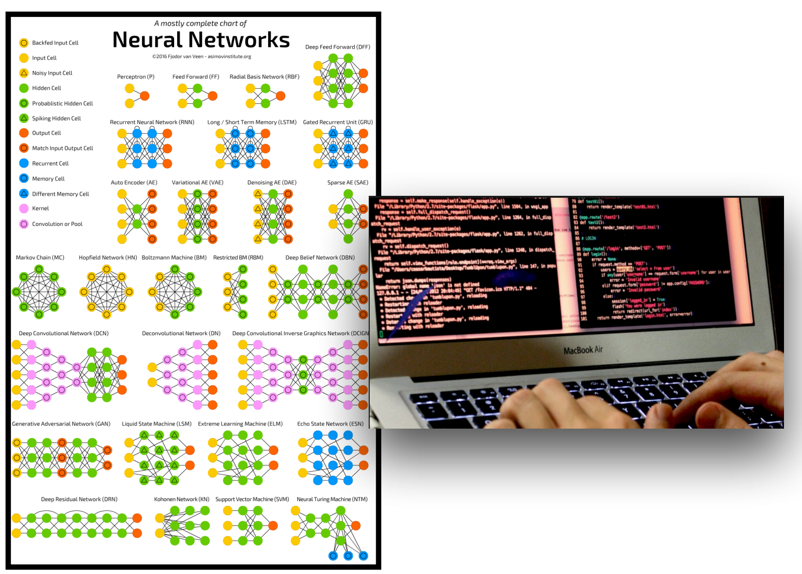

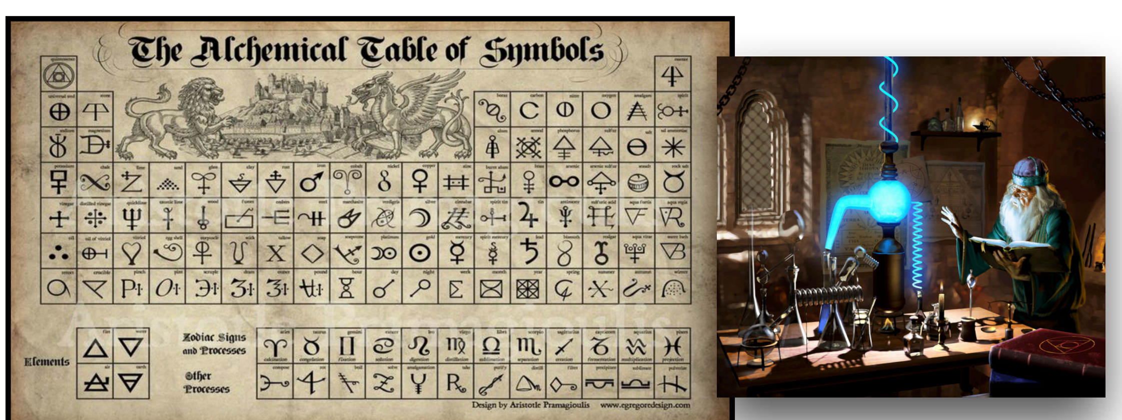

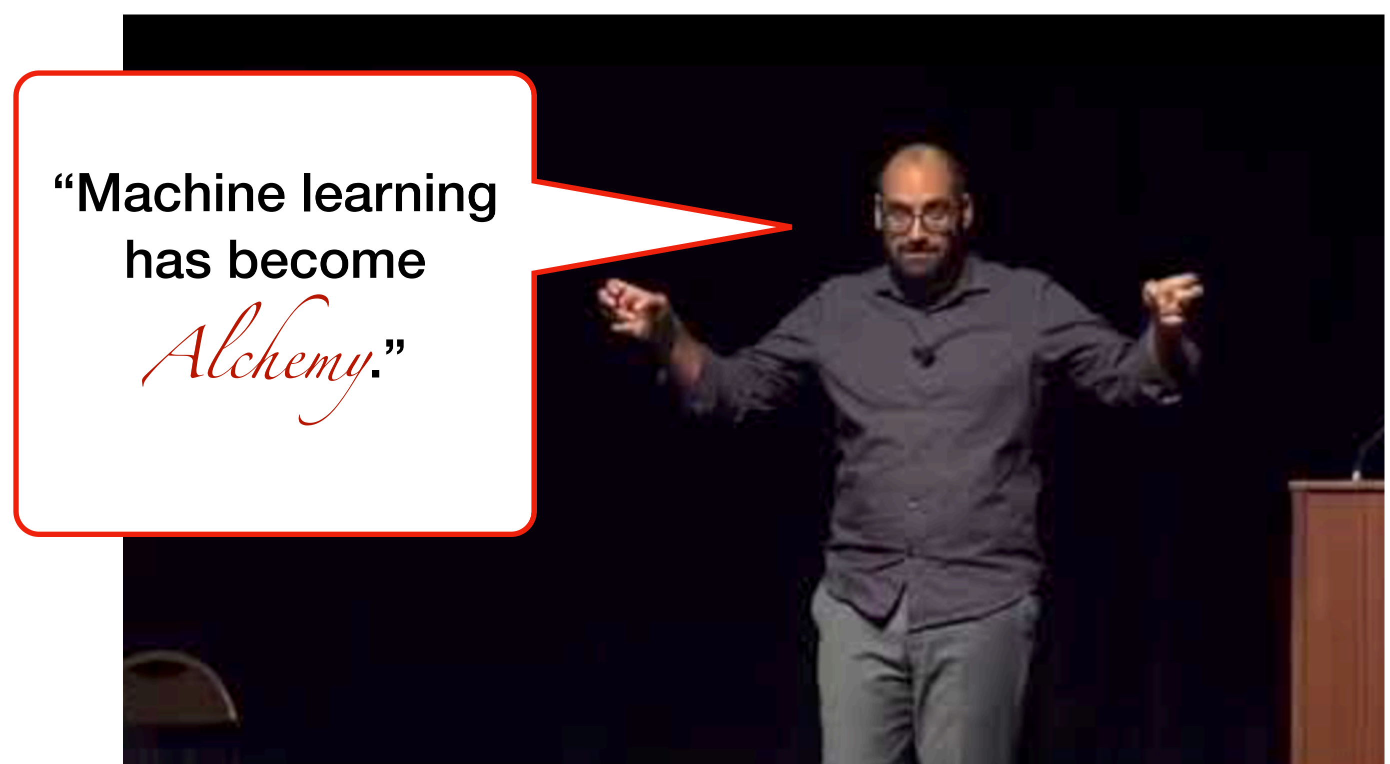

Ali Rahimi (Google) at *NIPS* 2017

Statistical Sequence Modeling

Next word prediction

$$P(x_n \mid x_{n-1}, \ldots, x_1)$$

Statistical Sequence Modeling

Next word prediction

I LOVE ?

$$P(x_n \mid x_{n-1}, \ldots, x_1)$$

Sentiment Analysis

"This is a great movie!!" $\sigma = +1$

"This is a boring movie…" $\sigma = -1$

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In Deep Learning era, typically parametrised by Recurrent Neural Networks (RNNs).

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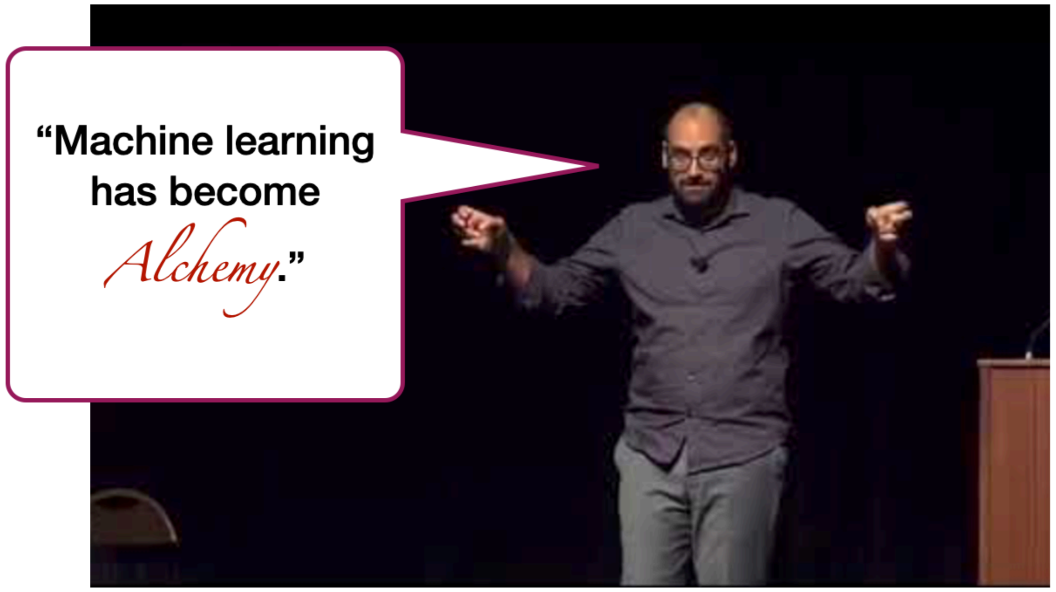

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Sequence Modeling and Many-body Quantum Physics

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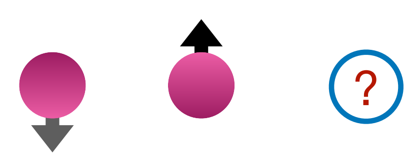
Many-body Quantum Physics

1-D Spin Chain



MPS, DMRG

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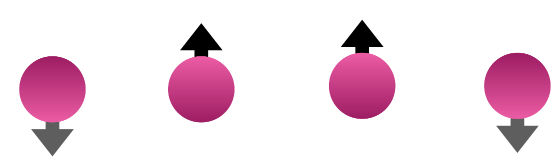
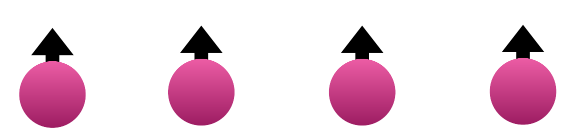


Classification of Phase of Matters

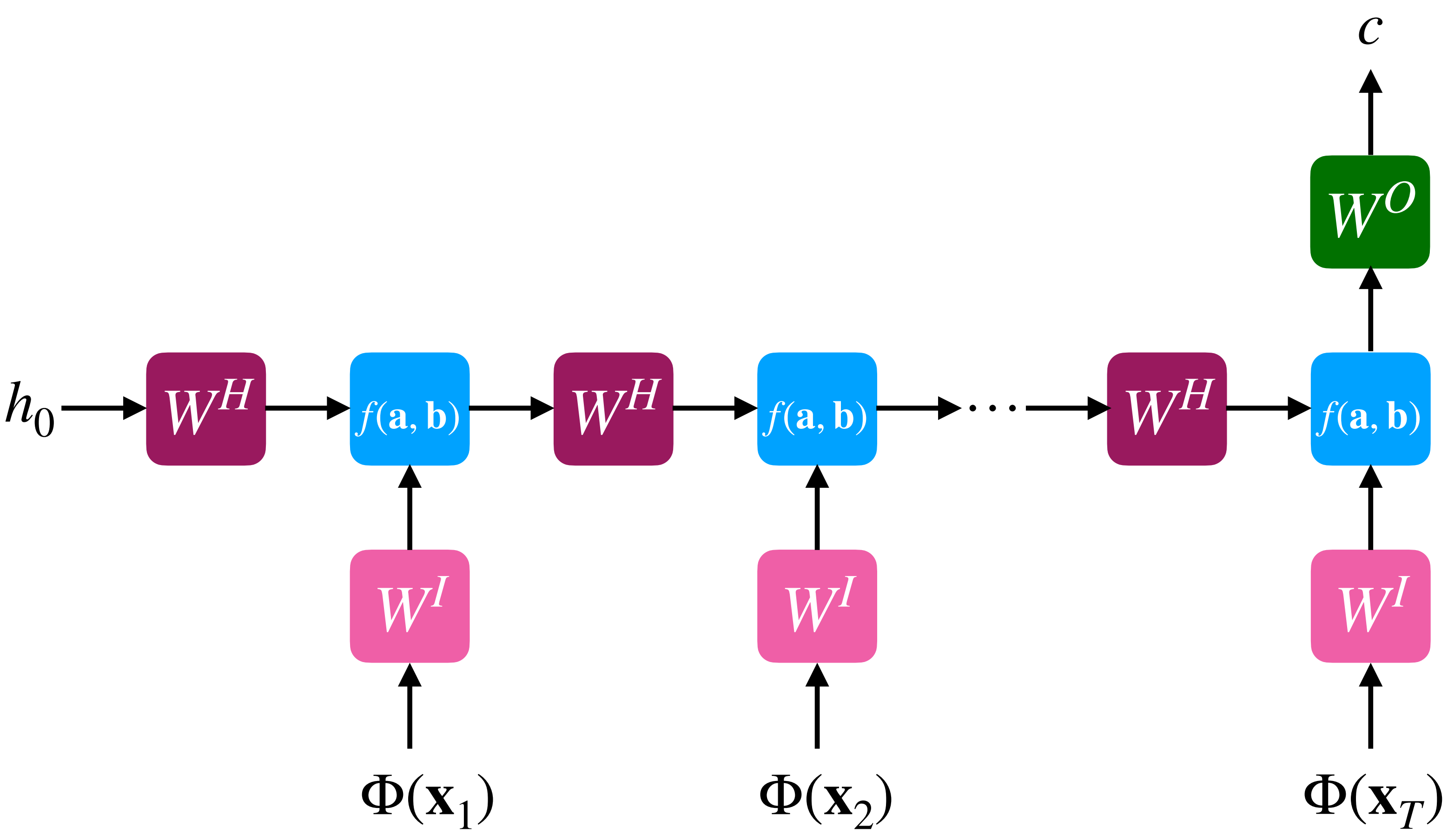


MPS, DMRG

“Ferromagnets”

Relatively well developed

Shallow Recurrent Neural Networks (RNNs) Architecture for Sentiment Analysis



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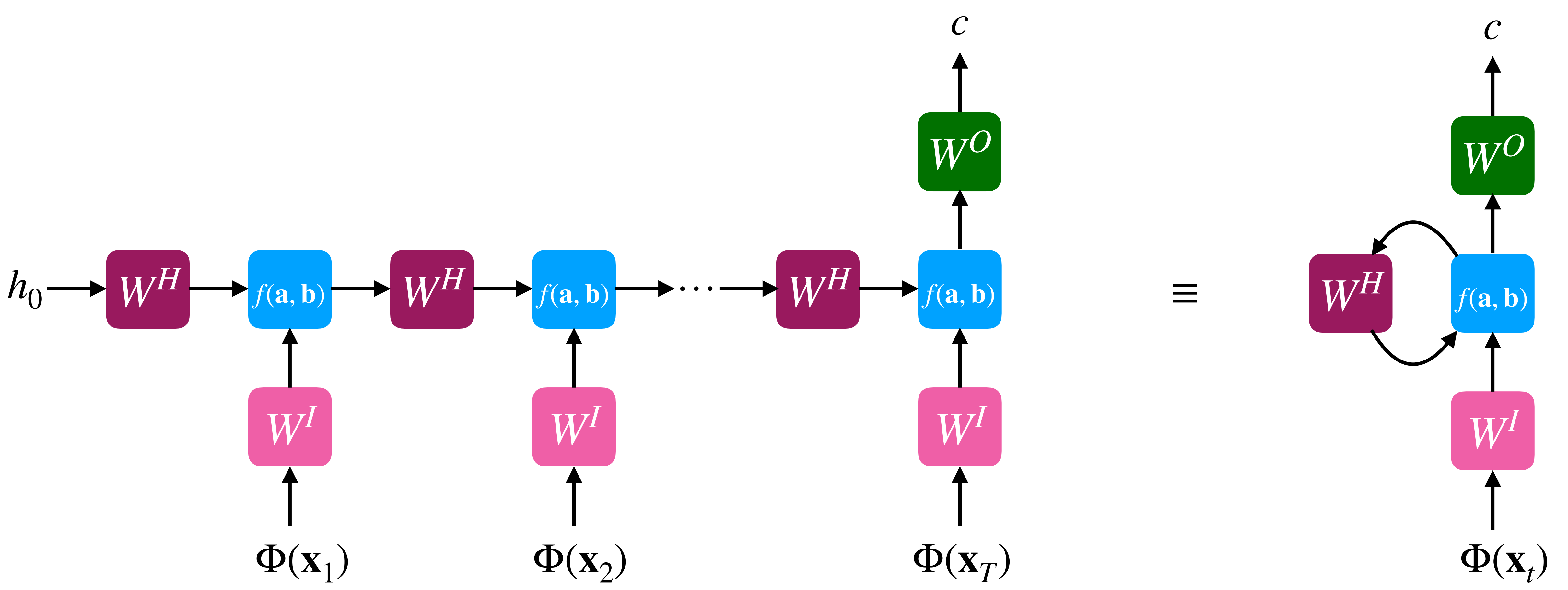

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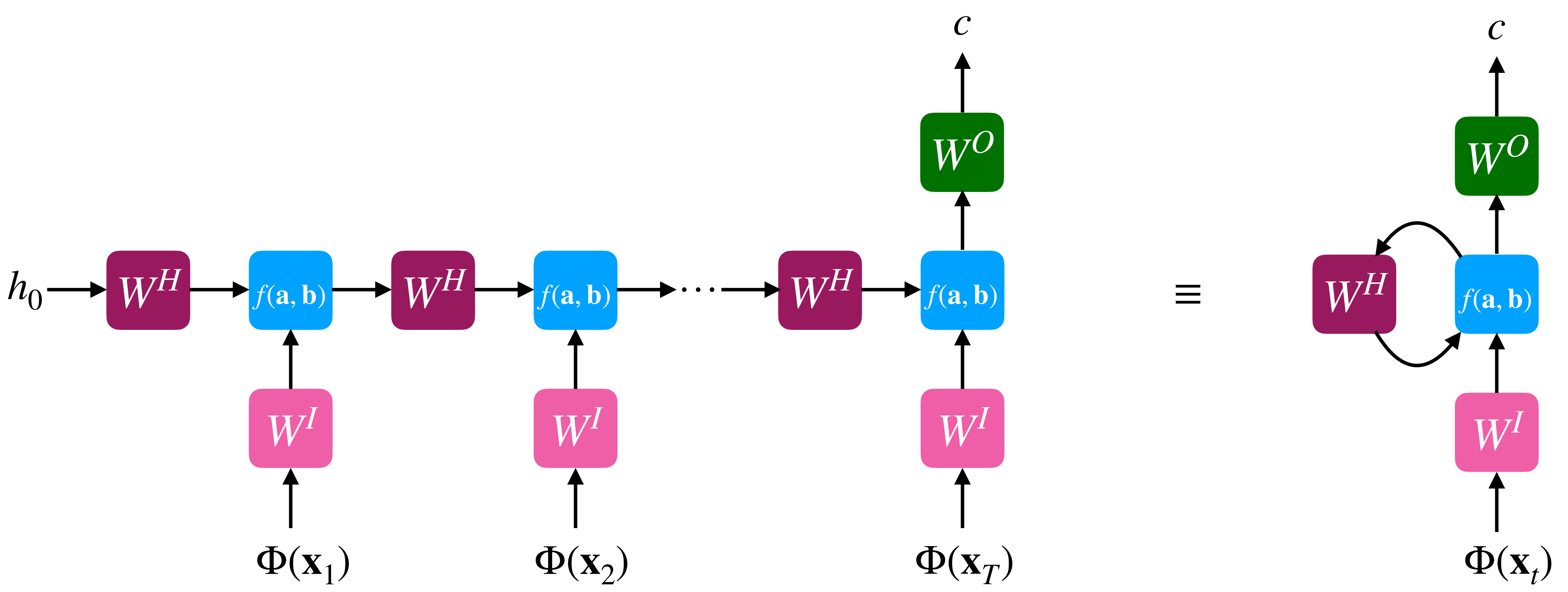

$$\mathbf{h}^t = f\left(W^{\mathrm{H}}\mathbf{h}^{t-1}, W^{\mathrm{I}}\Phi\left(\mathbf{x}_t\right)\right)$$

$$c = \sigma(W^{\mathrm{O}}\mathbf{h}^T) \qquad \approx \qquad P(c\,|\,x_T, \ldots, x_1)$$

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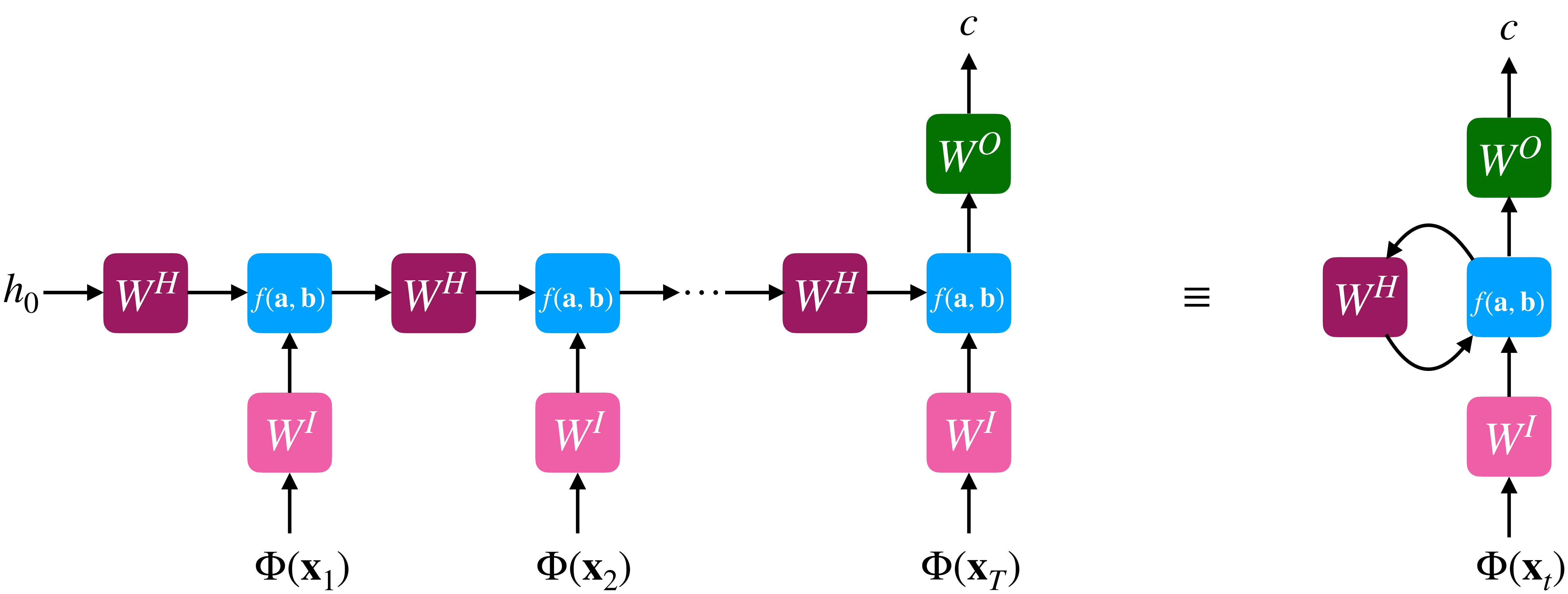

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However, for a specific type of activation function called Recurrent Arithmetic Circuits (RACs), there's a mapping to a translational invariant Matrix Product State (MPS)

$$f(\mathbf{a}, \mathbf{b}) \equiv f^{\mathrm{RAC}}(\mathbf{a}, \mathbf{b}) = \mathbf{a} \odot \mathbf{b}$$

Levine, Y., et. al. *On the Long-Term Memory of Deep Recurrent Networks*, ICRL, 2018.
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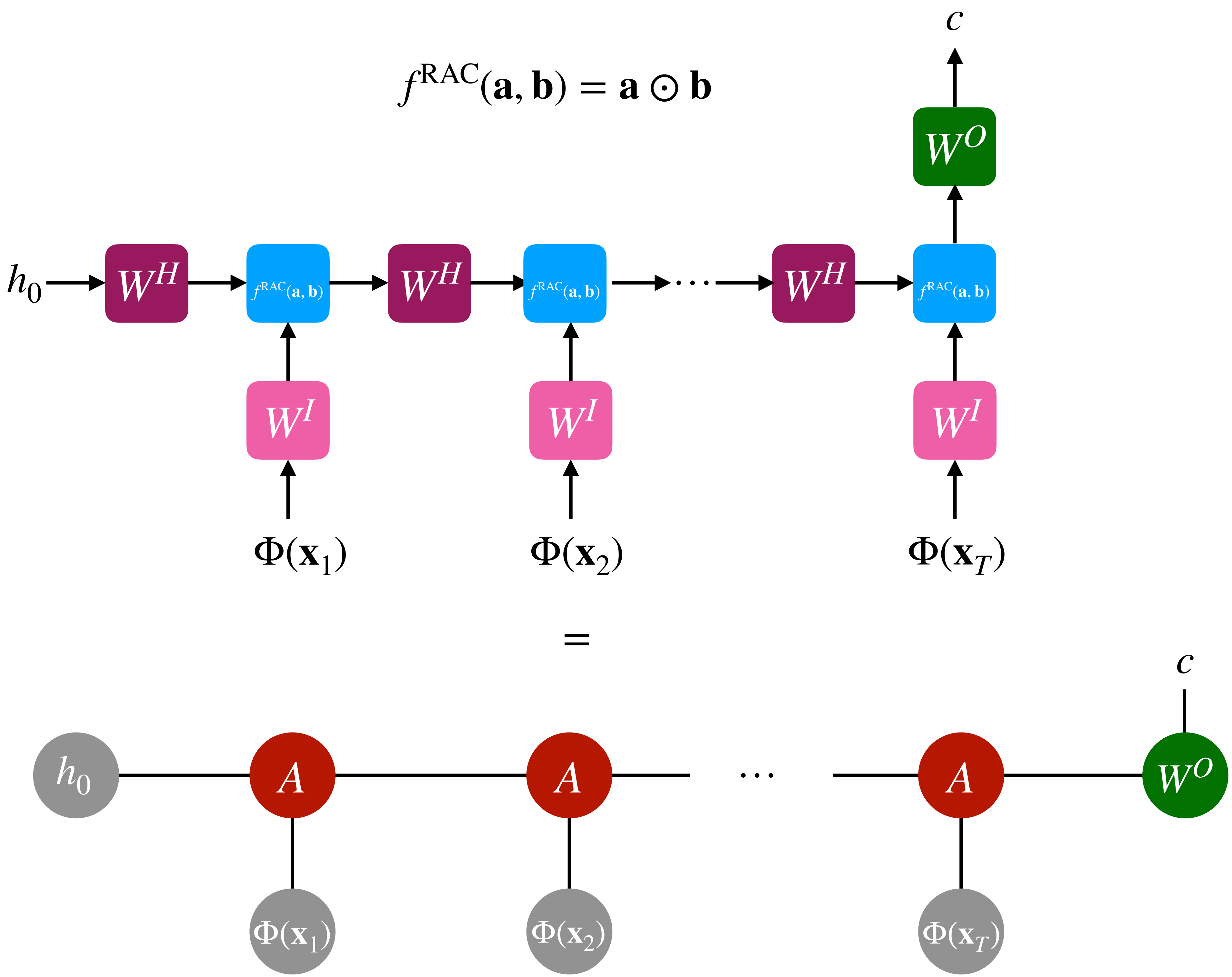

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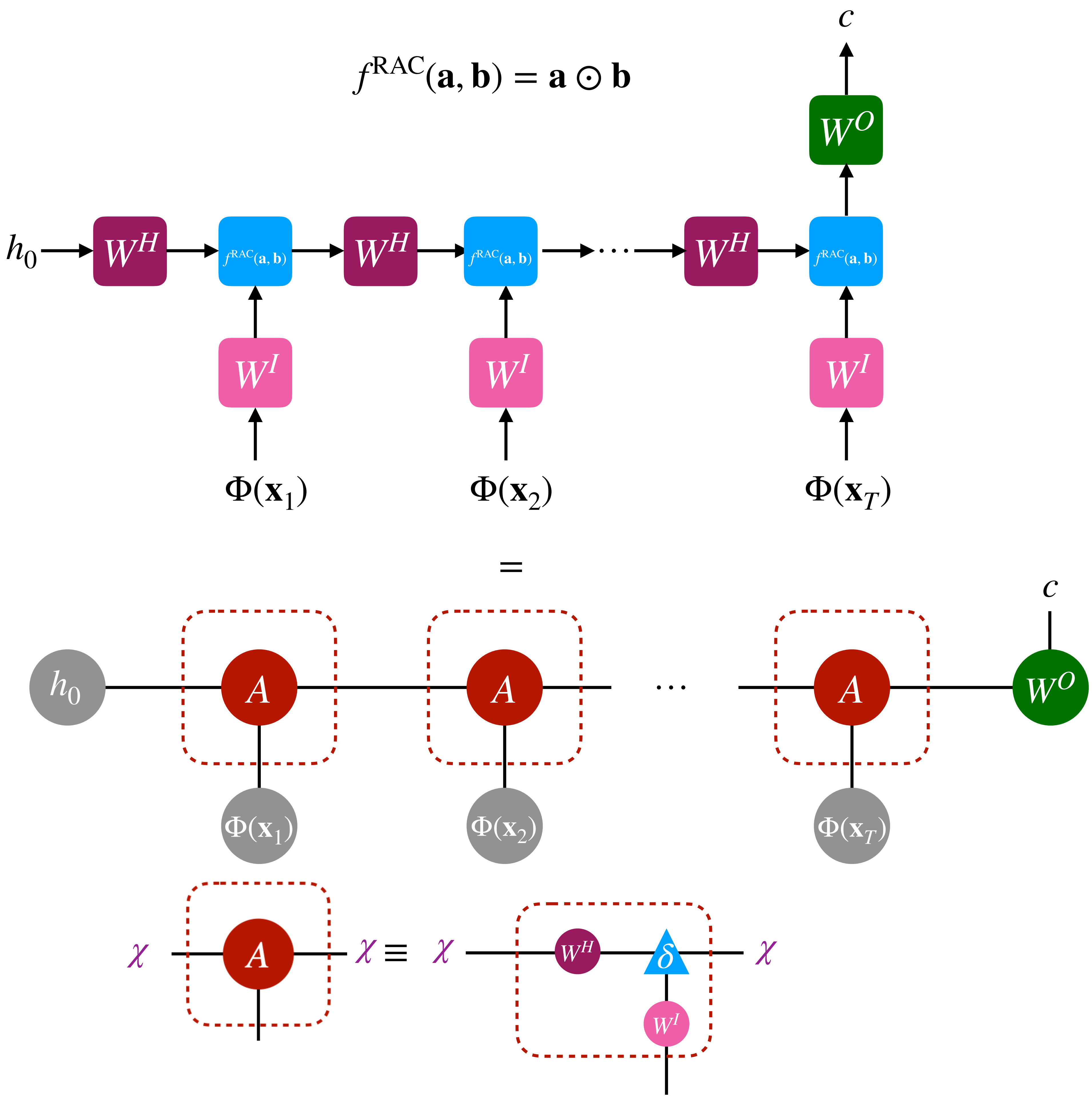

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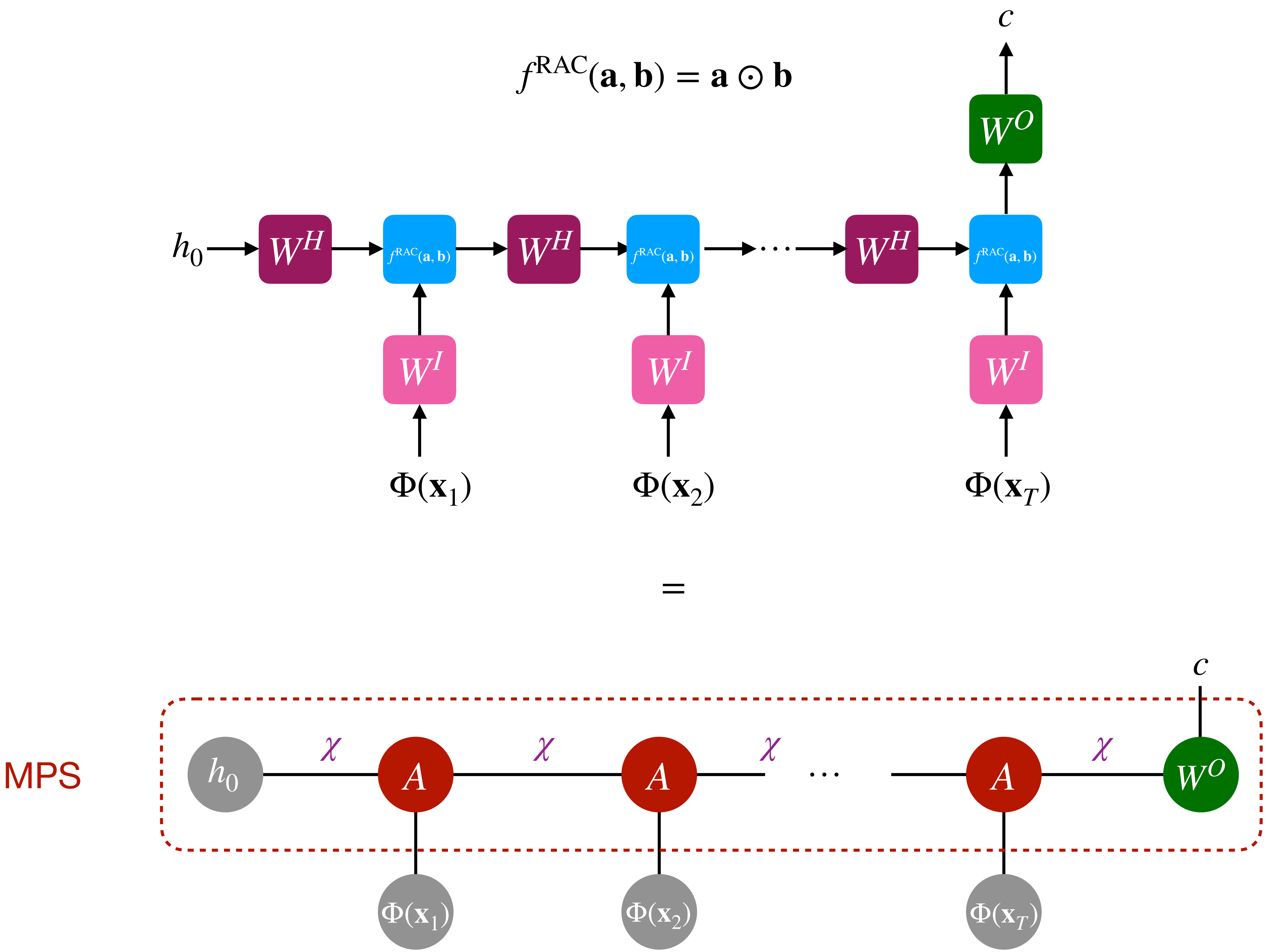

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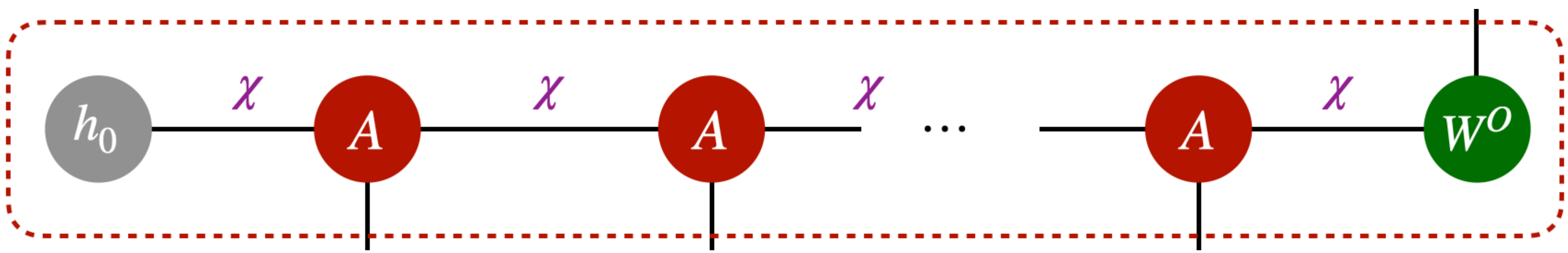
Entanglement Entropy as a Proxy of Information Propagation in RACs



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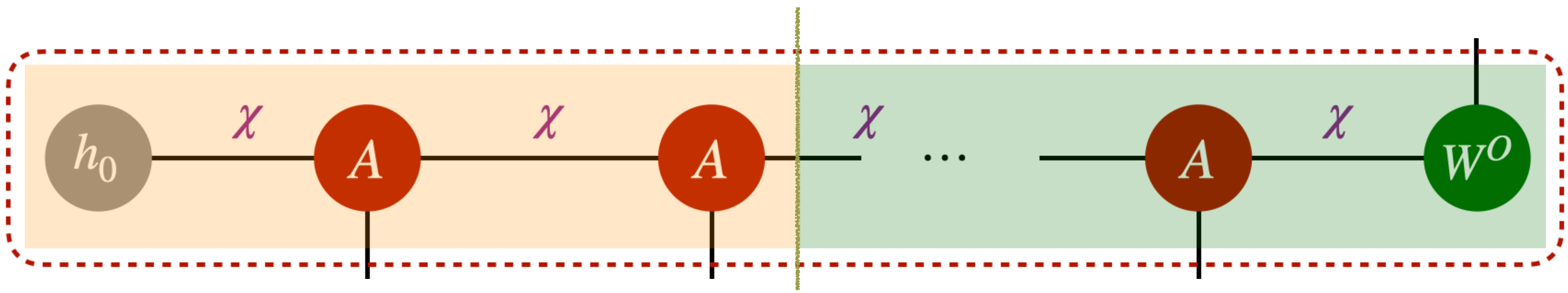

$$|\psi_{MPS}\rangle = \sum_{\alpha=1}^{r} \lambda_\alpha \left|\phi_\alpha^L\right\rangle \otimes \left|\phi_\alpha^R\right\rangle$$

Entanglement Entropy

$$S = -\sum_{\alpha=1}^{r} \left|\lambda_\alpha\right|^2 \ln \left|\lambda_\alpha\right|^2$$

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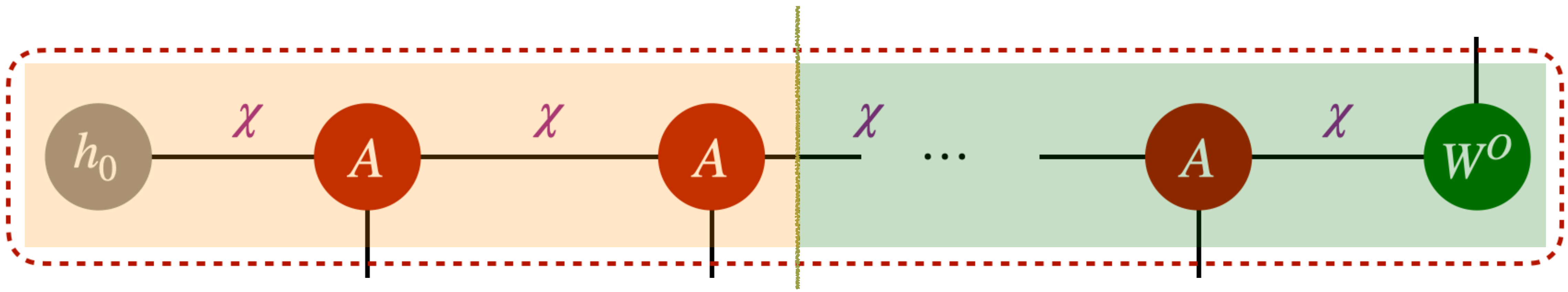

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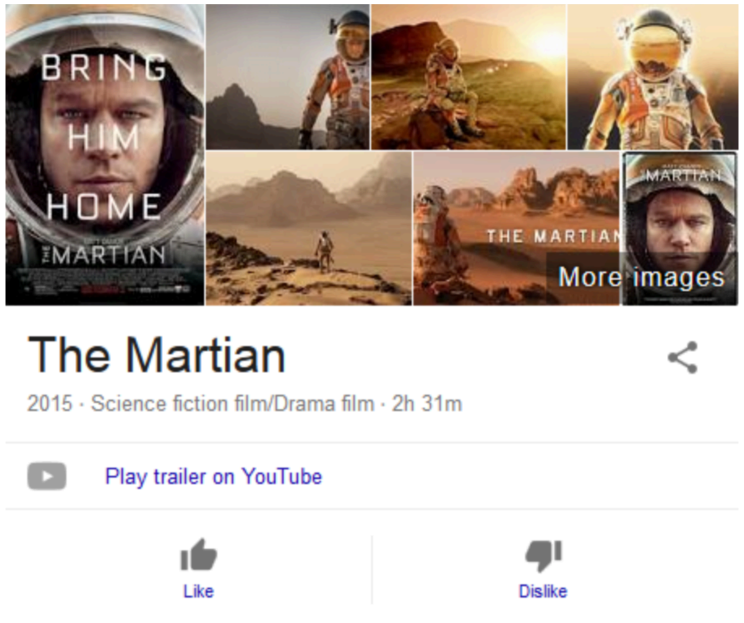
If $r \ll \chi$, then $|\psi_{MPS}\rangle$ does not possess long-range correlation.

Thus S can be a good proxy to test whether the learned RACs has long-range information propagation.

Sentiment Analysis for IMDB dataset



10/10

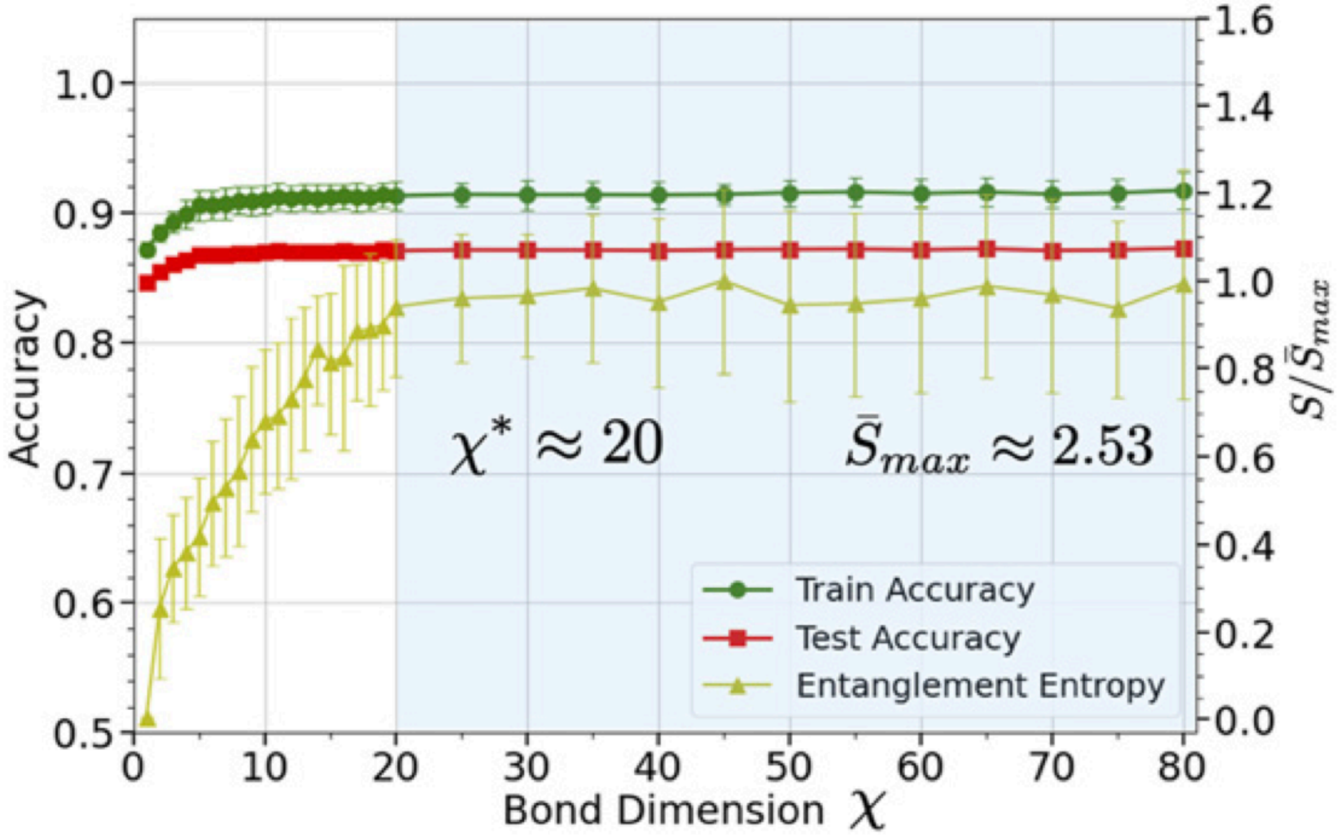
pleasantly surprised

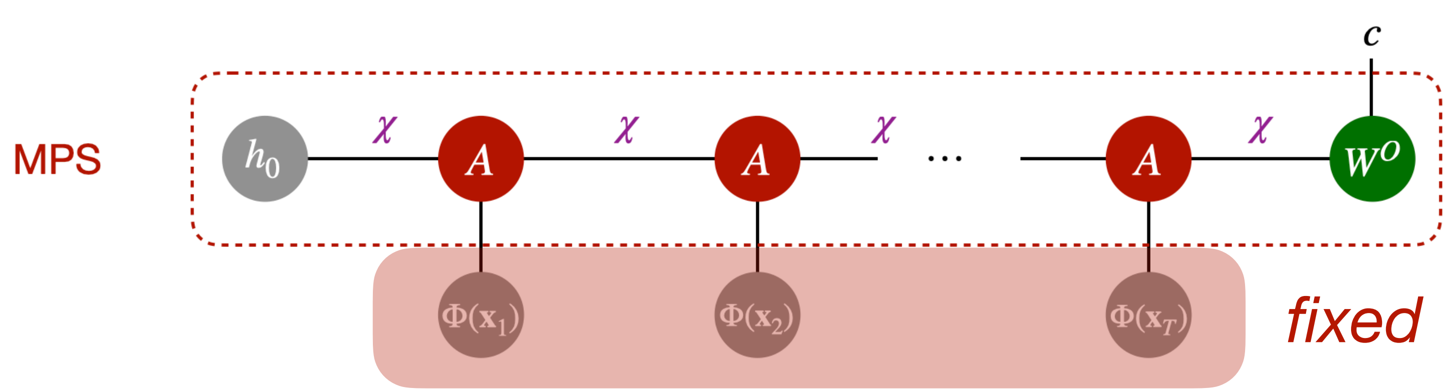
whammo-79346 17 January 2016

Seeing that the movie was over 2 hrs long, and knowing that the person was going to be stuck on the planet by their self for the majority, I didn't have high hopes for it. Usually these types of movies are boring. Not a lot of writers can pull this off. This movie was really good tho. A group of us watched it and really enjoyed. There were some things they failed to explain, that we collectively came up with our own answer for. Other than that, it was great. I never felt bored or left waiting for more. Overall, I feel it was very

Sentiment Analysis for IMDB dataset: fixed word embedding

Fix the pre-trained $\mathbf{\Phi}(w) \in \mathbb{R}^4$





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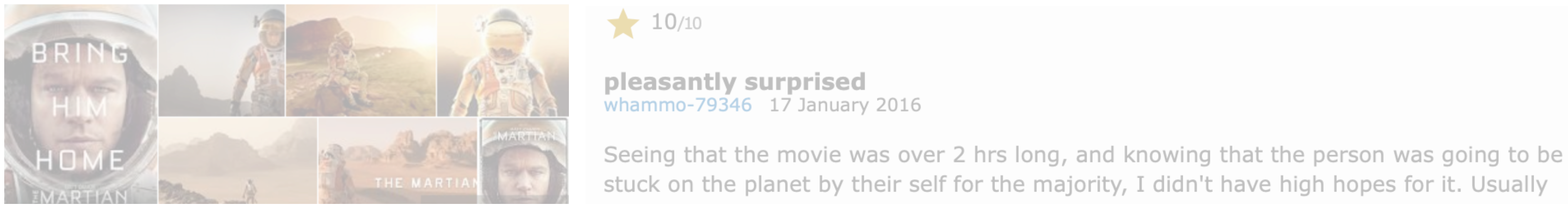

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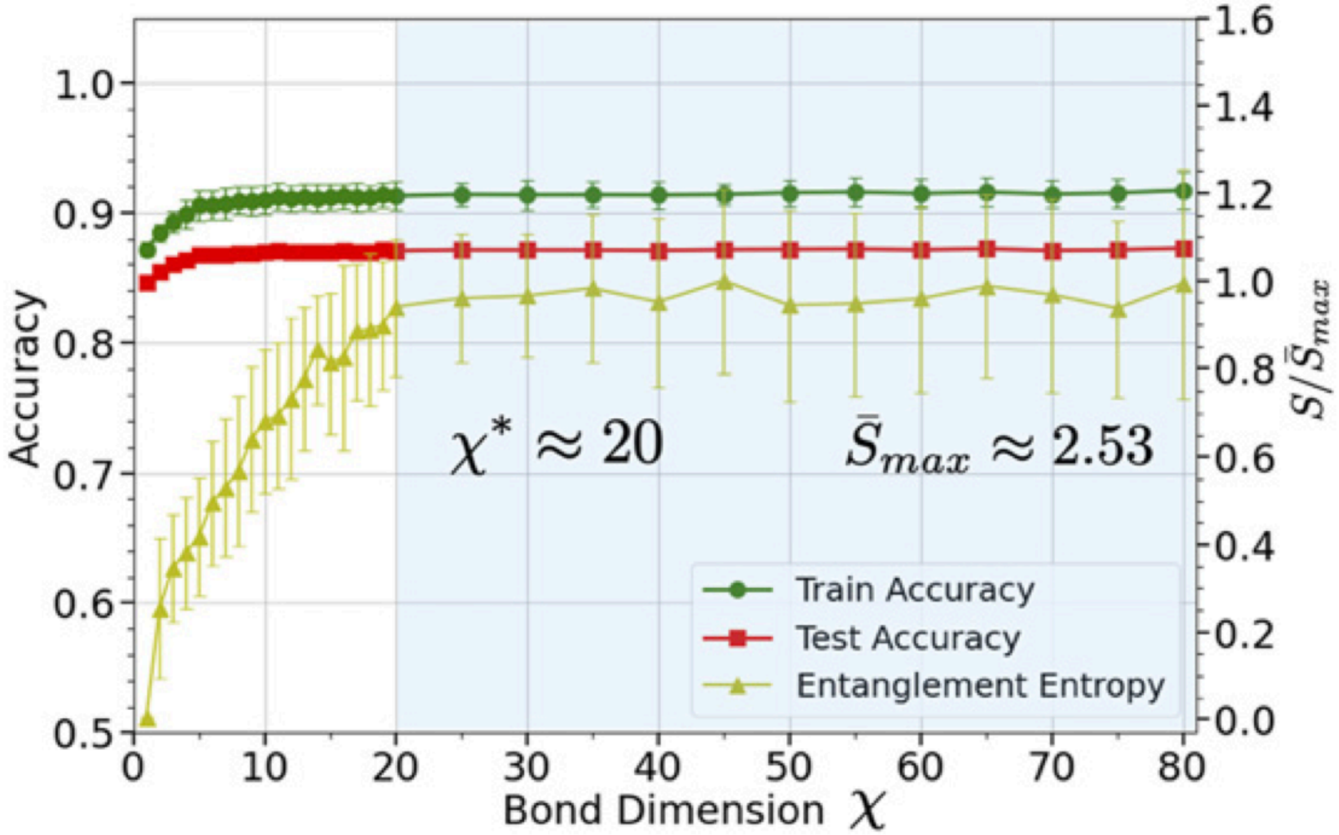
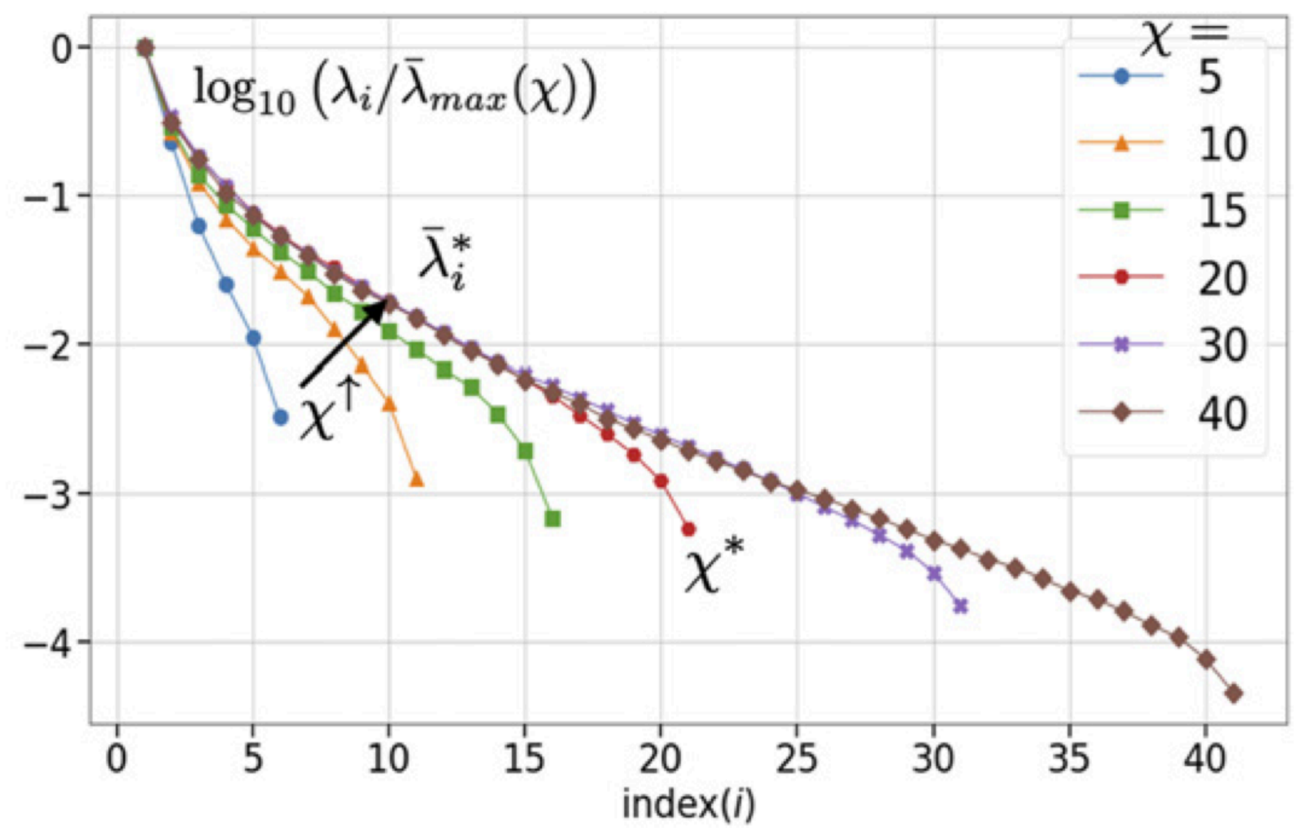
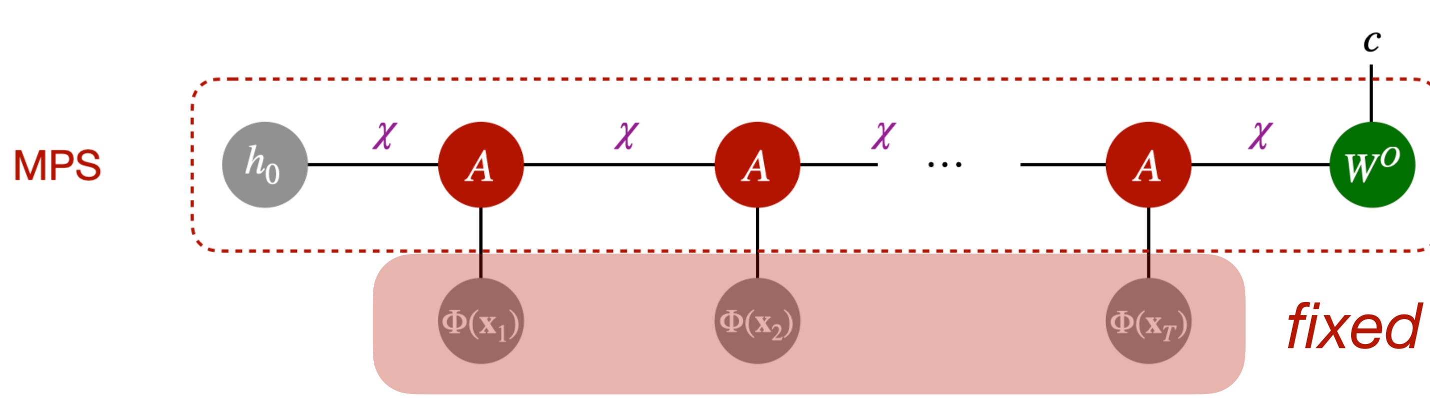
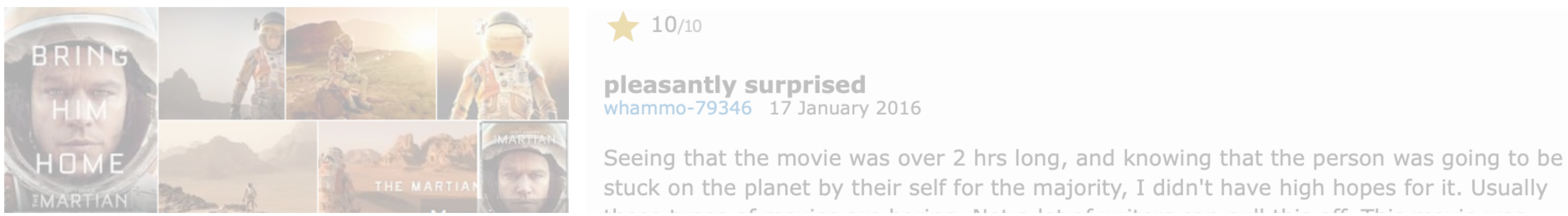


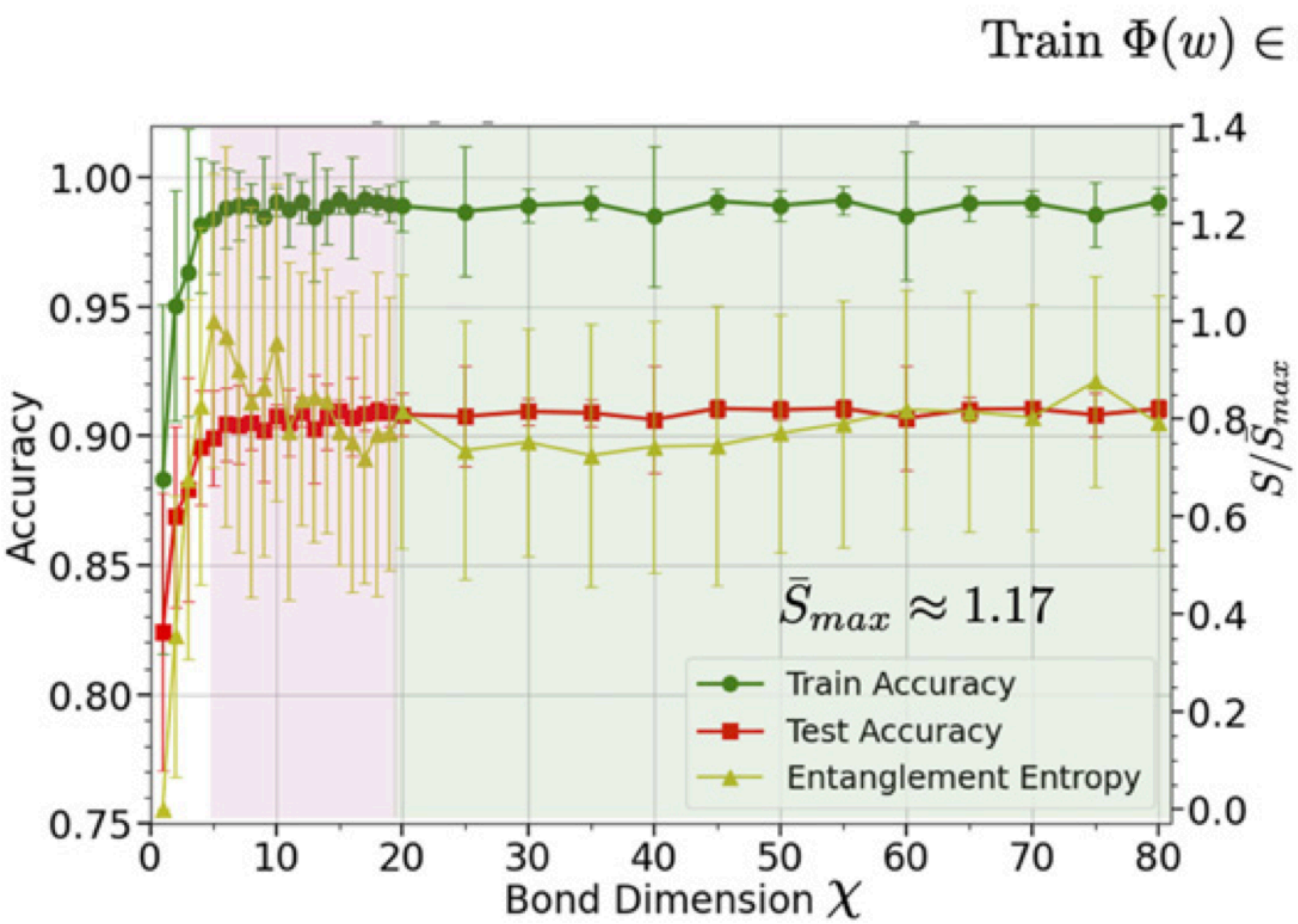
Collapse of entanglement spectrum determines model bias

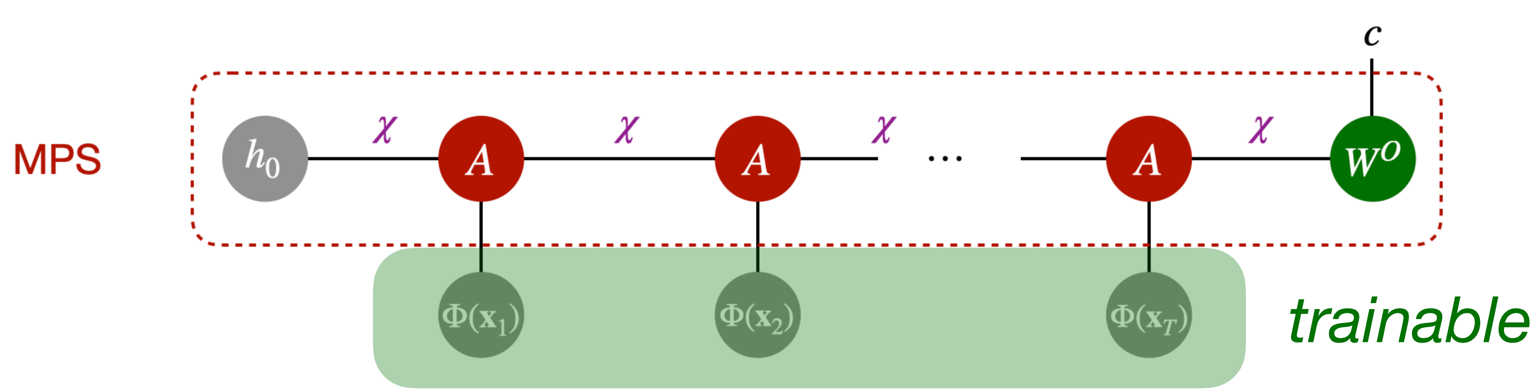




Sentiment Analysis for IMDB dataset: trainable word embedding







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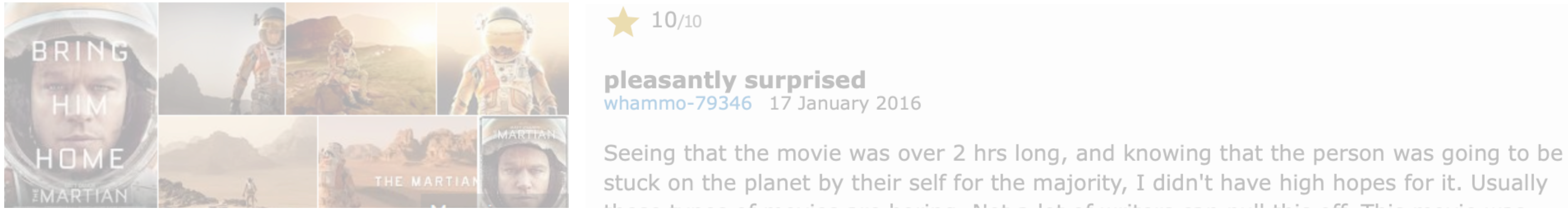
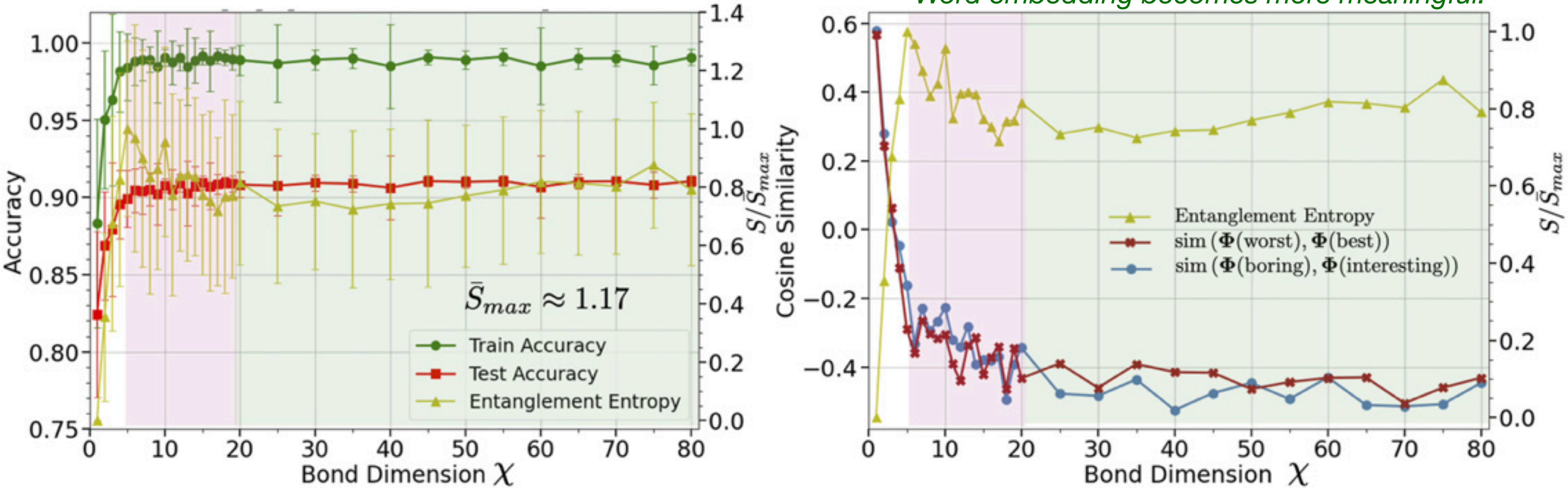
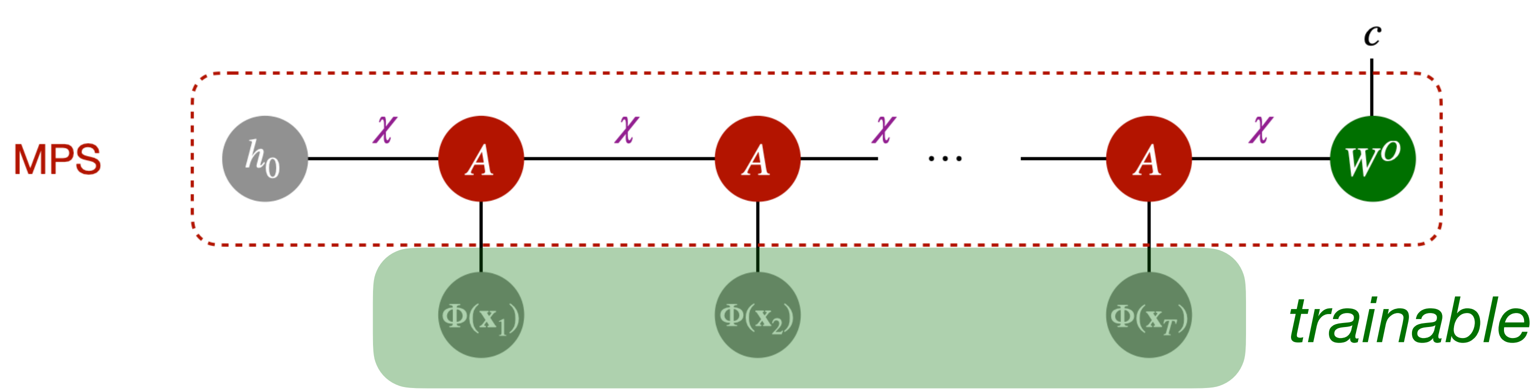


Train $\Phi(w) \in \mathbb{R}^4$ with RACs

Word embedding becomes more meaningful!





Summary

Mapping RACs to MPS allows one to exploit entanglement entropy as a measure of long-range correlation in natural language modeling.

Machine learning model bias in sentiment analysis is closely related to the saturation of information propagation, arising from the collapse of MPS's entanglement spectrum.

Word embedding plays a very crucial role in expressing data. Although long-range information propagation is limited by the area law of MPS, the expressiveness of model is boosted by more meaningful word embeddings.

Tangpanitanon, J., Mangkang, C., Bhadola, P., Minato, Y., Angelakis, D., **Chotibut, T.** *Explainable Natural Language Processing with Matrix Product States,* **New Journal of Physics 2022** (arxiv:2112.08628)

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J. Tangpanitanon, ...,T. Chotibut NJP 2022

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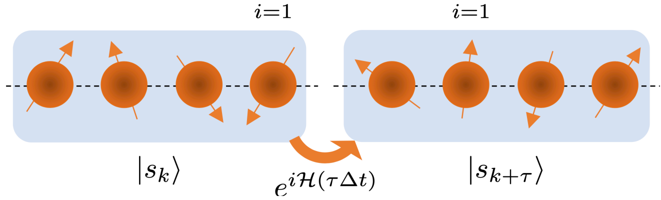

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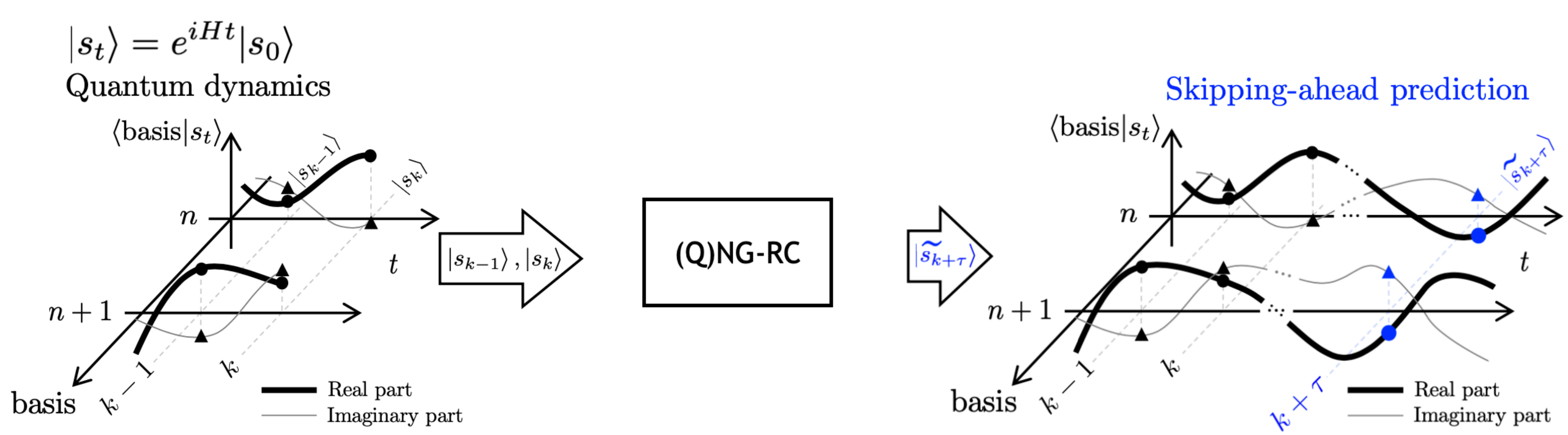

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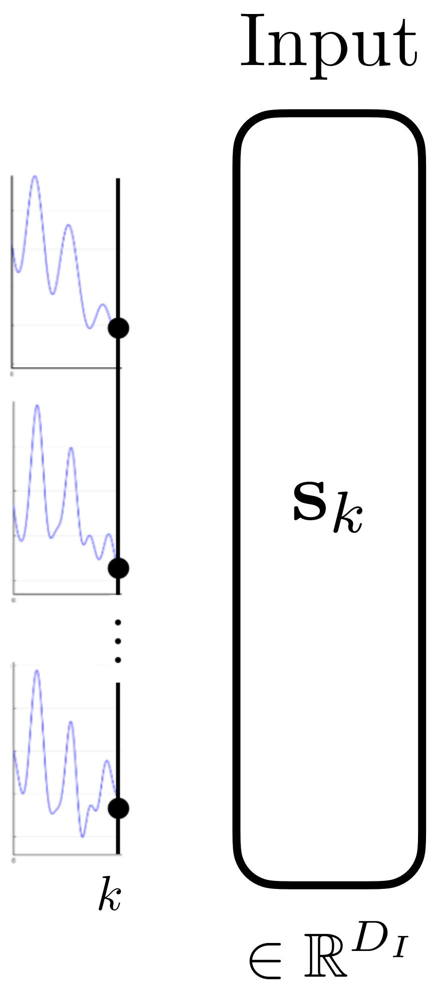
Reservoir Computing (RC) in a nutshell



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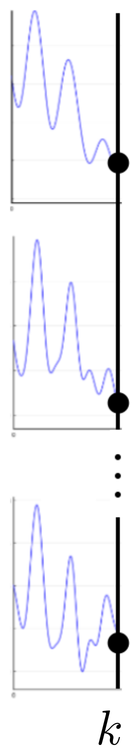

Input

$\mathbf{s}_k$

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

Reservoir state update

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

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

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$D_I \ll D_R$

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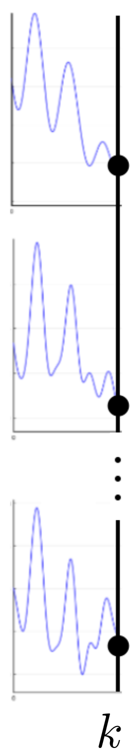

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The current state of the reservoir is influenced by the past inputs

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

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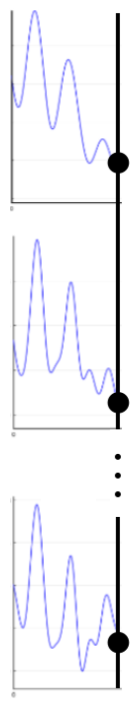

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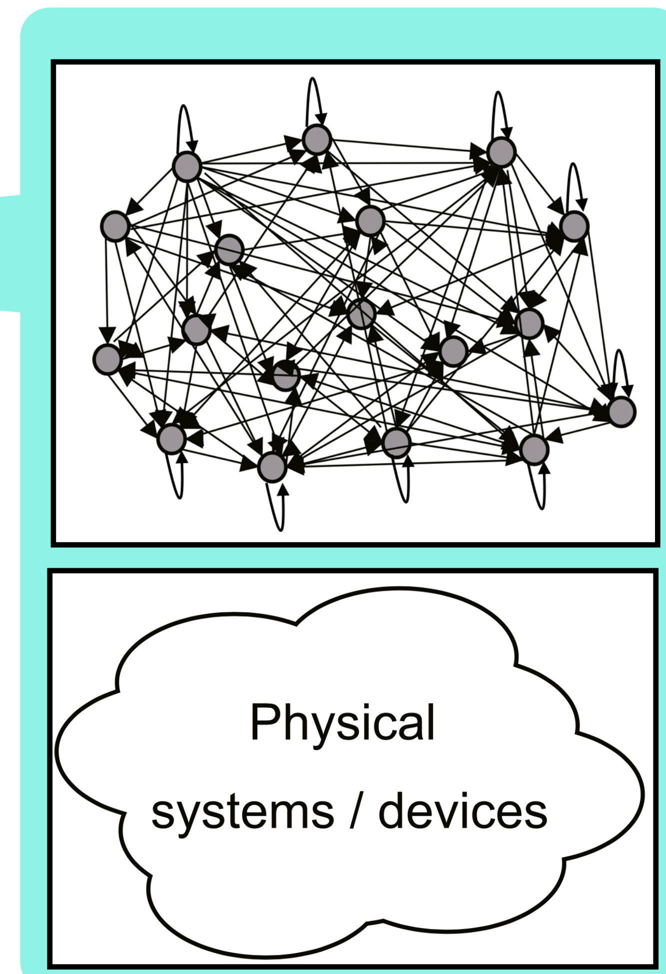

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G. Tanaka et. al. Recent advances in physical reservoir computing: a review, *Neural Networks*, (**115**) 100-123, 2019

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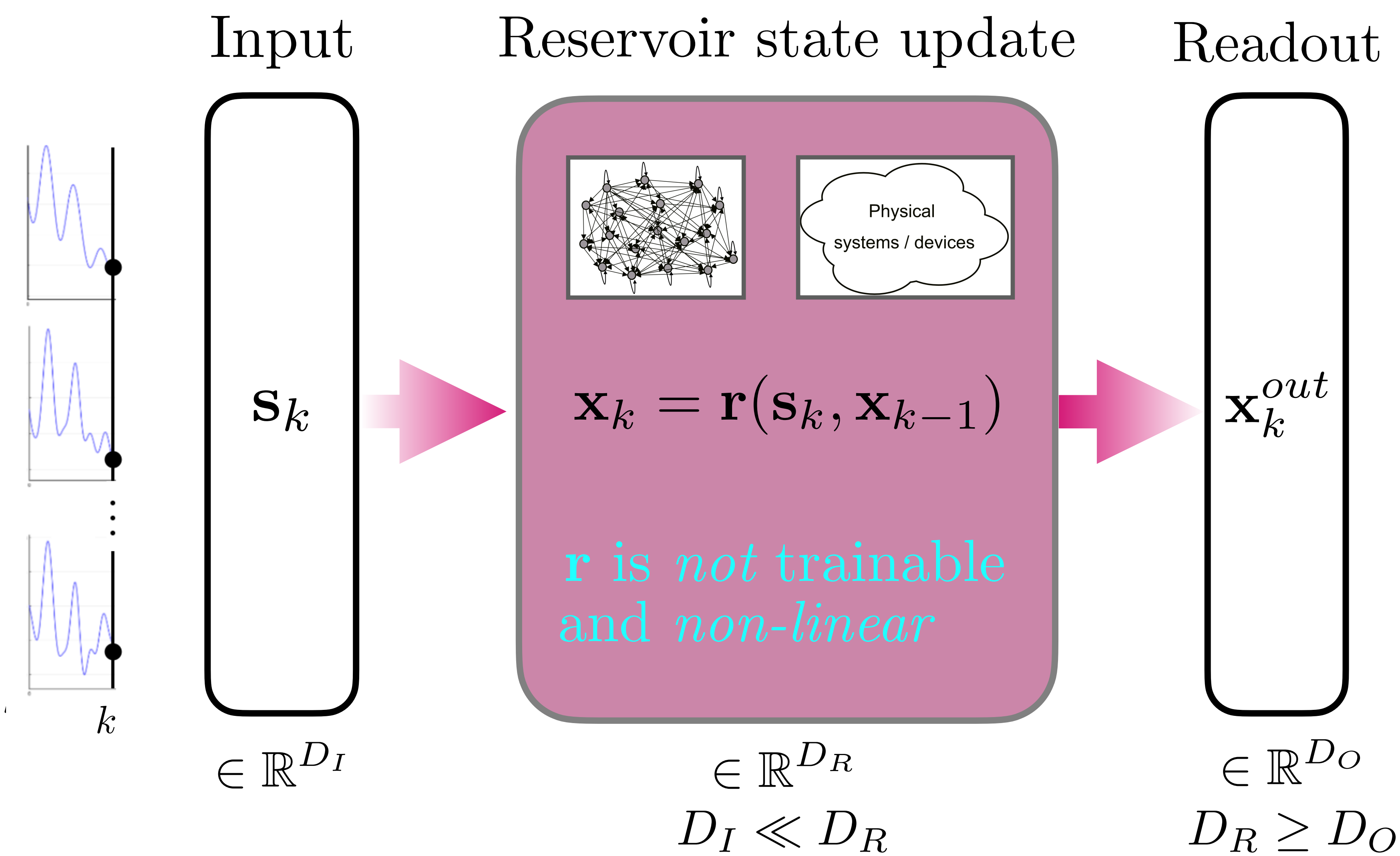
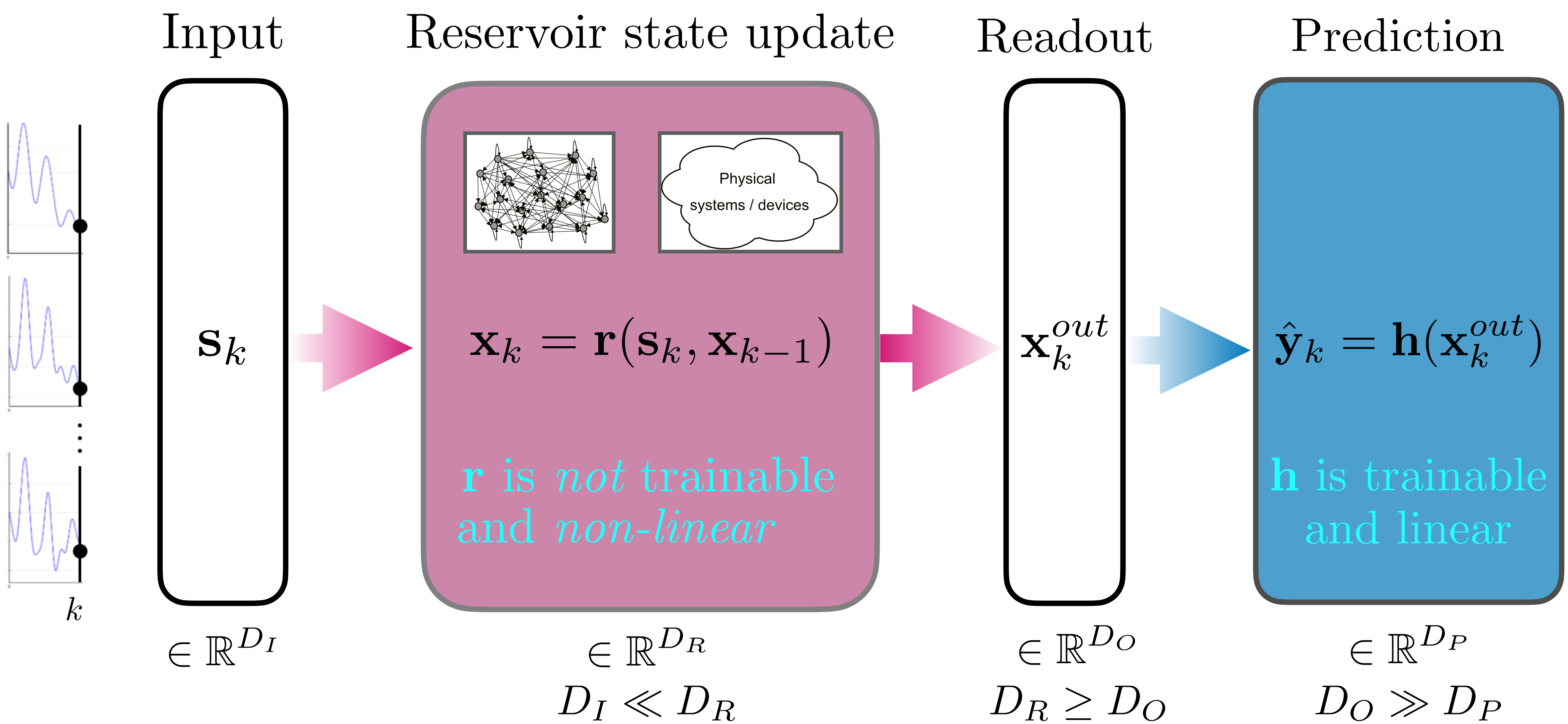


Reservoir Computing (RC) in a nutshell



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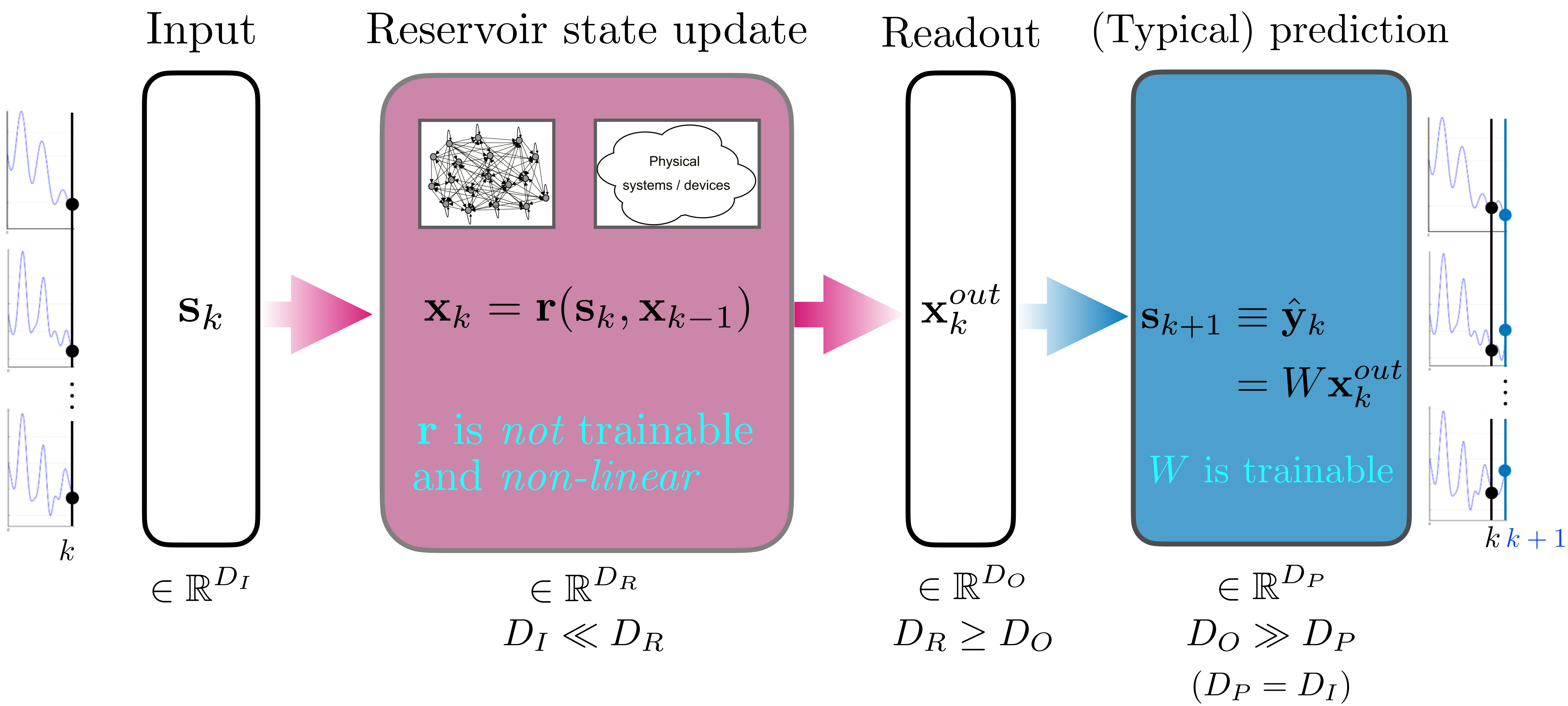
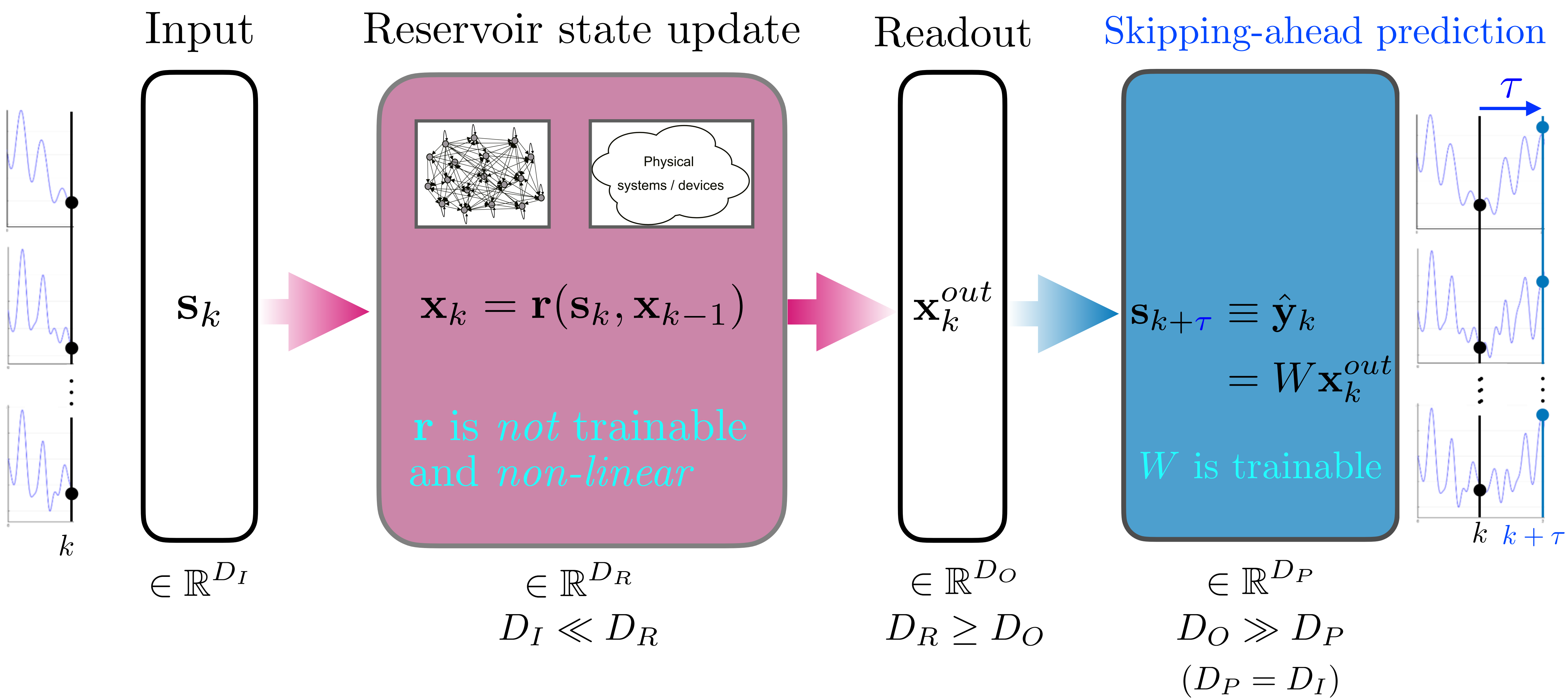


Reservoir Computing (RC) in a nutshell



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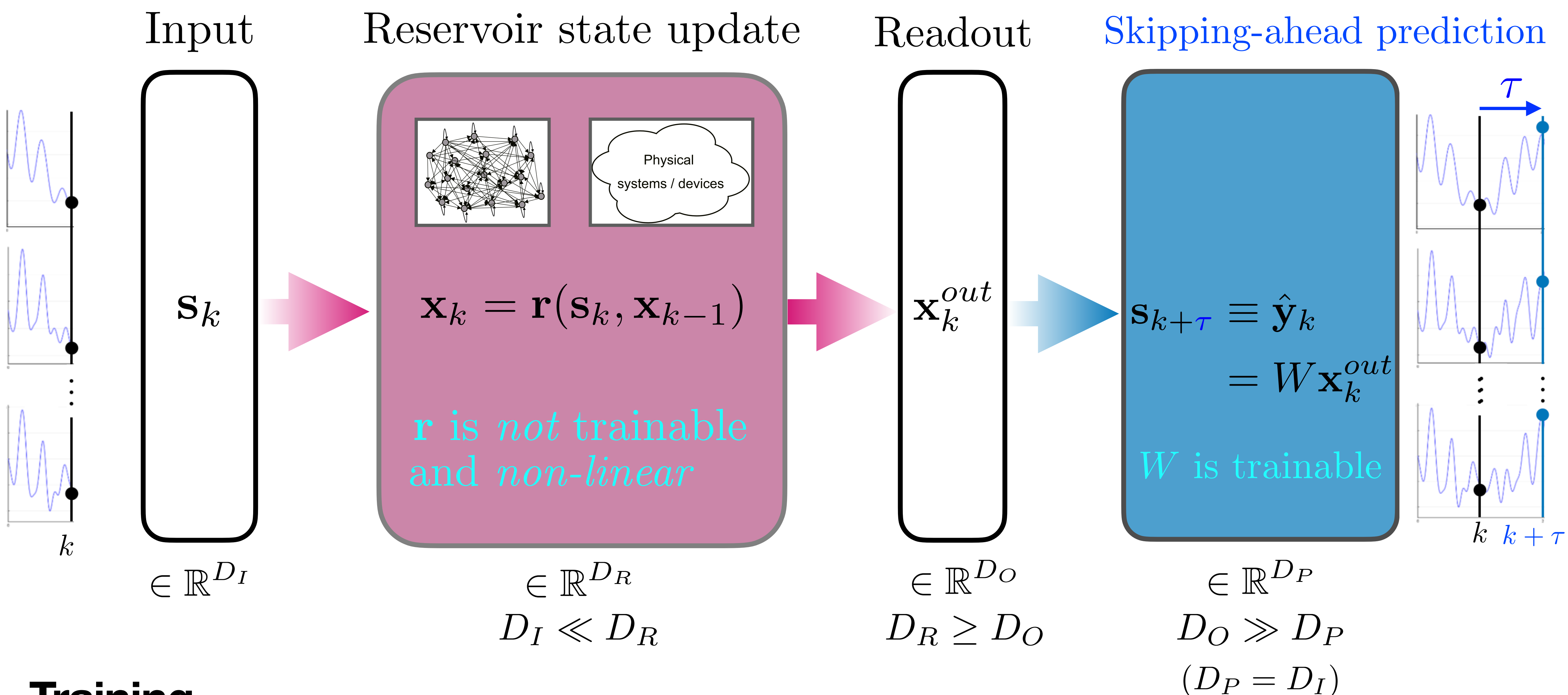
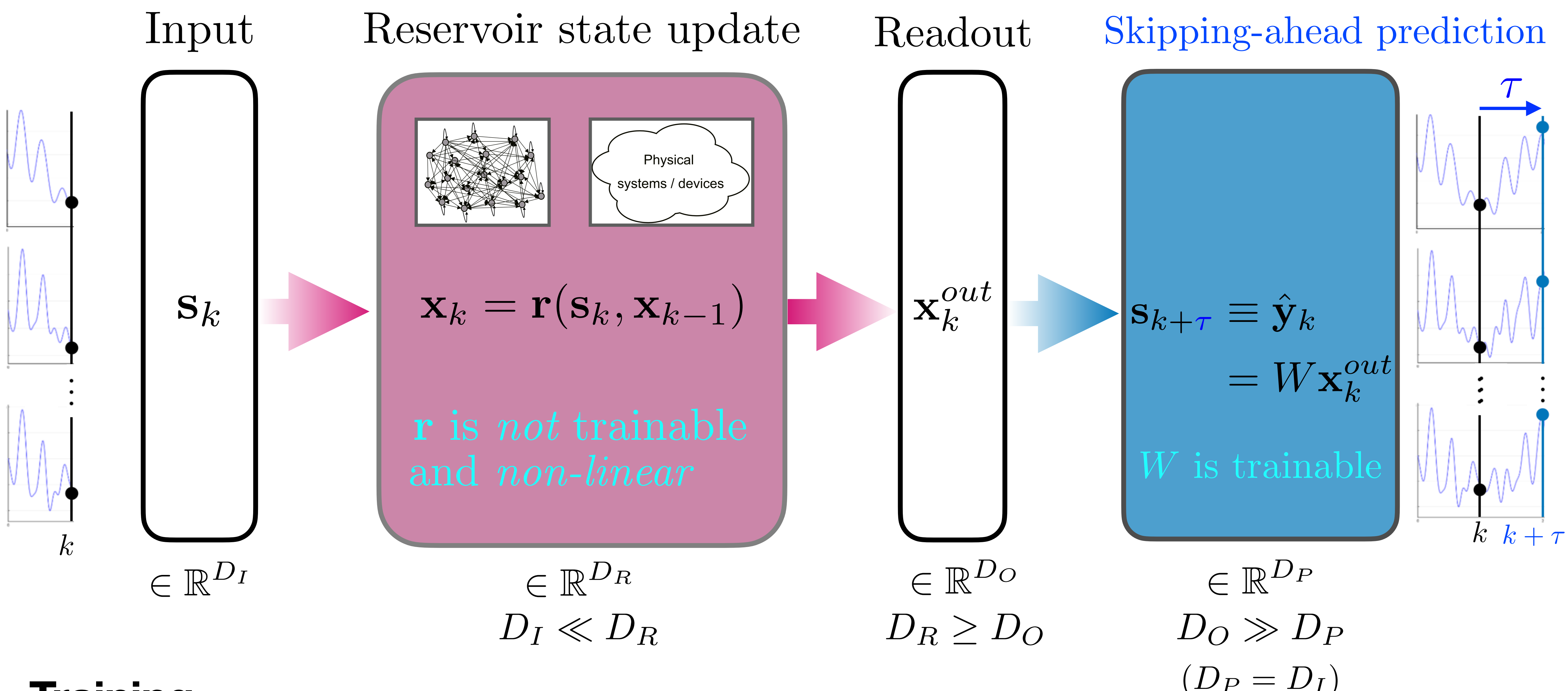


Training

W is "trained" by minimizing

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

Reservoir Computing (RC) in a nutshell



Training

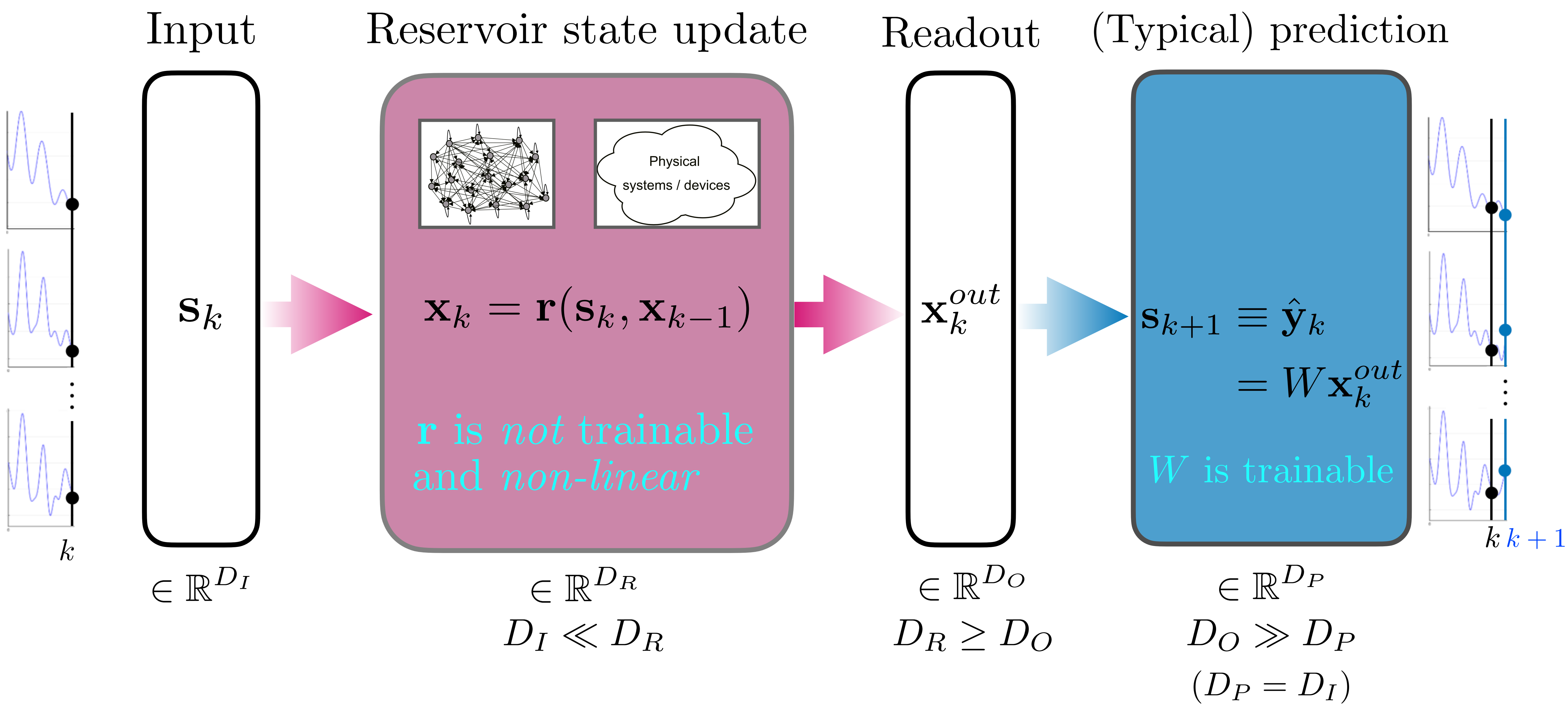
W is "trained" by minimizing $\displaystyle \frac{1}{T}\sum_{k=0}^{T-1} ||\hat{\mathbf{y}}_k - W\mathbf{x}_k^{out}||_2^2 + \lambda||W||^2$

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

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

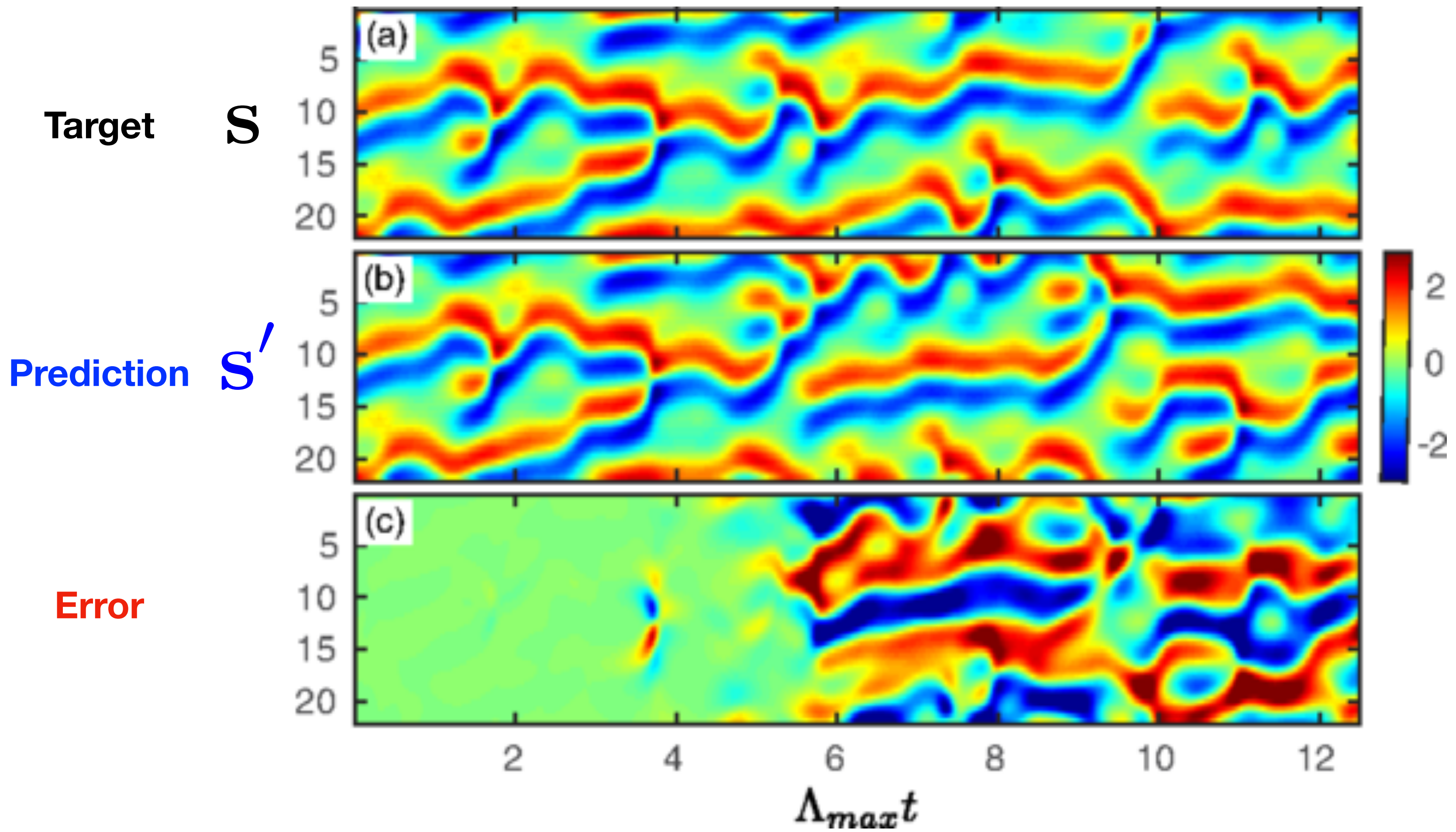
$$(\mathbf{x}_k^{out} = \mathbf{x}_k)$$

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

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

$$\vdots$$

kuramoto-sivashinsky spatiotemporal chaos



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

kuramoto-sivashinsky spatiotemporal chaos

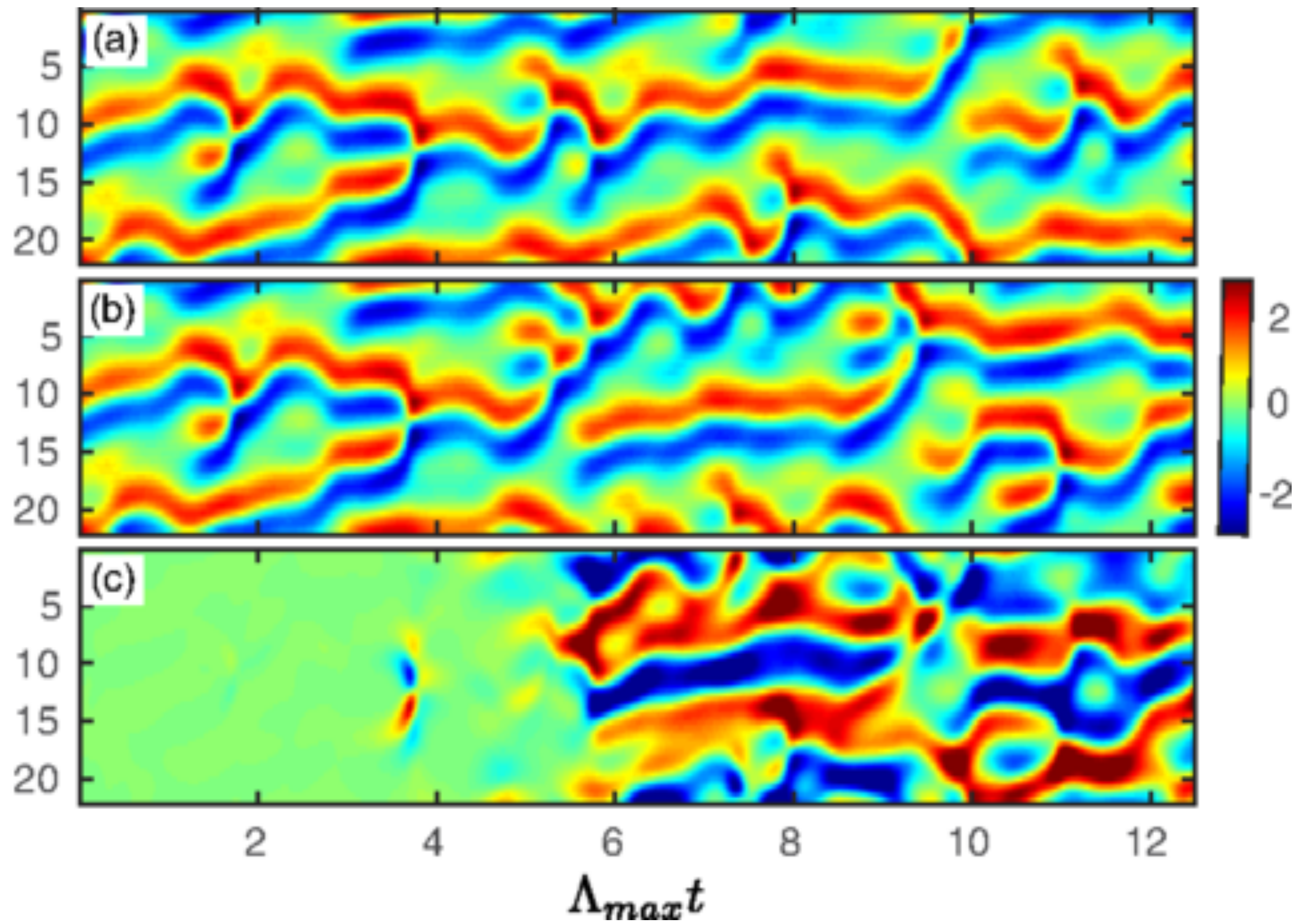
reservoir

RNN

Target $\mathbf{S}$

Prediction $\mathbf{S}'$

Error



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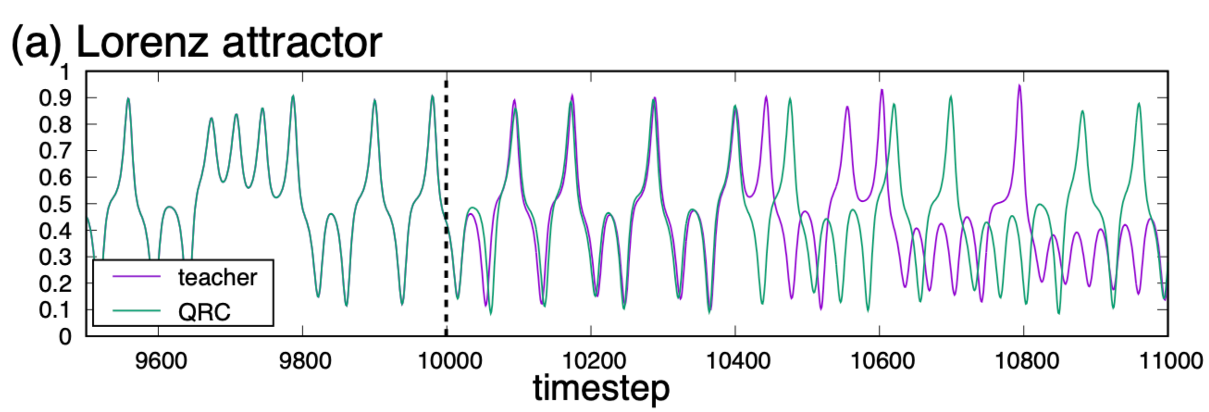
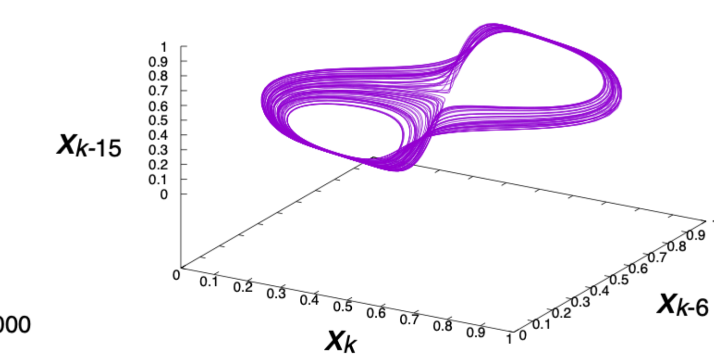
reservoir

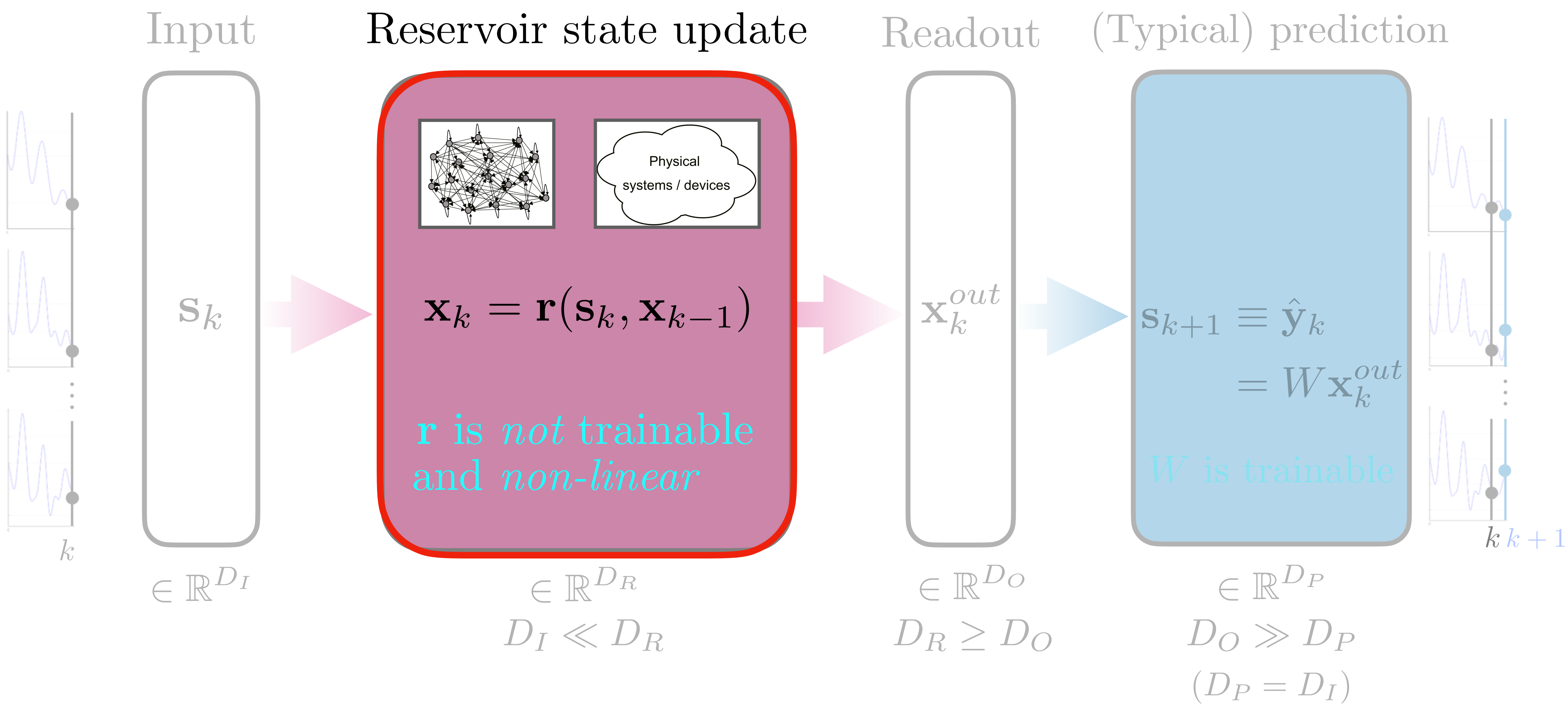
quantum Ising





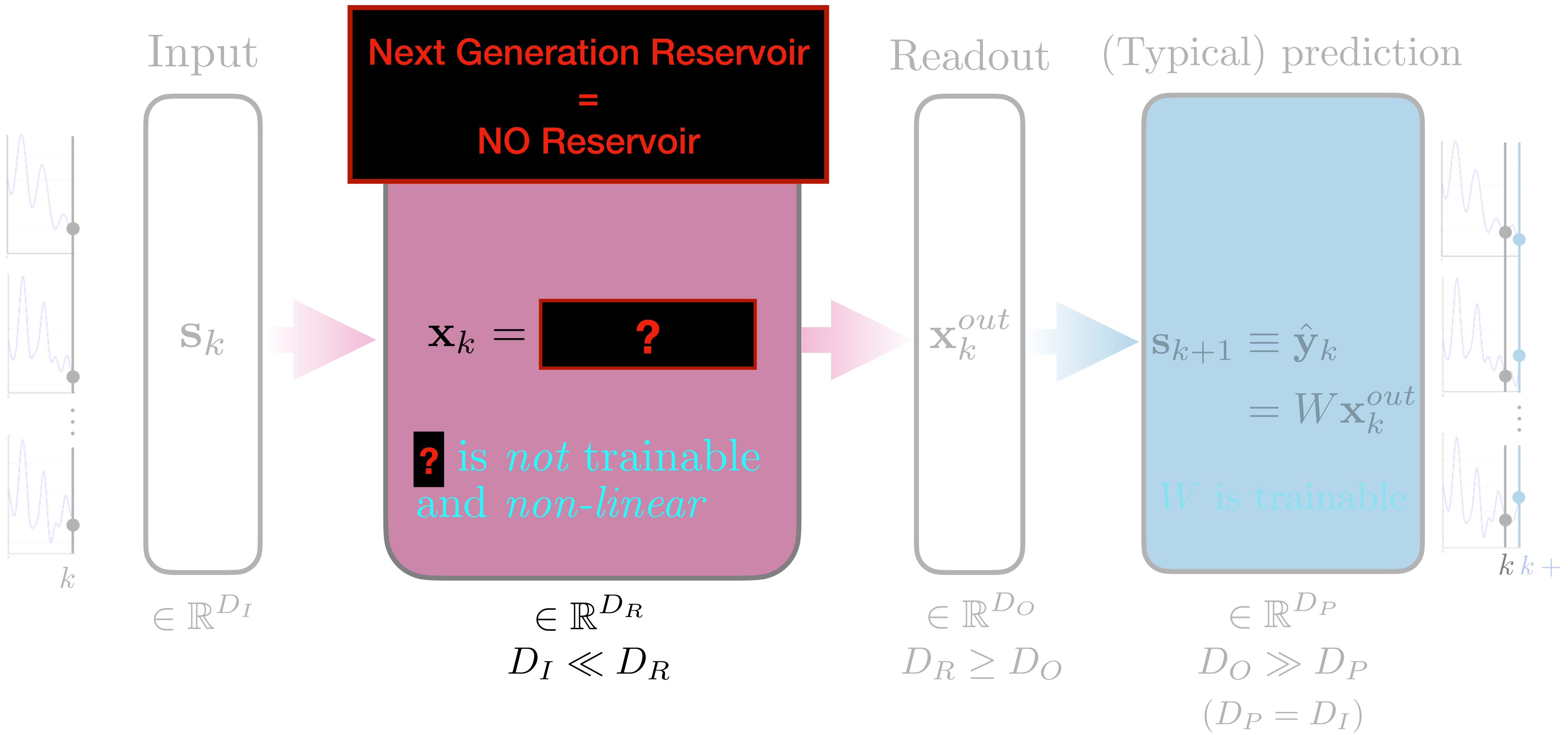
K. Fujii, K. Navajoma Quantum Reservoir Computing: A Reservoir Approach Toward Quantum Machine Learning Near-Term Devices, *Reservoir Computing* 423-450, 2021

Reservoir Computing (RC) in a nutshell



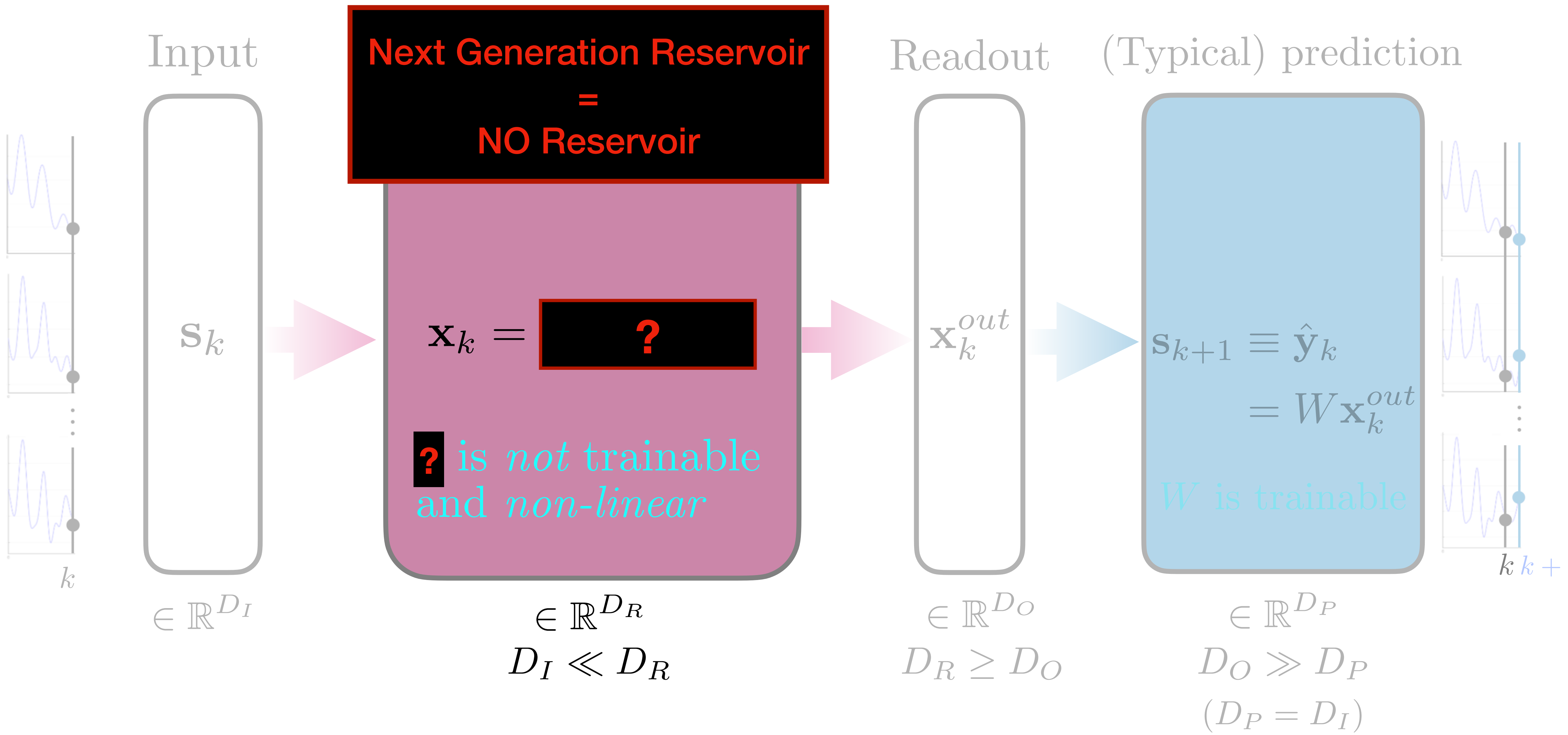
! No clear strategy on how to initialize different types of reservoir !

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



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

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



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

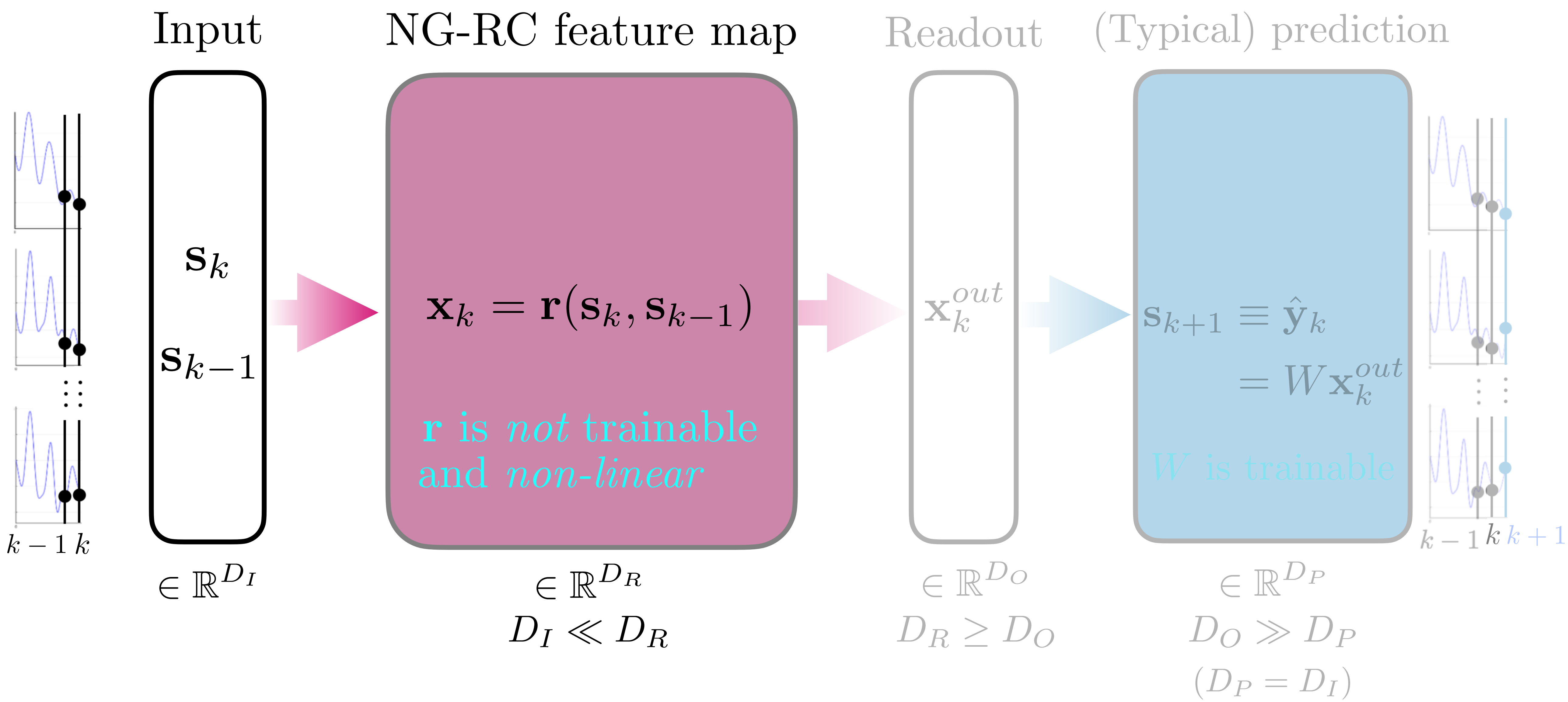
$$\boldsymbol{o}_k = \mathbf{s}_k \oplus \mathbf{s}_{k-\Delta} \oplus \mathbf{s}_{k-2\Delta} \oplus \ldots \oplus \mathbf{s}_{k-(m-1)\Delta}$$

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

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

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

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

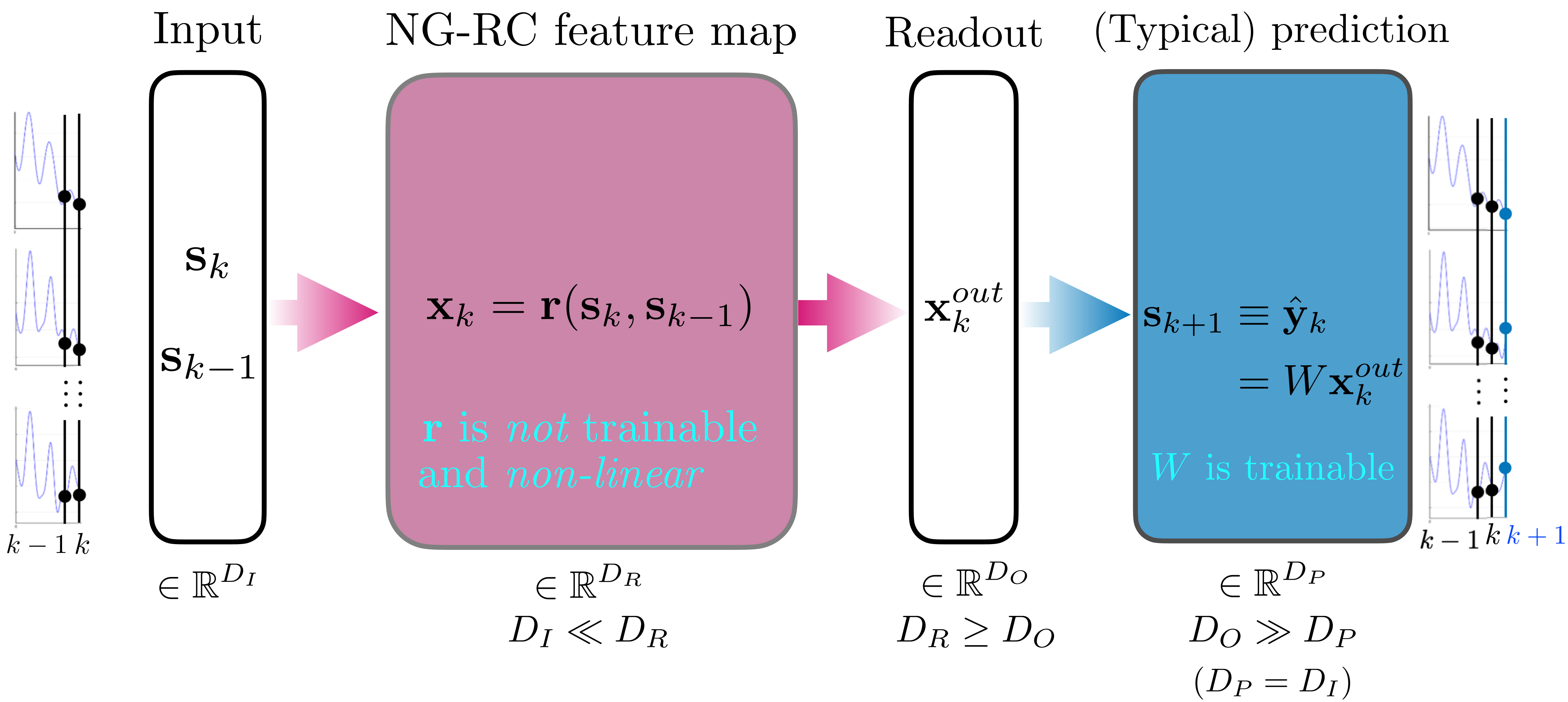


For example $\Delta = 1, m = 2, p = 2$

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

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

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



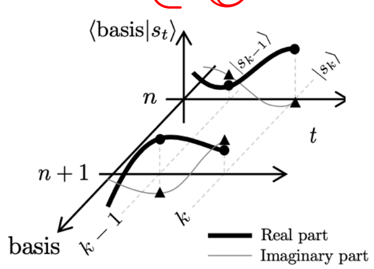
Training $$W = YX^\dagger(XX^\dagger + \lambda I)^{-1}$$

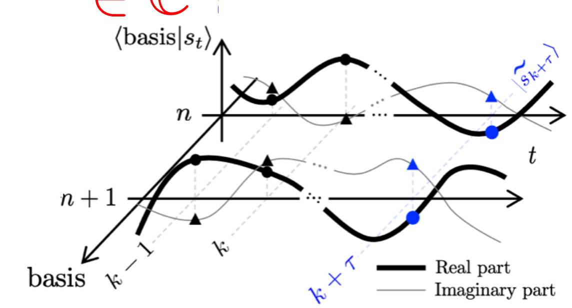
Typical prediction $$\mathbf{s}'_{k+1} = W\mathbf{x}_k = W\mathbf{r}(\mathbf{s}'_k, \mathbf{s}'_{k-1}) \qquad (\mathbf{x}_k^{out} = \mathbf{x}_k)$$

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

NG-RC for forecasting quantum dynamics

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

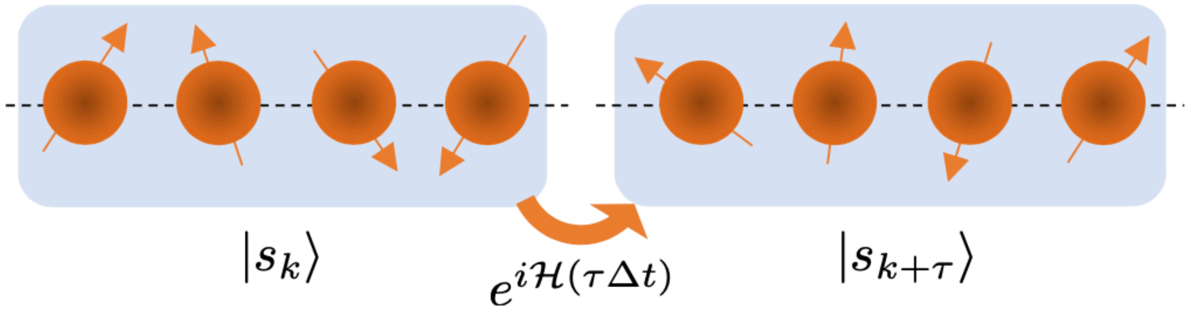
$$W = YX^{\dagger}(XX^{\dagger} + \lambda I)^{-1}$$

Skipping-ahead prediction

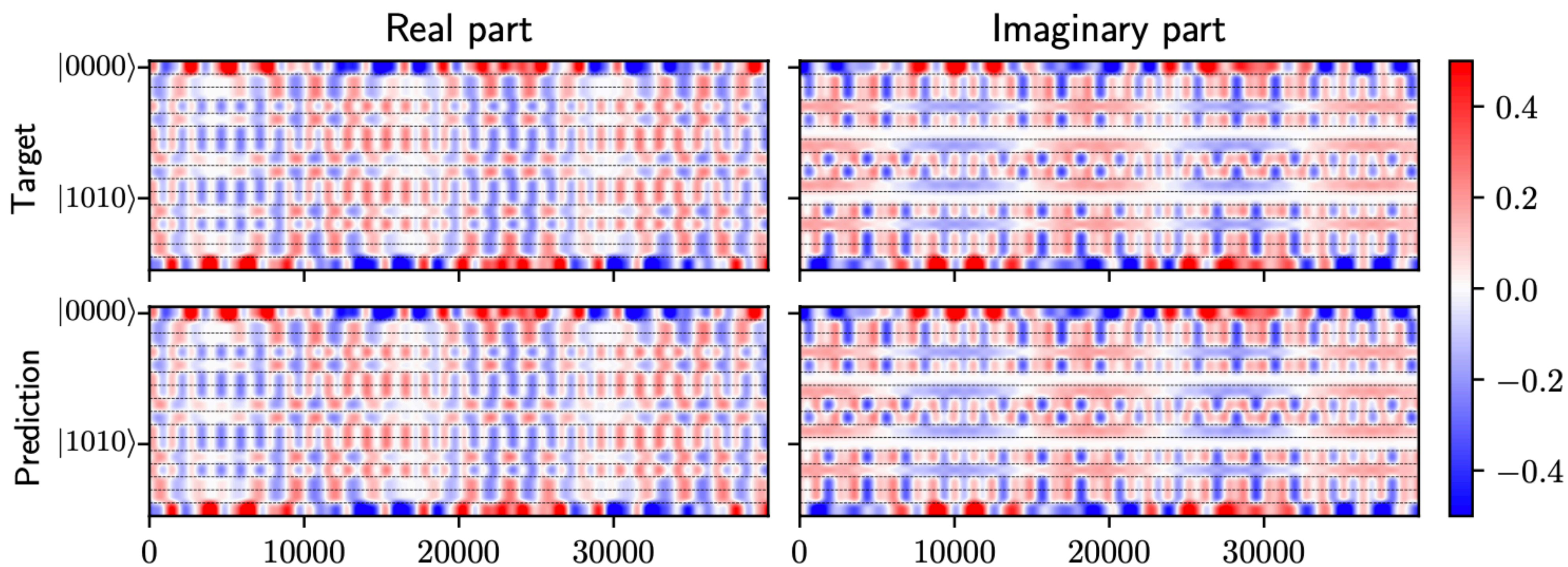
$$\mathbf{s}'_{k+\tau} = W\mathbf{x}_k = W\mathbf{r}(\mathbf{s}'_k, \mathbf{s}'_{k-1})$$

NG-RC for forecasting integrable quantum dynamics

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

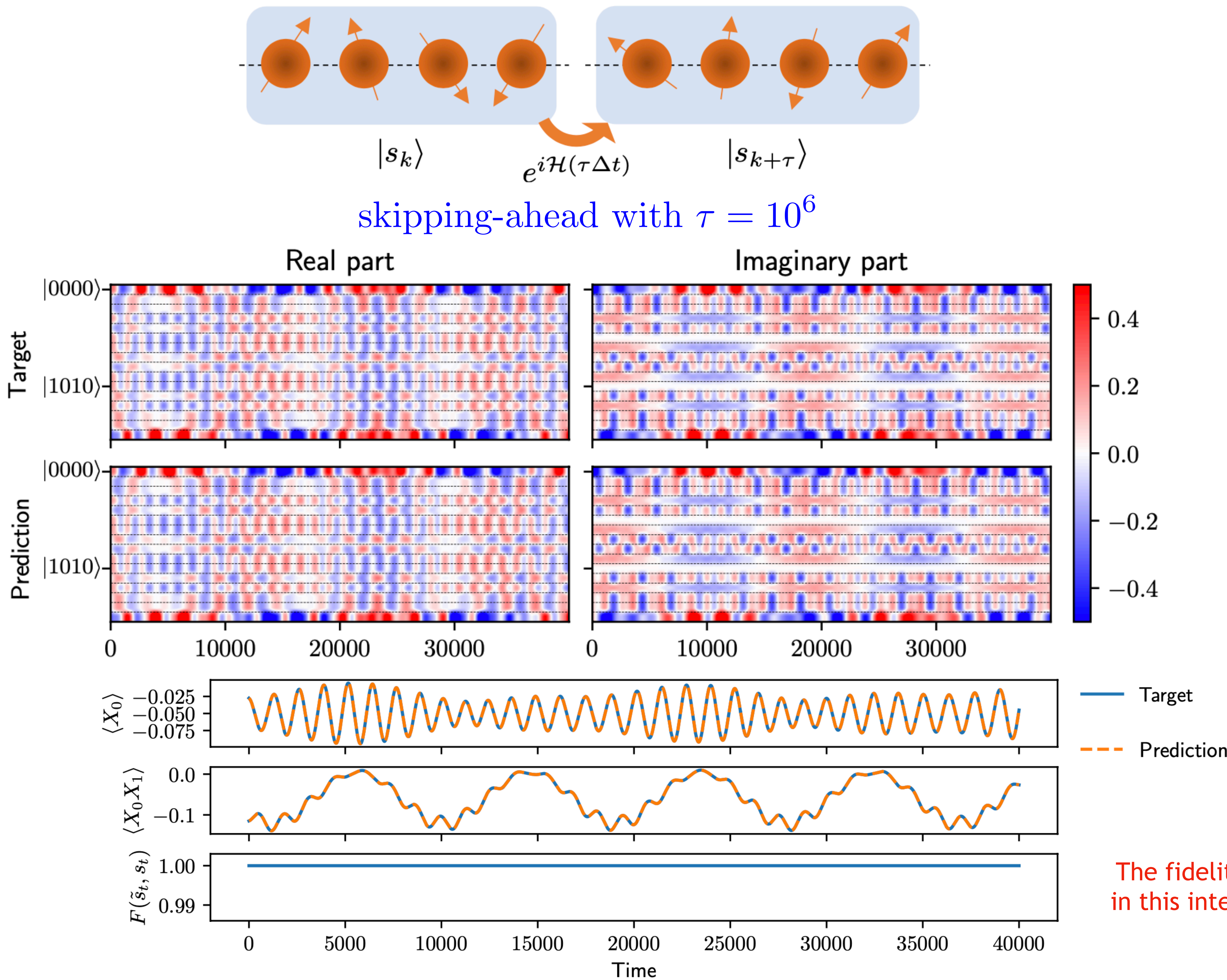


skipping-ahead with $\tau = 10^6$



NG-RC for forecasting integrable quantum dynamics

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



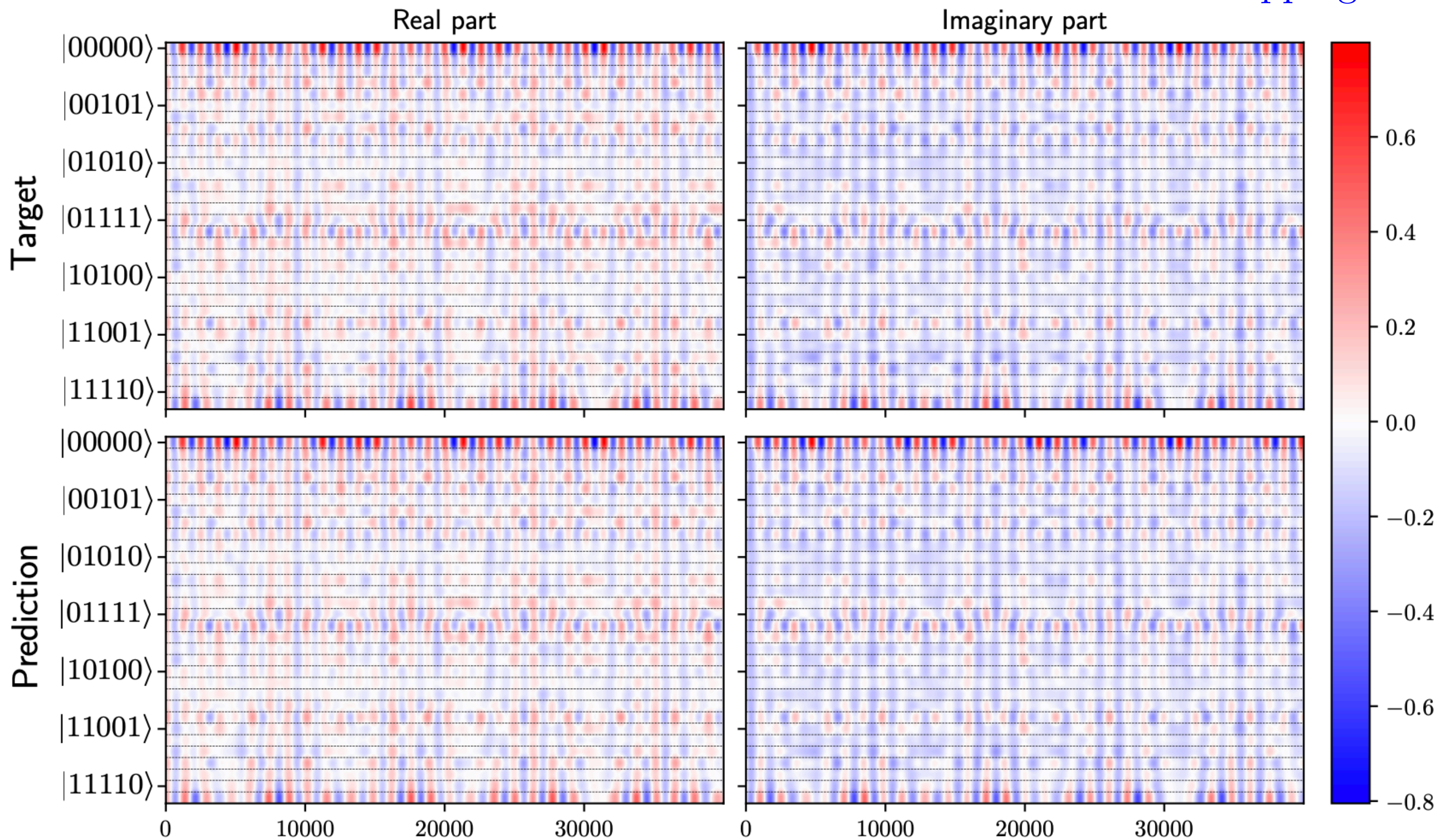
The fidelity is almost 1 in this integrable model

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 $\tau = 10^6$

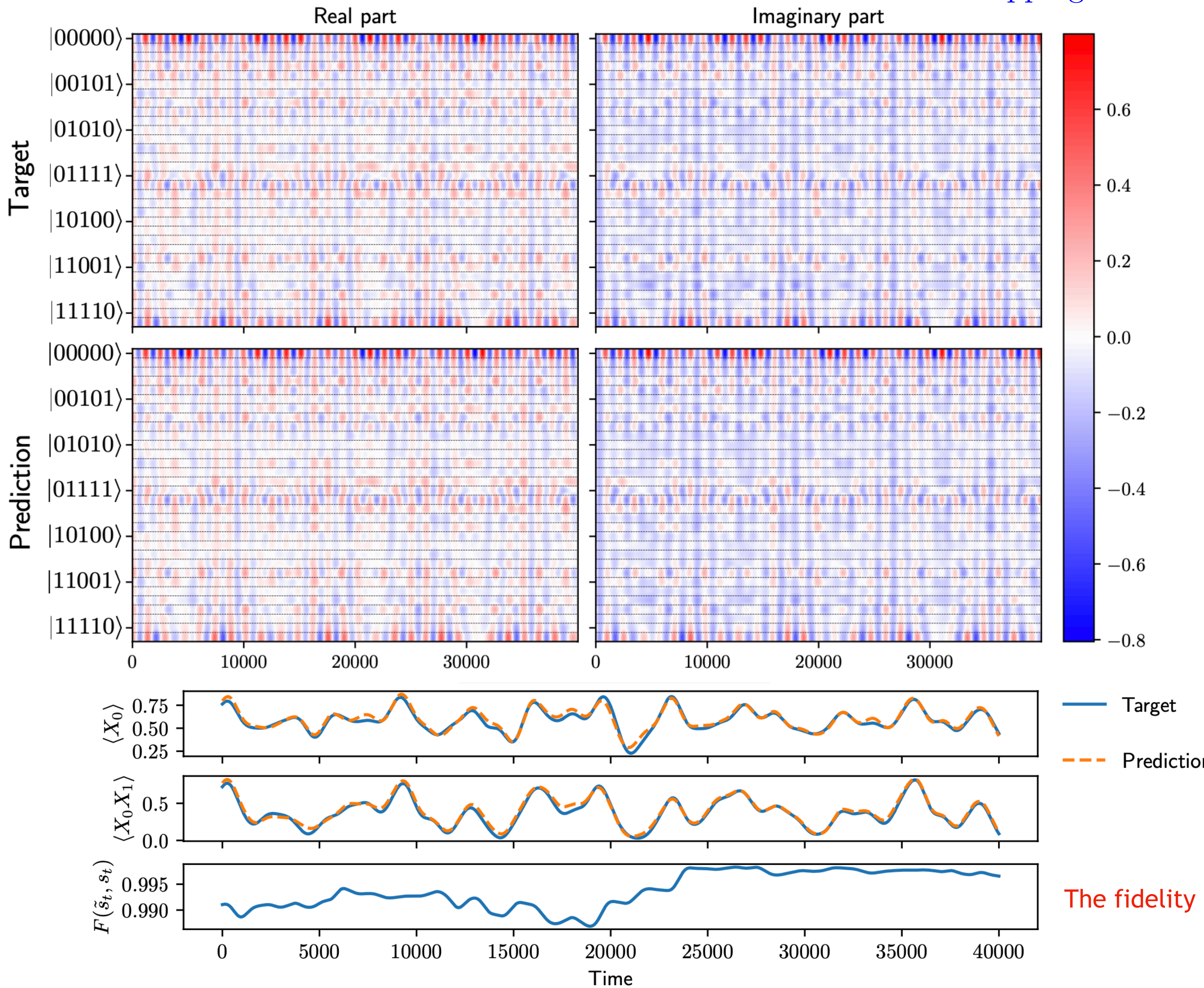


NG-RC for forecasting *chaotic* quantum dynamics

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

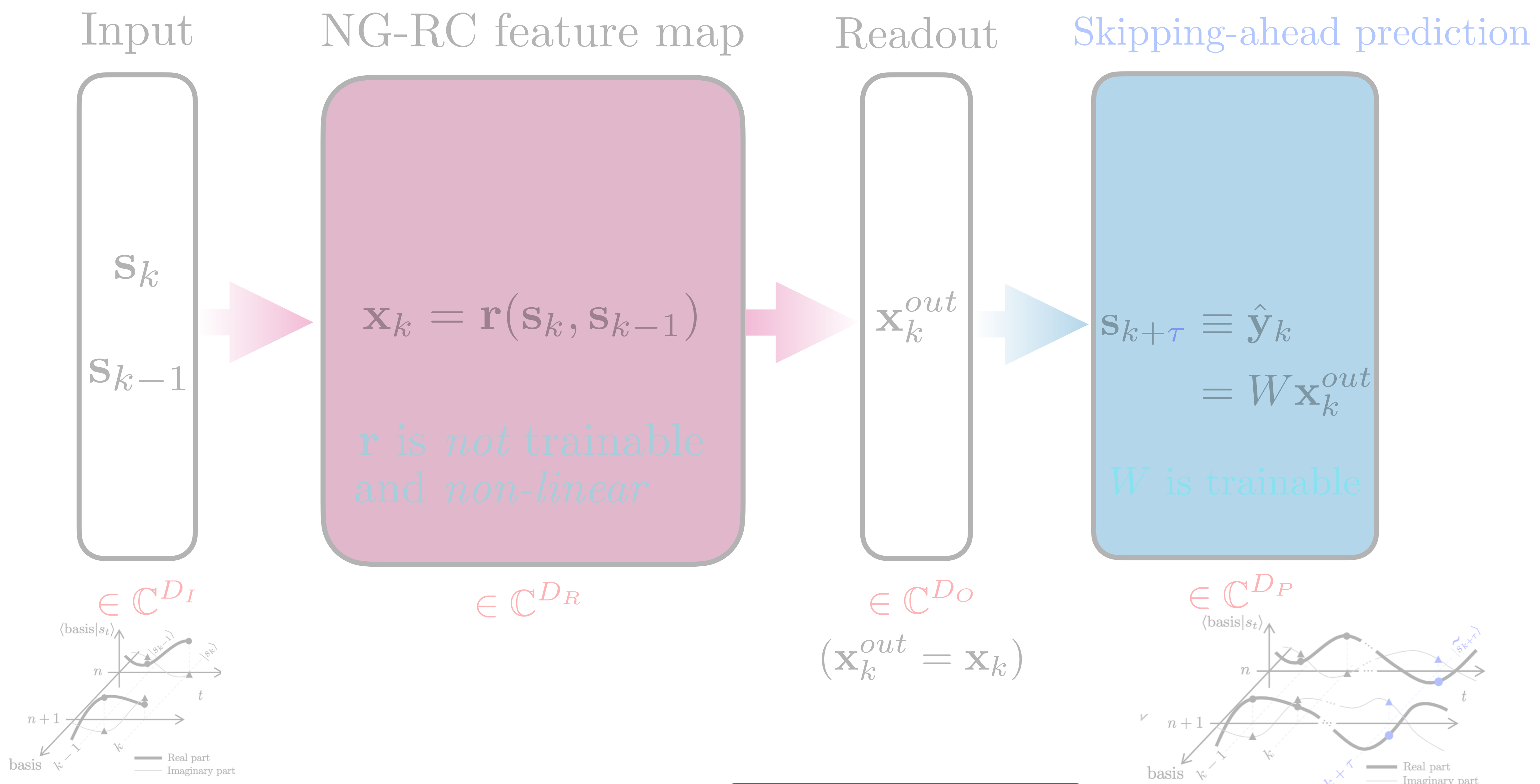
$d = 5, \theta = 15\pi/32$

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



The fidelity is above 0.99

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



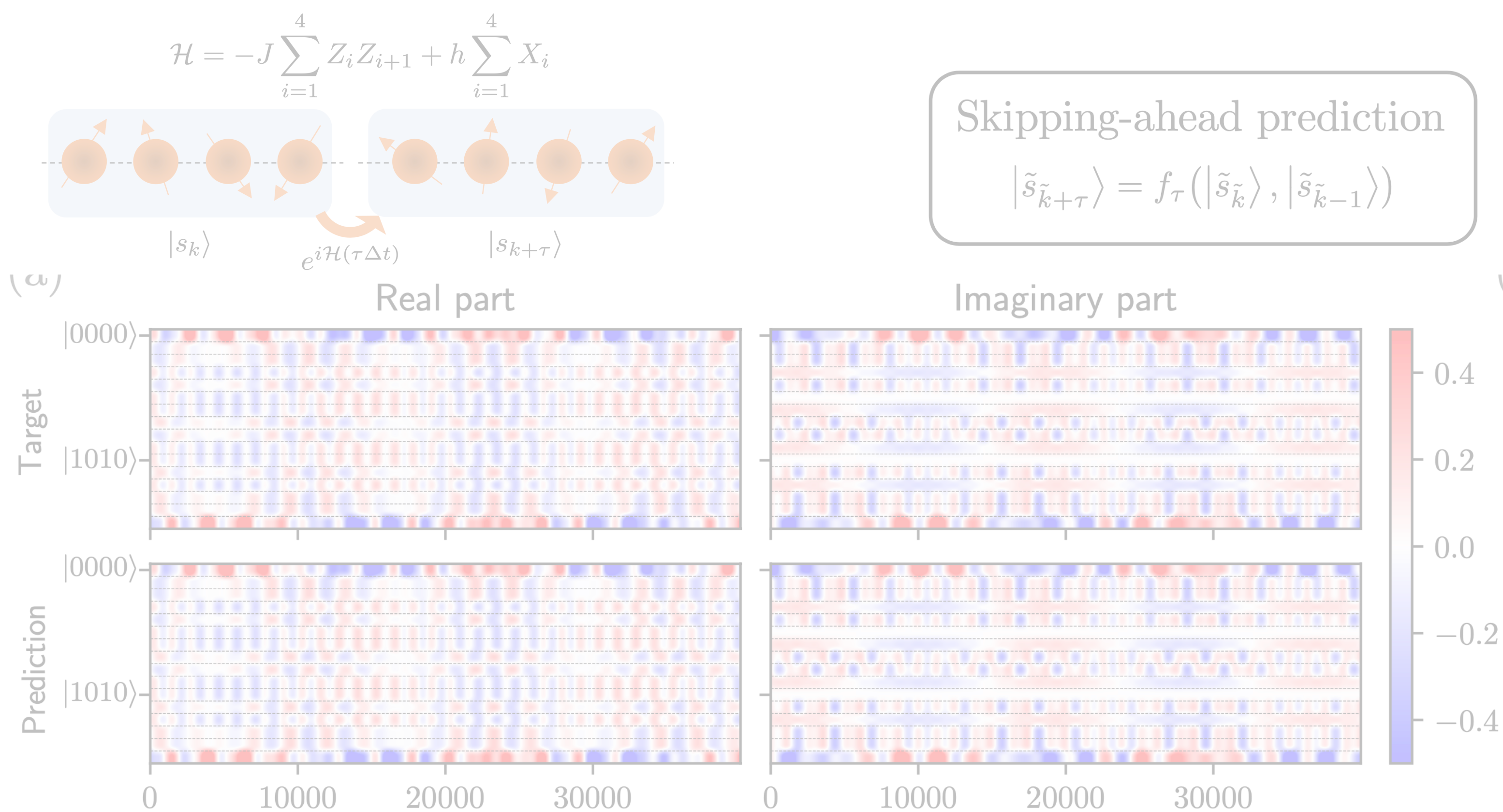
Training $$W = YX^{\dagger}\boxed{(XX^{\dagger} + \lambda I)^{-1}}$$ $O(2^{2d}T)$

Pseudoinverse Computation
d = # of qubits

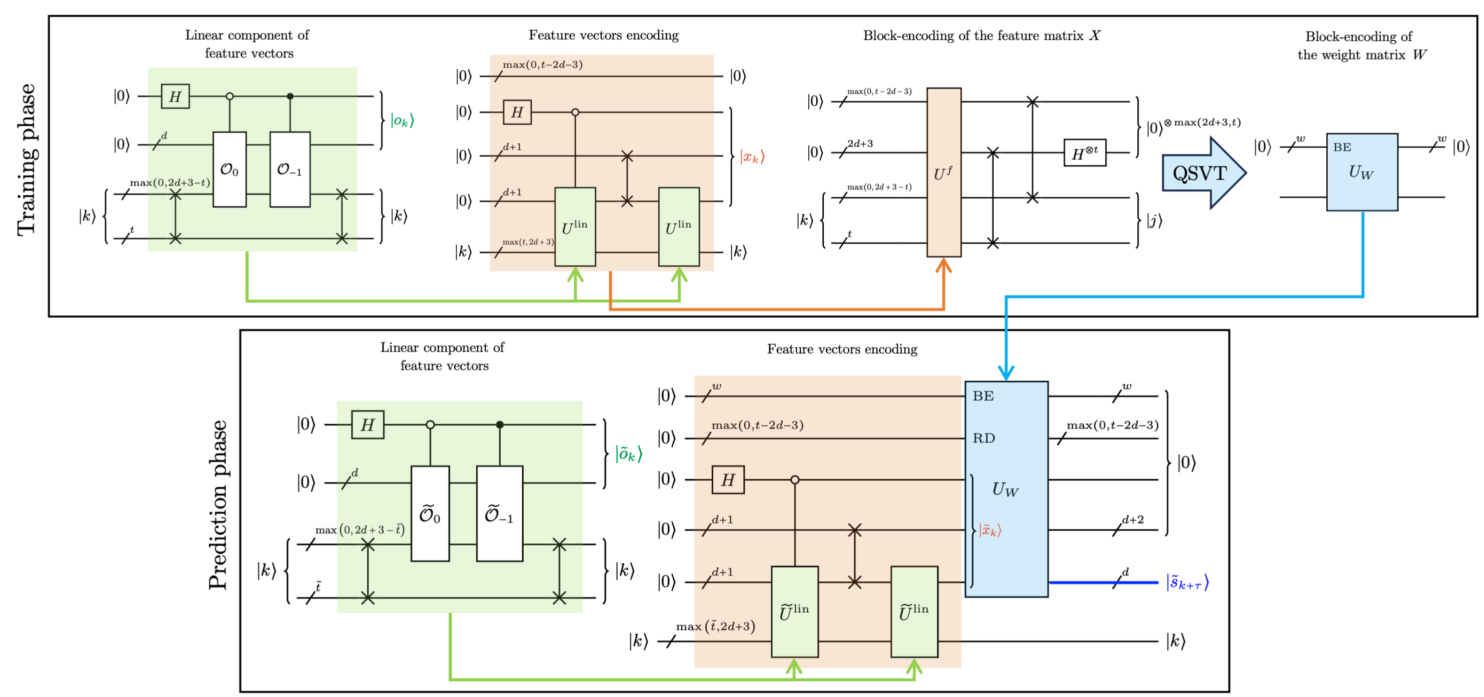
Skipping-ahead prediction $$\mathbf{s}'_{k+\tau} = W\mathbf{x}_k = W\mathbf{r}(\mathbf{s}'_k, \mathbf{s}'_{k-1})$$

Outline

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

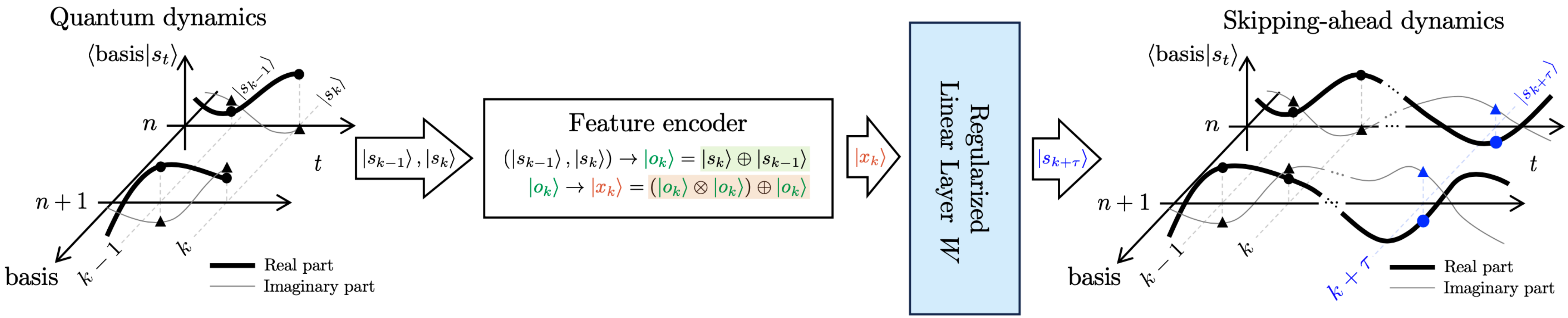


Part 2: Quantum Algorithm for NG-RC (QNG-RC)

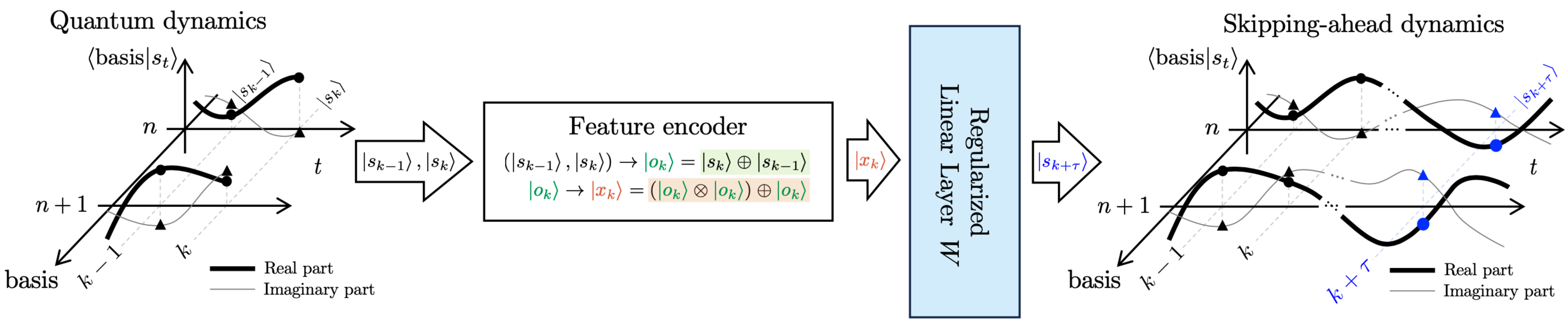


A. Sornsaeng, N. Dangniam, **T. Chotibut** arXiv: 2308.14239

Quantum Algorithm for NG-RC (QNG-RC)



Quantum Algorithm for NG-RC (QNG-RC)



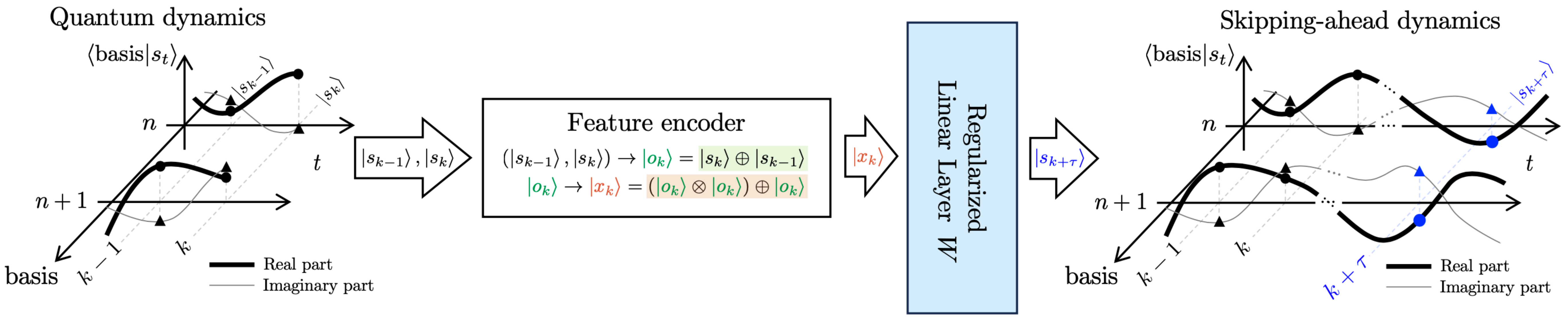
Training

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

Skipping-ahead prediction

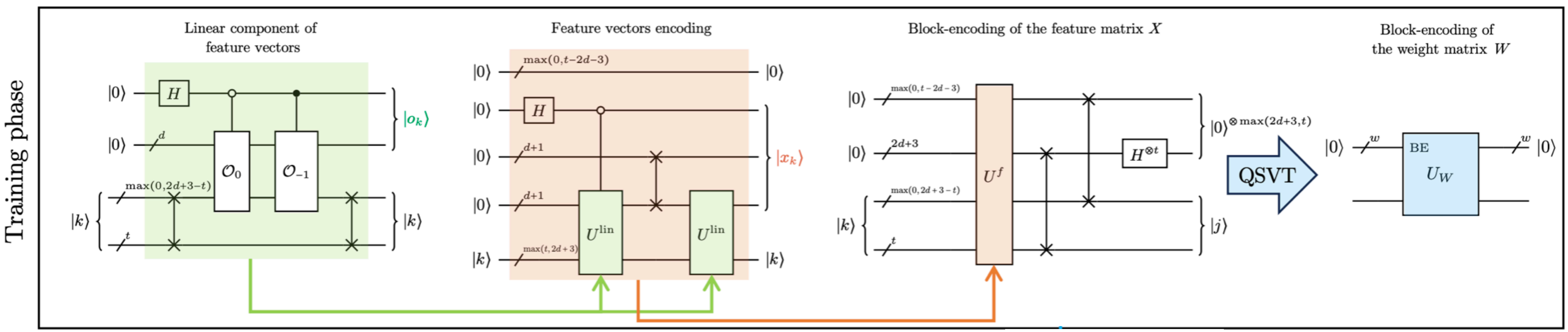
$$|s'_{k+\tau}\rangle = W |x_k\rangle = W \mathbf{r} \left(|s'_k\rangle, |s'_{k-1}\rangle \right)$$

Quantum Algorithm for NG-RC (QNG-RC)

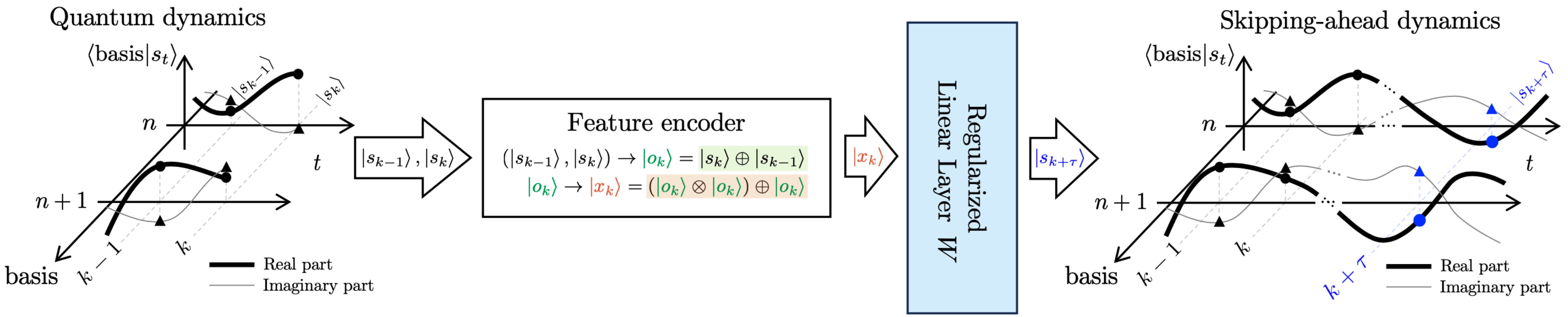


Training

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

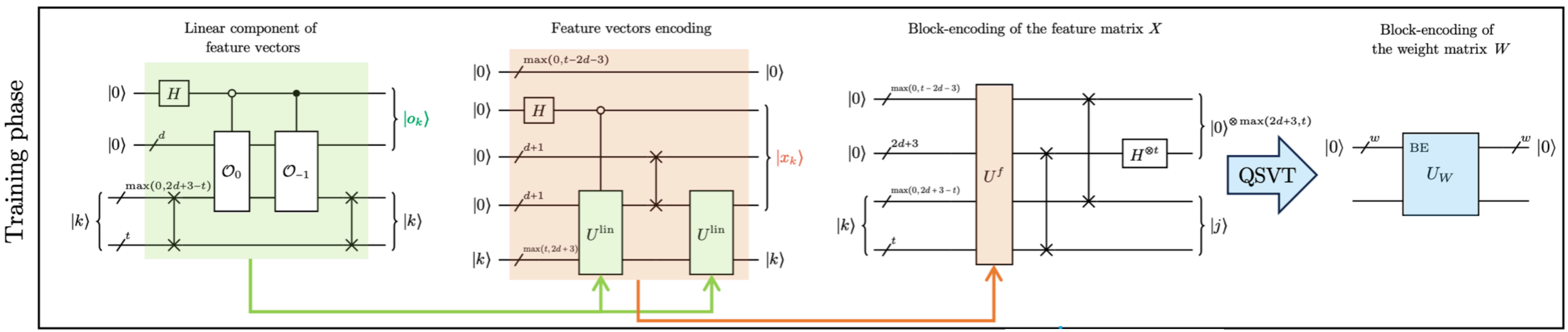


Quantum Algorithm for NG-RC (QNG-RC)



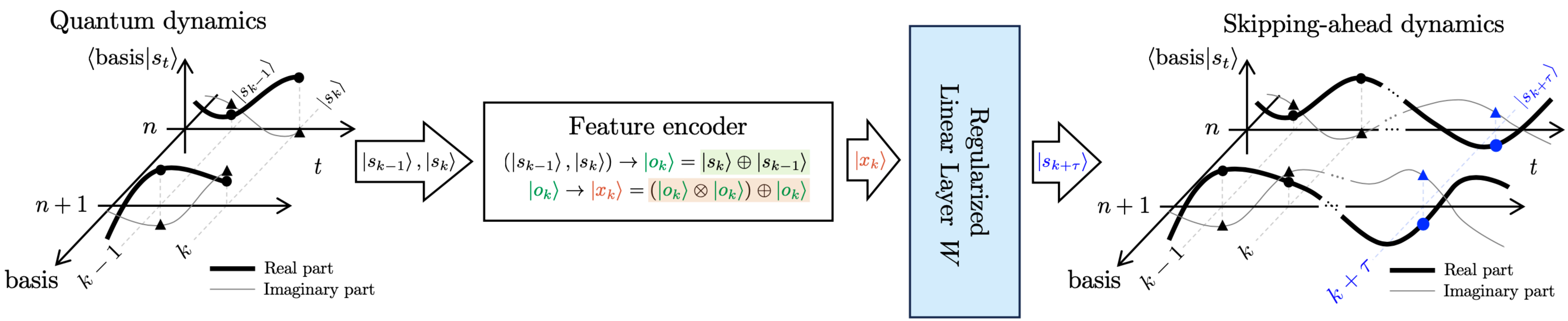
Training

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



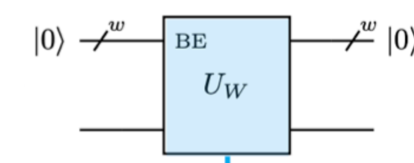
Theorem Given the block-encoded feature matrix X and target matrix Y, constructed in time T_O , and κ being a condition number of the Tikhonov-regularized feature matrix $\begin{pmatrix} X & \sqrt{\lambda} I \\ 0 & 0 \end{pmatrix}$, then the block-encoding of W, with error $\delta_W \in (0,1)$, can be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

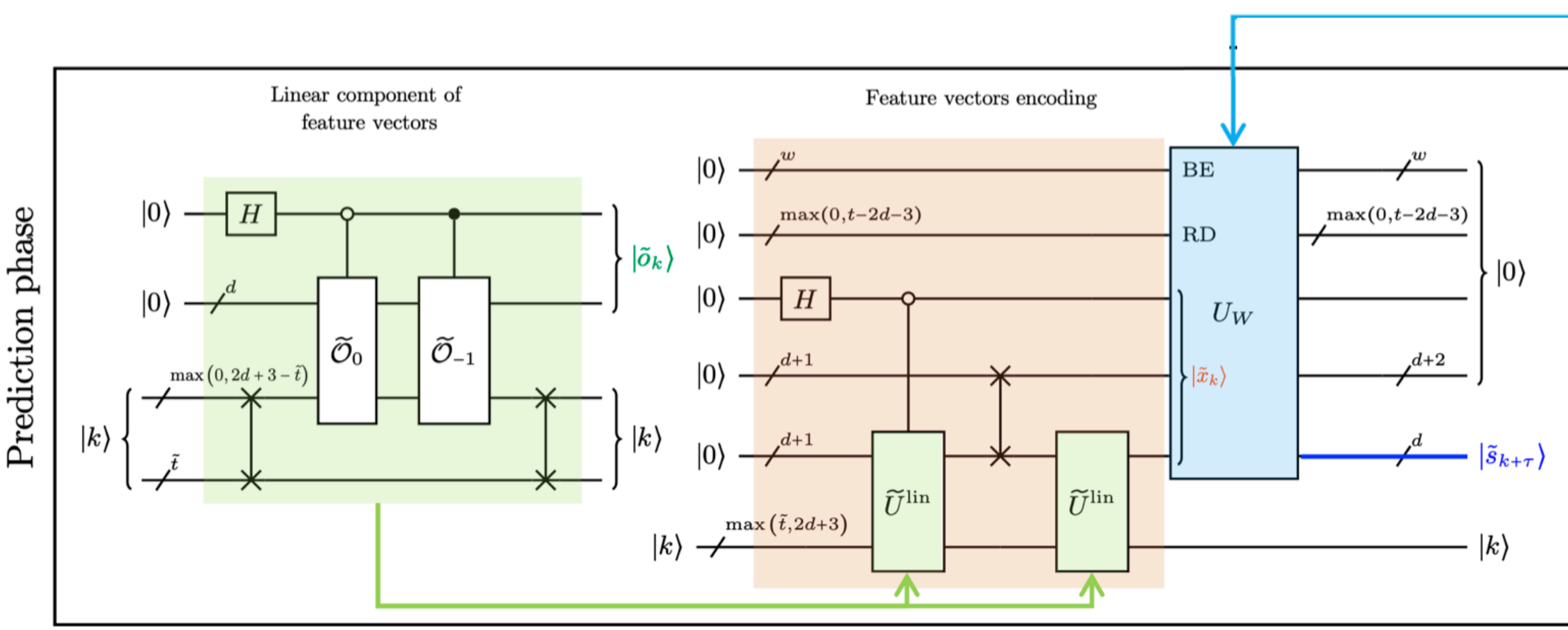
Quantum Algorithm for NG-RC (QNG-RC)



Skipping-ahead prediction

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





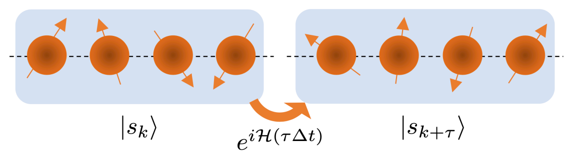
requires

$O(d)$ # of qubits

Summary

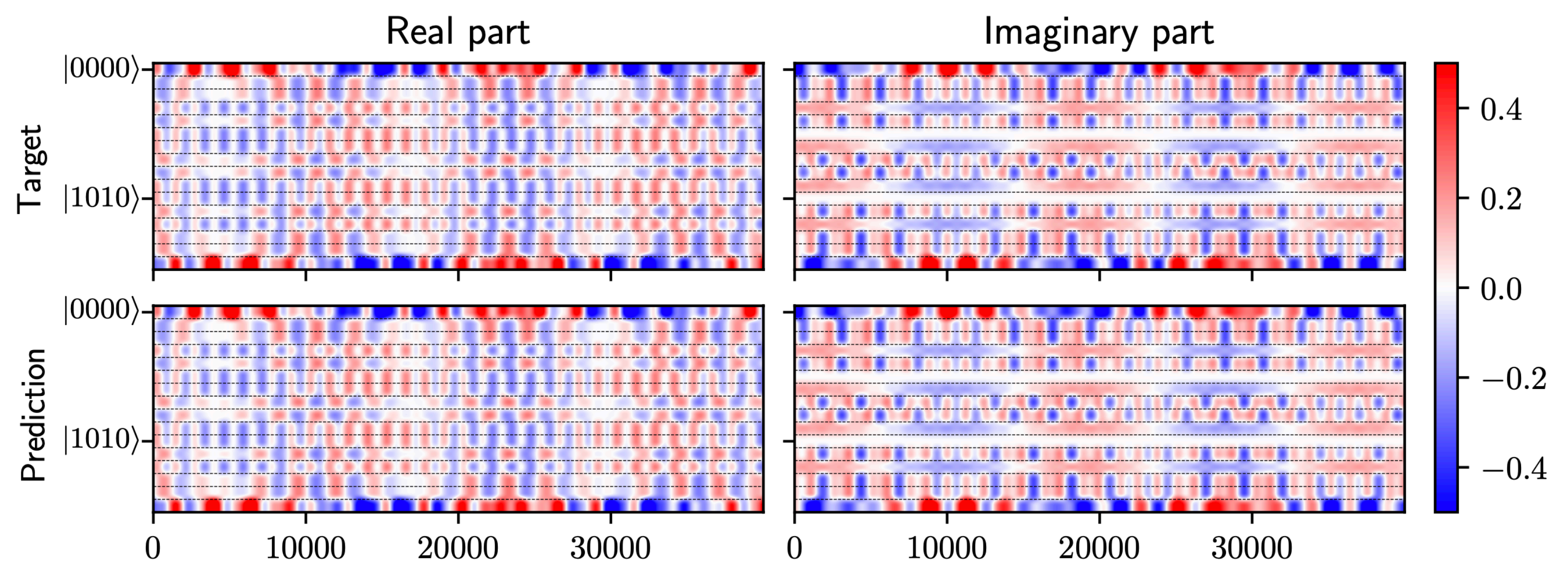
1. NG-RC can be applied to forecast *full* many-body dynamics far into the future, but with the time cost that scales as $O\left(2^{2d}\right)$

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

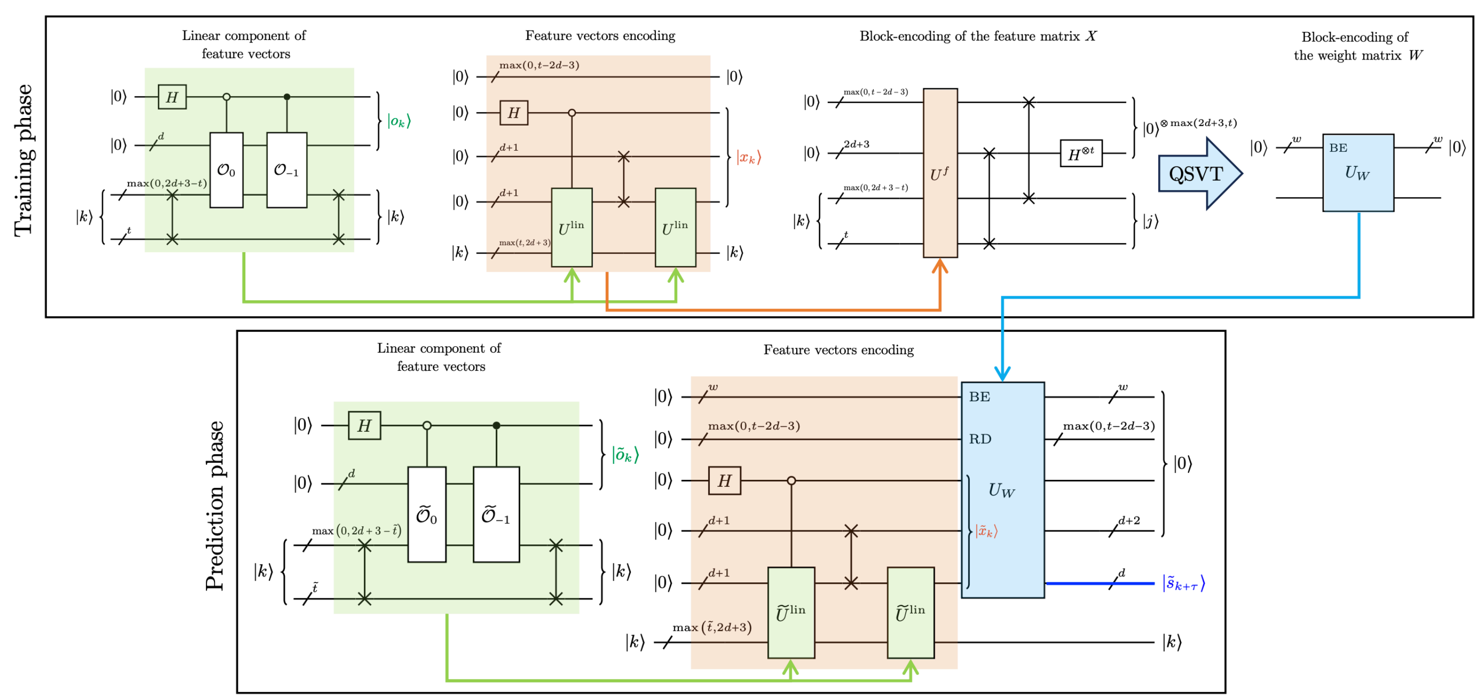


Skipping-ahead prediction

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



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

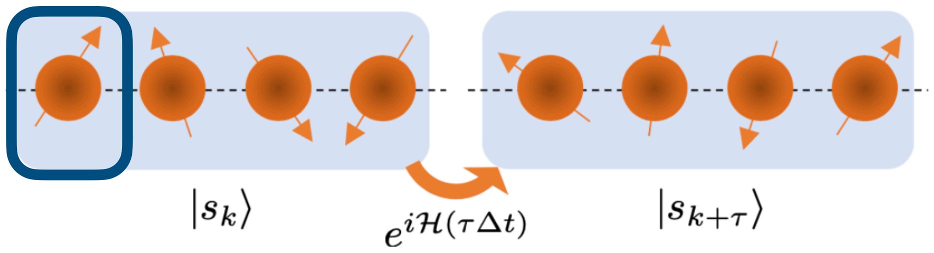


A. Sornsaeng, N. Dangniam, **T. Chotibut** arXiv: 2308.14239

Question Inspired by Experiments:

Can we measure *one* observable dynamics and reconstruct ALL the observables dynamics?

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



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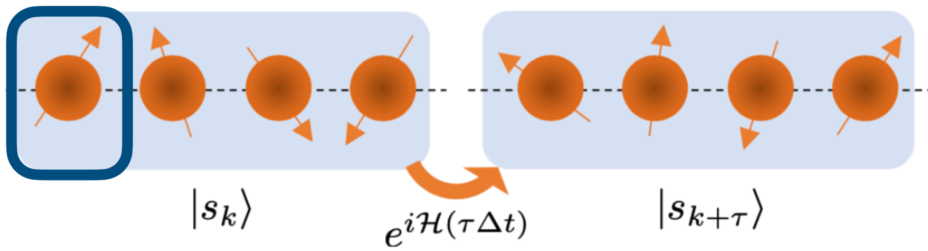
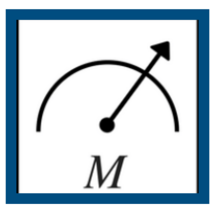
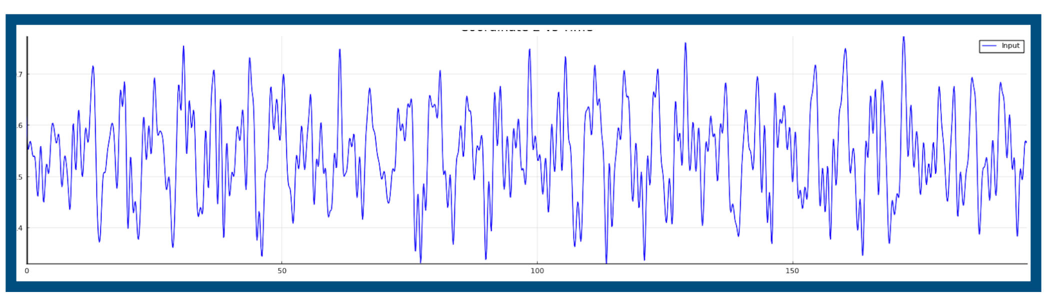




***Partial* observation of the past**

$\langle X_1 \rangle$



t

Question Inspired by Experiments:

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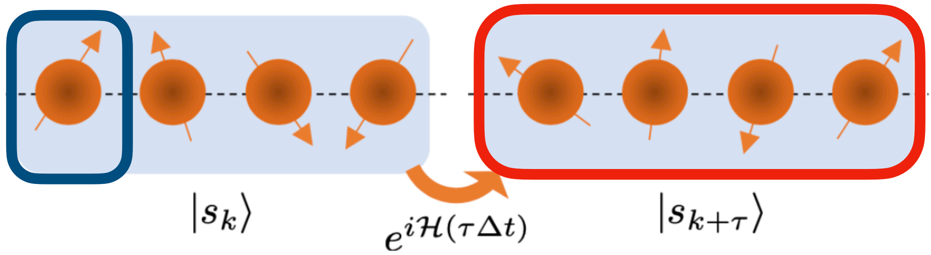

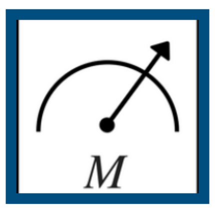

Partial **observation of the past**

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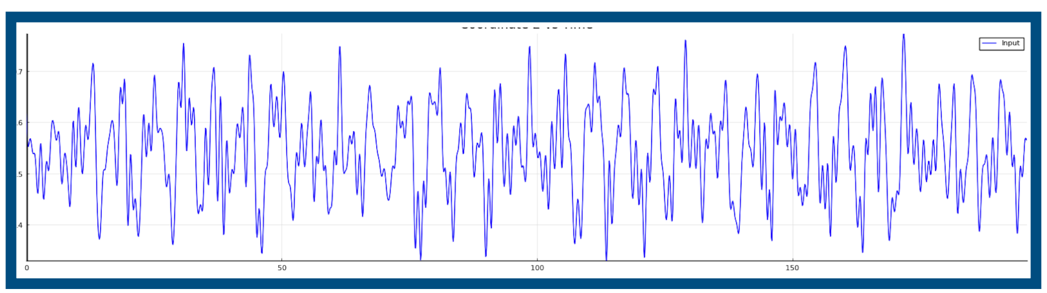

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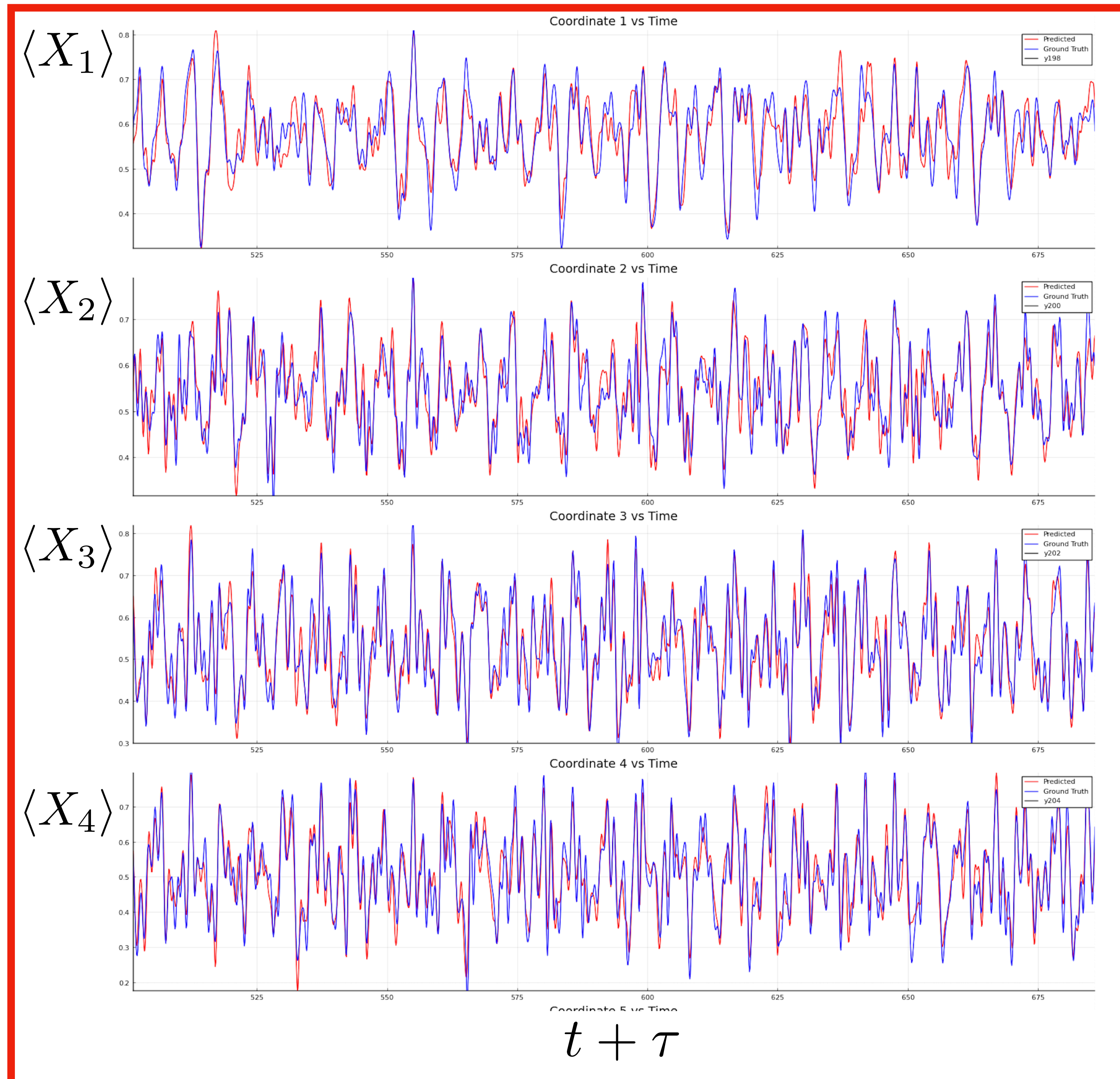
Reconstruction of *ALL* observables into the far future ($\tau = 10^6$)



Acknowledgement

Apimuk Sornsaeng

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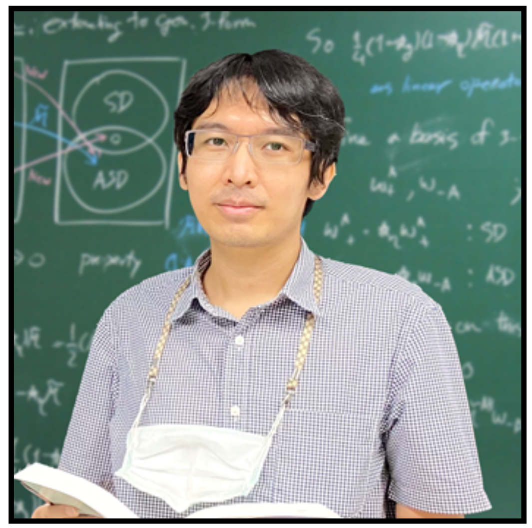
Ninnat Dangniam



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Thailand

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PMU-B

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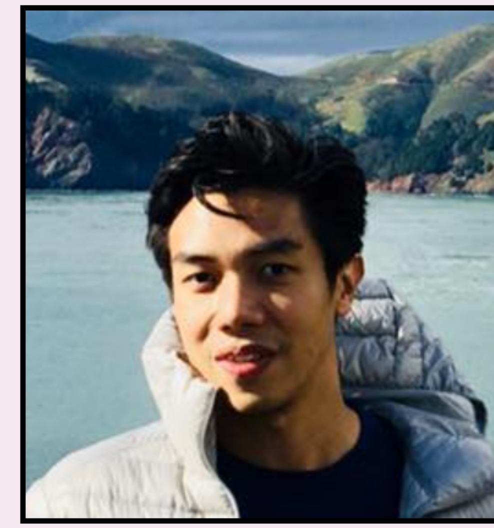

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Lab website: www.chics.ai

Benefits of Matrix Product States: Exponential Data Compression

$$|\Psi\rangle = \sum_{d_1,d_2,\ldots,d_N} c_{d_1,d_2,\ldots,d_N} |d_1 \; d_2 \ldots d_N\rangle$$

If the Hilbert space of each particle has dimension d, need to specific all d^N tensor coefficients.

However, for a gapped 1D systems, a useful ansatz is the MPS

$$|\tilde{\Psi}\rangle_{\mathrm{MPS}} \approx \sum_{\{\alpha\}} A_{d_1}^{\alpha_1} \ldots A_{d_i}^{\alpha_{i-1}\alpha_i} \ldots A_{d_N}^{\alpha_{N-1}} |d_1\rangle|d_2\rangle \ldots |d_N\rangle$$

α_i denotes the interaction with particle i with an effective dimension χ, called the *bond dimension*.

number of parameters d^N $N\chi^2 d$