

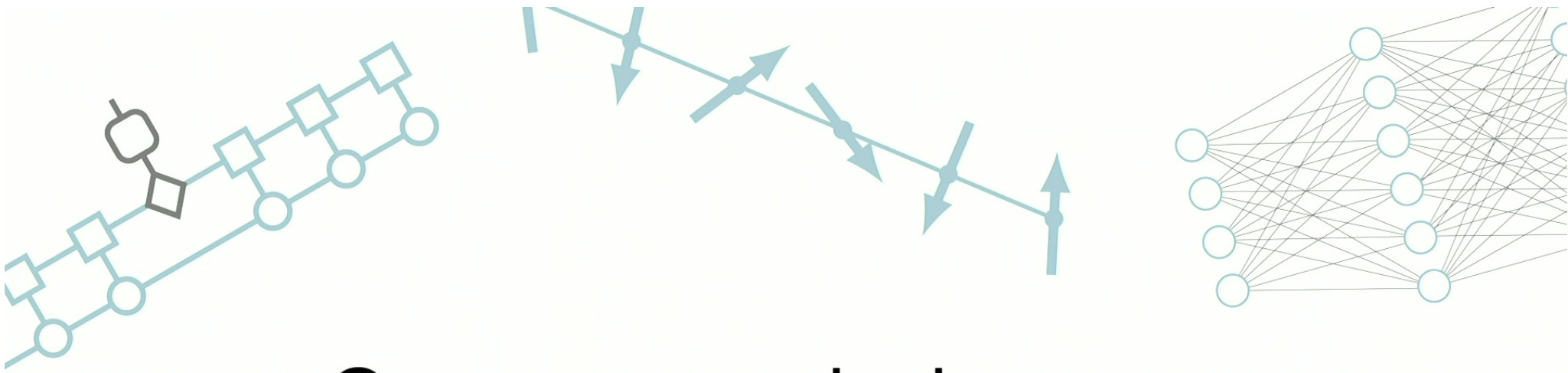
Title: Keynote

Speakers: Friederike Metz

Collection: PSI 15th Anniversary Reunion

Date: June 19, 2024 - 4:00 PM

URL: <https://pirsa.org/24060007>



Quantum many-body systems

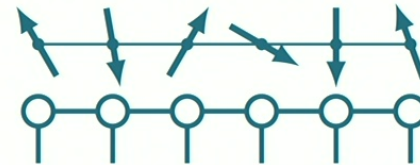
how to tame and control them

Friederike Metz @ EPFL - Switzerland

19.06.2024 — PSI 15th Anniversary Reunion

OUTLINE

- My academic journey
- My research interests
 - Computational quantum many-body physics
 - Quantum control & reinforcement learning
 - Efficient quantum many-body control using reinforcement learning



FM, M. Bukov, *Nature Machine Intelligence* **5**, 780-791 (2023)

MY JOURNEY



Standard Model of Elementary Particles

	three generations of matter (fermions)			interactions / force carriers (bosons)	
	I	II	III		
mass	$\approx 2.2 \text{ MeV}/c^2$	$\approx 1.28 \text{ GeV}/c^2$	$\approx 173.1 \text{ GeV}/c^2$	0	$\approx 125.11 \text{ GeV}/c^2$
charge	$\frac{2}{3}$	$\frac{2}{3}$	$\frac{2}{3}$	0	0
spin	$\frac{1}{2}$	$\frac{1}{2}$	$\frac{1}{2}$	1	0
	u up	c charm	t top	g gluon	H higgs
	d down	s strange	b bottom	γ photon	
	e electron	μ muon	τ tau	Z Z boson	
	ν_e electron neutrino	ν_μ muon neutrino	ν_τ tau neutrino	W W boson	

QUARKS
LEPTONS
GAUGE BOSONS
VECTOR BOSONS
SCALAR BOSONS

Image from Wikimedia

High school

— 2011

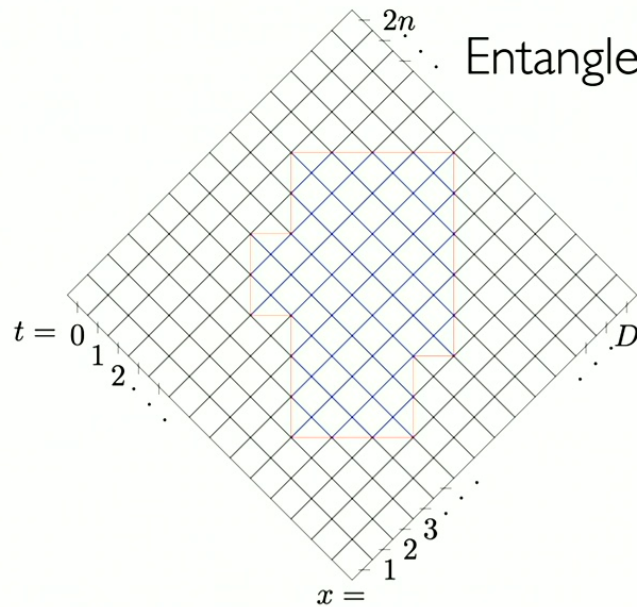
MY JOURNEY



Undergraduate

2011–2015

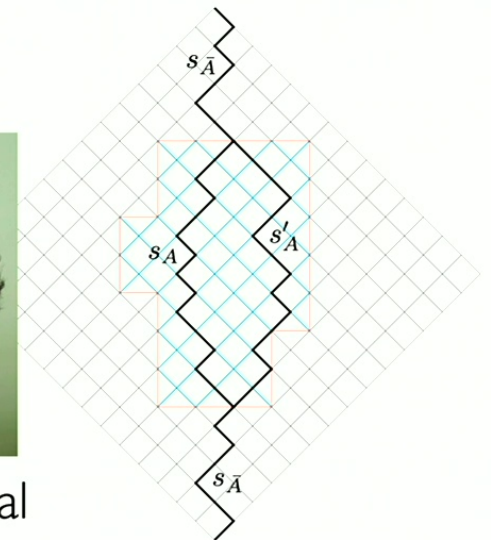
MY JOURNEY



Entanglement entropy of space-time regions



Barbara Terhal



Undergraduate

2011–2015

MY JOURNEY



“PSI is like trying to drink from a firehose.”



Image from DALL-E

PSI Program

2015–2016

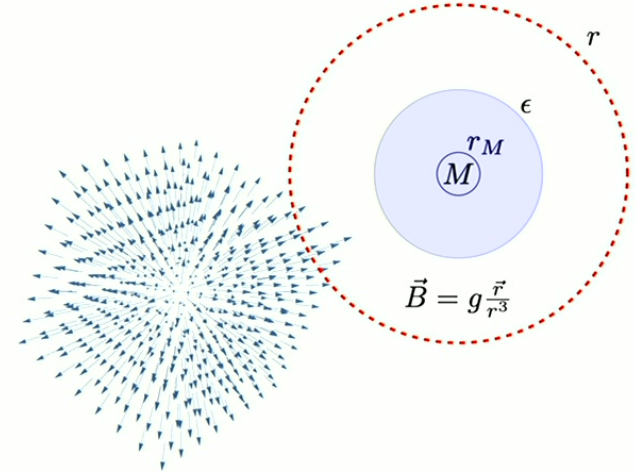
MY JOURNEY



Effective Theory of Monopole
- Fermion Scattering



Cliff Burgess



PSI Program

2015–2016

MY JOURNEY



Studying \neq Doing research

PSI Program

2015–2016

MY JOURNEY



PhD

2017–2023



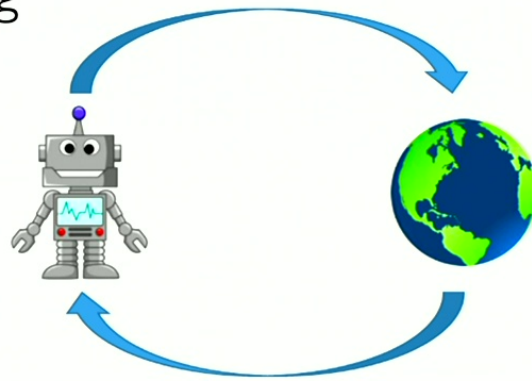
Okinawa Institute of
Science and Technology

MY JOURNEY

Reinforcement learning



D. Silver et al. Nature 529, 484 (2016)



OIST

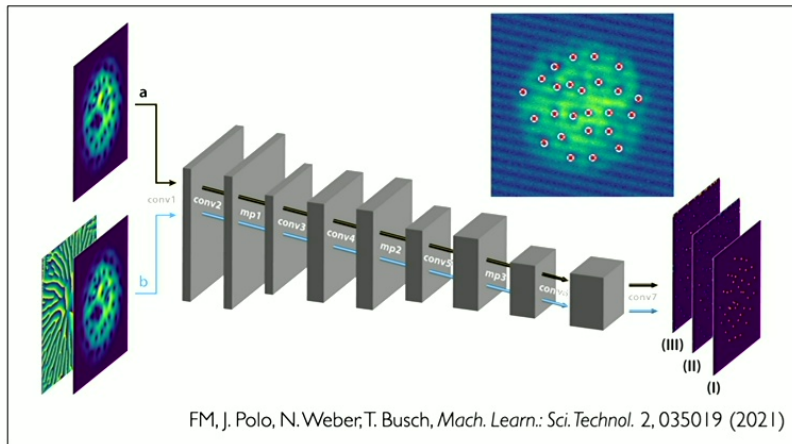
Okinawa Institute of
Science and Technology

PhD

2017–2023

MY JOURNEY

Machine learning applications to study and control quantum systems



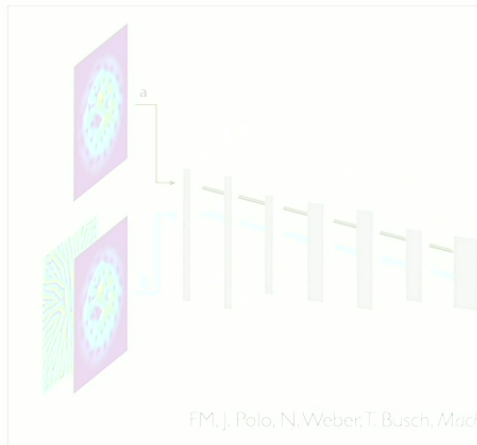
Deep-learning based vortex detection in rotating BECs

PhD

2017–2023

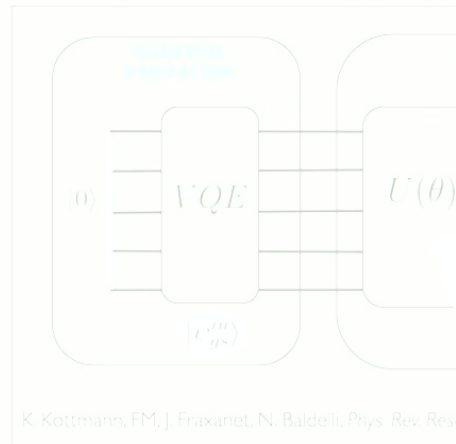
MY JOURNEY

Machine learning applications to study and control quantum systems

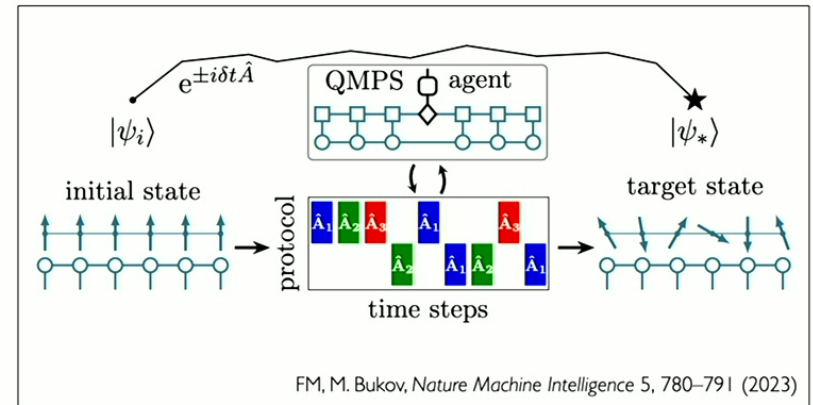


Deep-learning based detection in rotational systems

Variational quantum algorithms
Unsupervised mapping



Quantum many-body control using reinforcement learning with tensor networks

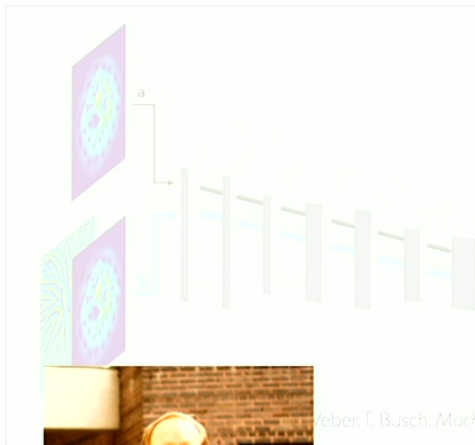


PhD

2017–2023

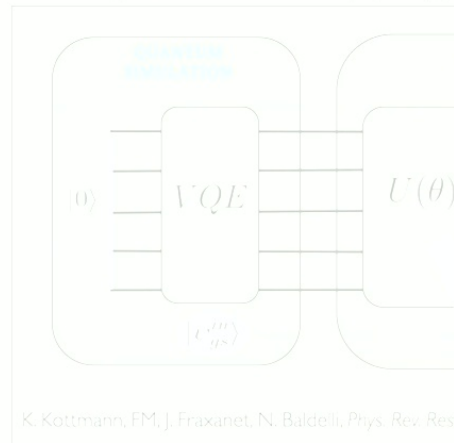
MY JOURNEY

Machine learning applications to study and control quantum systems

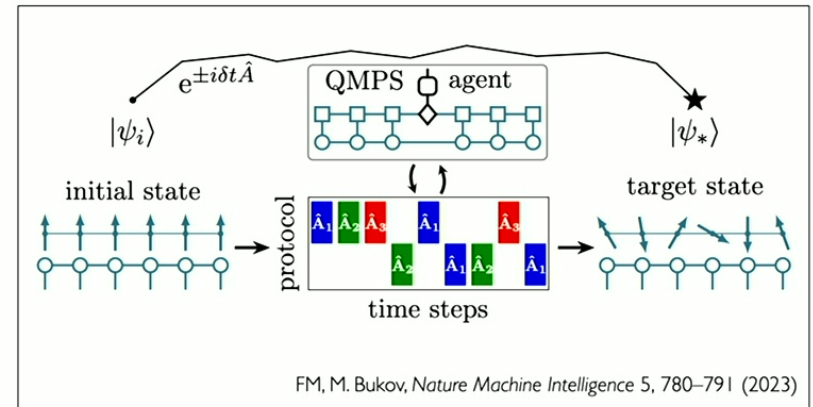


Thomas Busch

Variational quantum ar
Unsupervised mapping



Quantum many-body control using
reinforcement learning with tensor networks



PhD

2017-2023

MY JOURNEY



Max Planck Institute for the
Physics of Complex Systems

Visiting researcher

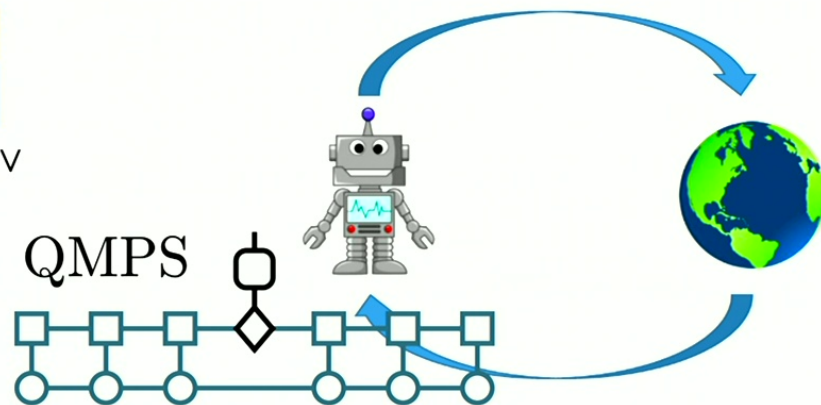
2022

MY JOURNEY



Marin Bukov

Quantum many-body control & reinforcement learning



Max Planck Institute for the
Physics of Complex Systems

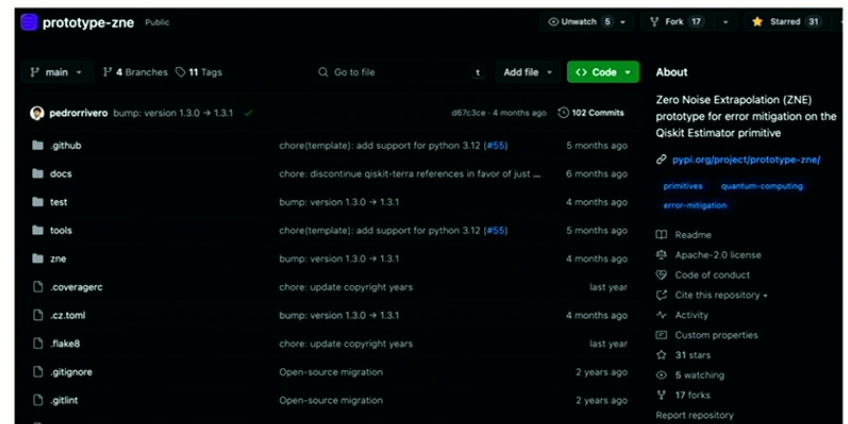
Visiting researcher

2022

MY JOURNEY



Quantum software development



Internship

2022

BIG PICTURE

Quantum chemistry

- Better catalysts
- New drugs
- More efficient batteries
- Carbon capture & storage

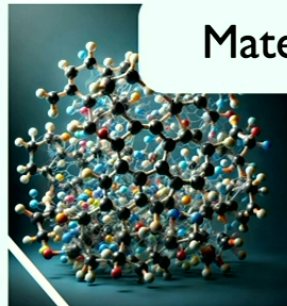
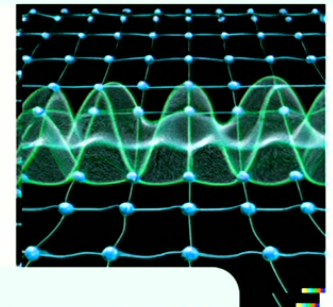


Image from DALL-E

Materials science

Condensed matter physics

- High temperature superconductivity
- Topologically ordered states
- Quantum spin liquids
- Exotic states of matter



DALL-E

Quantum physics

Atomic, molecular, and optical physics

Quantum information



More is different. -
Philip W. Anderson

BIG PICTURE

Quantum chemistry

- Better catalysts
- New drugs
- More efficient batteries
- Carbon capture & storage

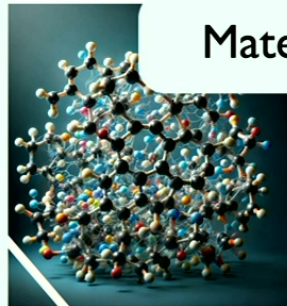
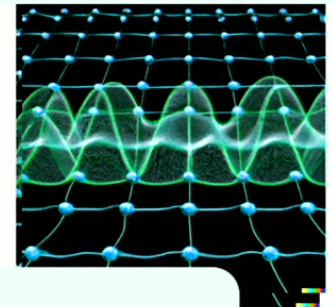


Image from DALL-E

Materials science

Condensed matter physics

- High temperature superconductivity
- Topologically ordered states
- Quantum spin liquids
- Exotic states of matter



DALL-E

Quantum many-body physics

Atomic, molecular, and optical physics

Quantum information



More is different. -
Philip W. Anderson

CURSE OF DIMENSIONALITY

Hilbert space dimension grows exponentially in system size!

N Spin-1/2 particles:

$$|\sigma\rangle = \left| \begin{array}{cccccccc} \uparrow & \downarrow & \downarrow & \uparrow & \downarrow & \uparrow & \uparrow & \downarrow \\ 0 & 1 & 1 & 0 & 1 & 0 & 0 & 1 \end{array} \right\rangle$$

2^N dimensional



$$|\Psi\rangle = \Psi_1|00\dots 0\rangle + \Psi_2|10\dots 0\rangle + \Psi_3|01\dots 0\rangle + \dots + \Psi_{2^N}|11\dots 1\rangle = \sum_{\sigma} \Psi_{\sigma}|\sigma\rangle$$

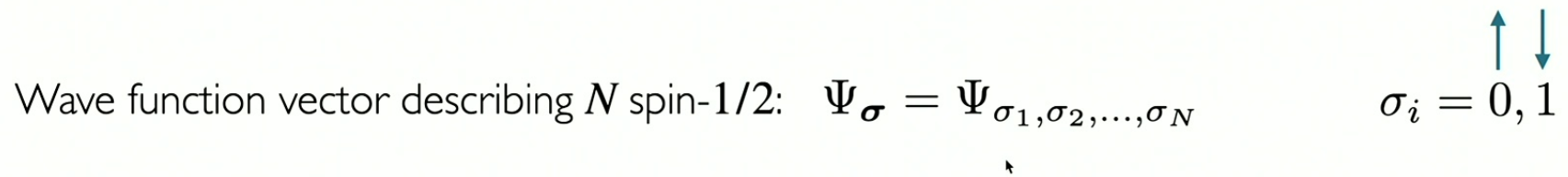


1 Petabyte: $10^{15} \sim 2^{50}$

TENSOR NETWORKS

Compressed representations/approximations of exponentially large quantum states

Wave function vector describing N spin-1/2: $\Psi_{\sigma} = \Psi_{\sigma_1, \sigma_2, \dots, \sigma_N}$ $\sigma_i = 0, 1$



TENSOR NETWORKS




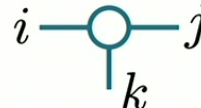
Compressed representations/approximations of exponentially large quantum states

Tensor diagrams 101 Roger Penrose 1971

Tensor with N indices = Shape with N legs

$$\Psi_{\sigma_1, \sigma_2, \dots, \sigma_N} = \text{Diagram of a horizontal bar with } N \text{ legs labeled } \sigma_1, \sigma_2, \dots, \sigma_N \text{ and } \Psi \text{ above it.}$$

Important examples:

			
S	V_i	M_{ij}	T_{ijk}


J. C. Bridgeman, C. T. Chubb, J. Phys. A: Math. Theor. 50 223001 (2017)


TENSOR NETWORKS

Compressed representations/approximations of exponentially large quantum states


Tensor diagrams 101 *Roger Penrose 1971*

Linear algebra operations:



 $\sum_i V_i W_i$


 $\sum_j A_{ij} B_{jk}$


Important examples:




S



V_i



M_{ij}



T_{ijk}


J. C. Bridgeman, C. T. Chubb, J. Phys. A: Math. Theor. 50 223001 (2017)


TENSOR NETWORKS

Compressed representations/approximations of exponentially large quantum states


Tensor diagrams 101 Roger Penrose 1971

Linear algebra operations:


 $\sum_i V_i W_i$



 $\sum_j A_{ij} B_{jk}$

Singular value decomposition & truncation




M

=



$U \quad \tilde{S} \quad V^\dagger$

=



$A_1 \quad A_2$

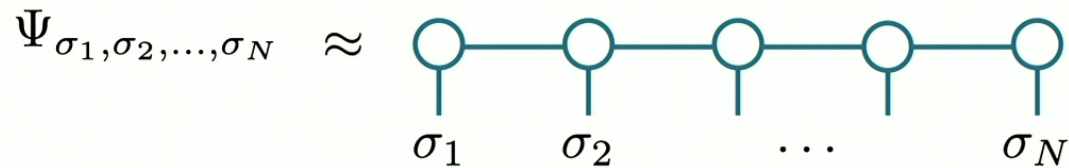
→

lower dimensional

J. C. Bridgeman, C. T. Chubb, J. Phys. A: Math. Theor. 50 223001 (2017)

TENSOR NETWORKS

Compressed representations/approximations of exponentially large quantum states



Matrix product state (MPS)

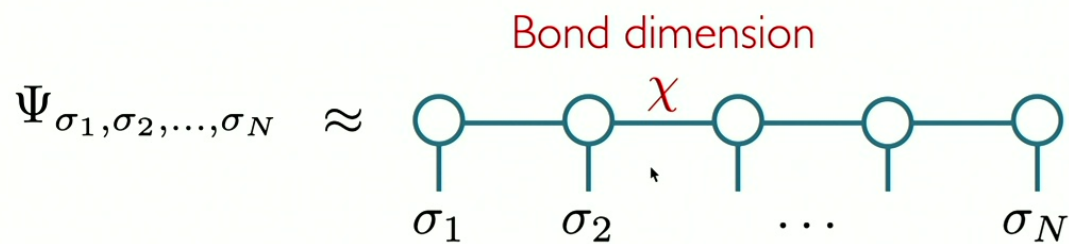
Tensor train (TT)

MPS reduces number of parameters: $2^N \rightarrow 2\chi^{2N}$

J. C. Bridgeman, C. T. Chubb, J. Phys. A: Math. Theor. 50 223001 (2017)

TENSOR NETWORKS

Compressed representations/approximations of exponentially large quantum states



Matrix product state (MPS)

Tensor train (TT)

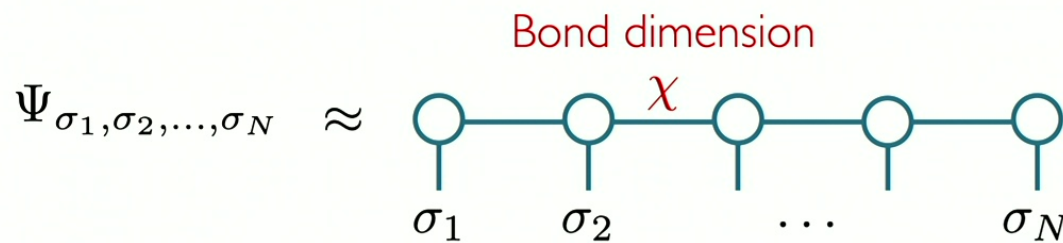
MPS reduces number of parameters: $2^N \rightarrow 2\chi^{2N}$

Linear scaling!

J. C. Bridgeman, C. T. Chubb, J. Phys. A: Math. Theor. 50 223001 (2017)

TENSOR NETWORKS

Compressed representations/approximations of exponentially large quantum states



Matrix product state (MPS)

Tensor train (TT)

MPS reduces number of parameters: $2^N \rightarrow 2\chi(N)^2N$

$$\chi \sim \begin{cases} \text{const} & \text{low-entangled} \\ 2^N & \text{highly-entangled} \end{cases}$$

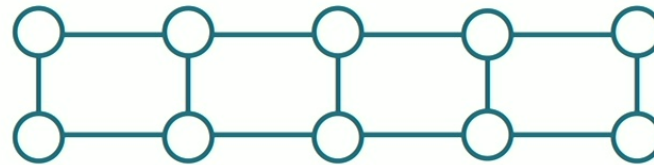
J. C. Bridgeman, C. T. Chubb, J. Phys. A: Math. Theor. 50 223001 (2017)

MATRIX PRODUCT STATES (MPS)

MPS allow for efficient computations:

- E.g. wave function overlaps

$$\langle \Psi | \Psi' \rangle = \sum_{\sigma} \Psi_{\sigma}^* \Psi'_{\sigma}$$



- Computing ground states: Density matrix renormalization group (DMRG) *Steven R. White 1992*

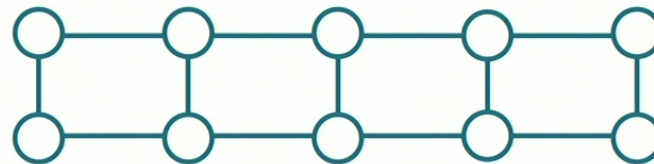
J. C. Bridgeman, C. T. Chubb, J. Phys. A: Math. Theor. 50 223001 (2017)

MATRIX PRODUCT STATES (MPS)

MPS allow for efficient computations:

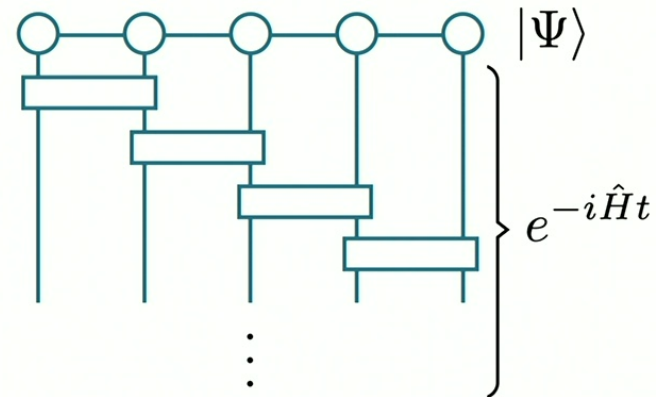
- E.g. wave function overlaps

$$\langle \Psi | \Psi' \rangle = \sum_{\sigma} \Psi_{\sigma}^* \Psi'_{\sigma}$$



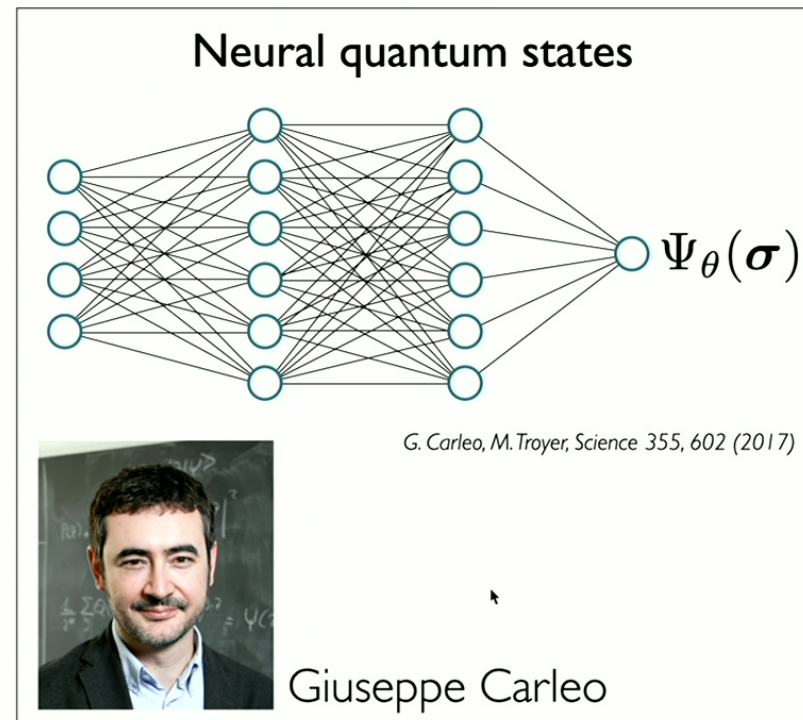
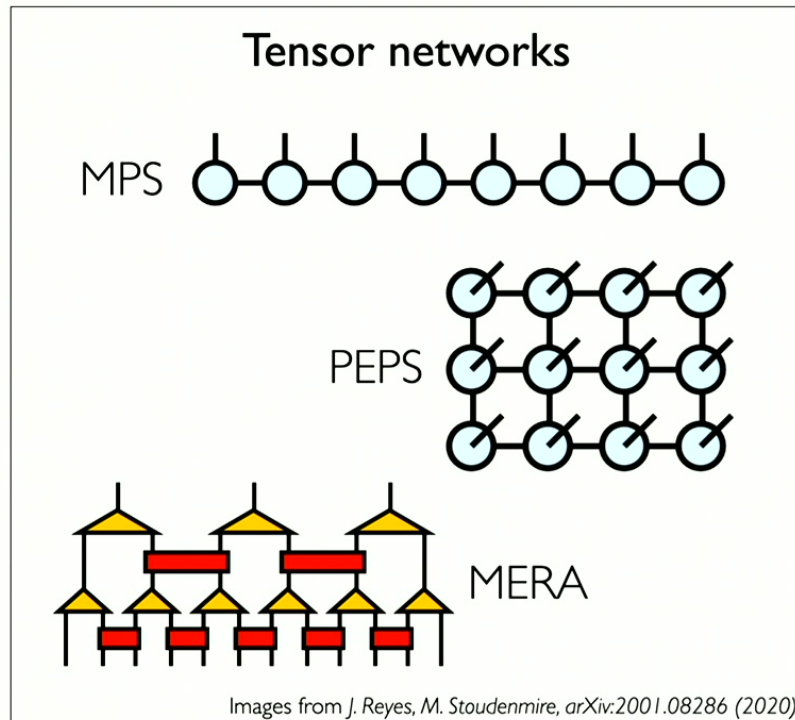
- Computing ground states: Density matrix renormalization group (DMRG) *Steven R. White 1992*

- Time evolution: $e^{-i\hat{H}t} |\Psi\rangle$



WAVE FUNCTION ANSATZE

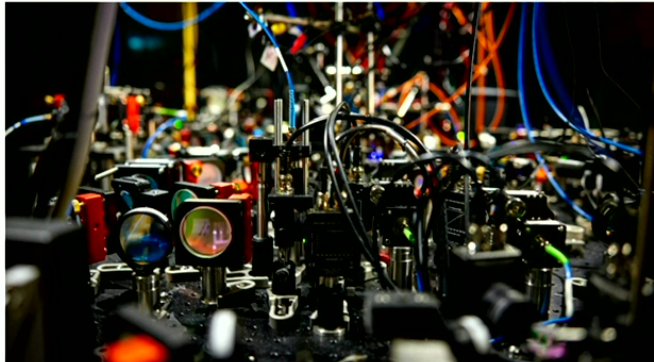
Compressed representations/approximations of exponentially large quantum states



QUANTUM SIMULATORS



Nature isn't classical, dammit, and if you want to make a simulation of nature, you'd better make it quantum mechanical. - *Richard Feynman 1981*



Optical table from Mikhail Lukin's cold atom experiment at Harvard
Image from Quanta Magazine

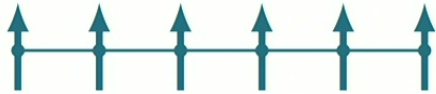
Experimental platforms

- Rydberg atoms trapped in optical tweezers
- Ultracold atoms in optical lattices
- Trapped ions
- Superconducting circuits
- Photonic systems
- ...

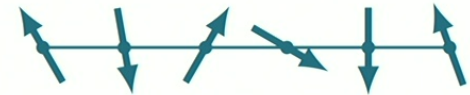
TOY QUANTUM SIMULATOR

$$\hat{H}_{\text{Ising}} = -J \sum_i \hat{Z}_i \hat{Z}_{i+1} - h_x \sum_i \hat{X}_i - h_z \sum_i \hat{Z}_i$$

Initial state

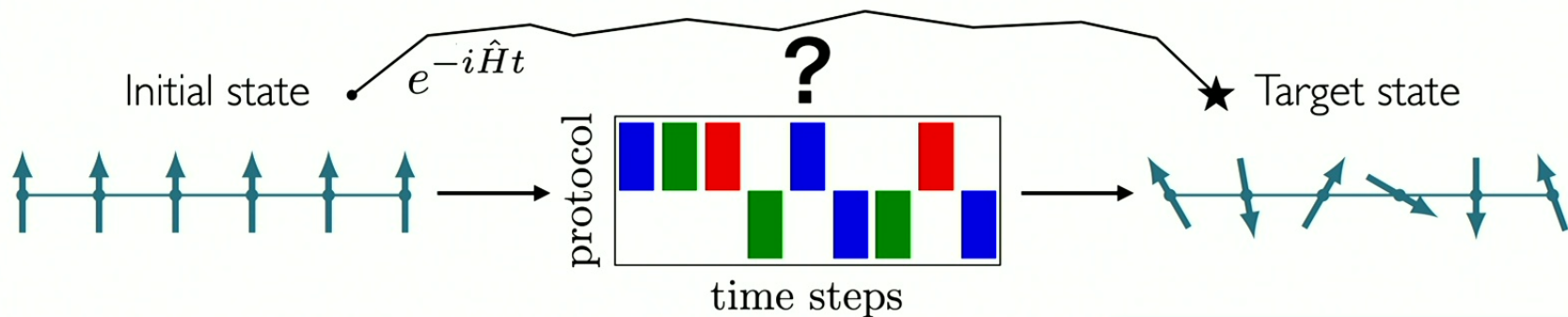


Target state



TOY QUANTUM SIMULATOR

$$\hat{H}_{\text{Ising}} = -J \sum_i \hat{Z}_i \hat{Z}_{i+1} - h_x \sum_i \hat{X}_i - h_z \sum_i \hat{Z}_i$$

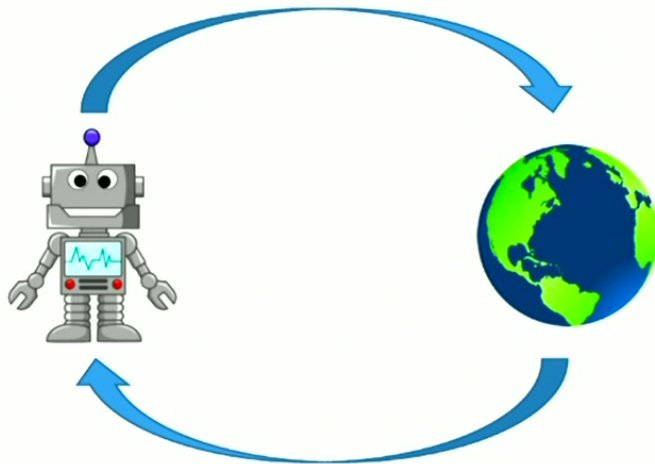


Optimal control problem!

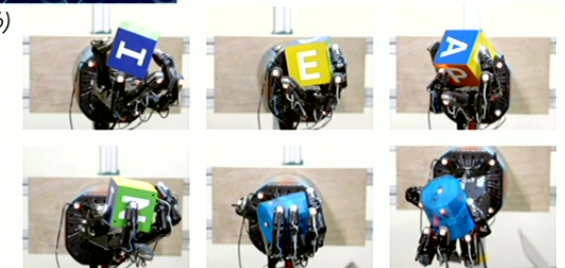
Optimal control

- Greedy search
- Beam search
- ...
- Reinforcement learning

REINFORCEMENT LEARNING (RL)



D. Silver et al. Nature 529, 484 (2016)



OpenAI et al. arXiv:1808.00177 (2019)

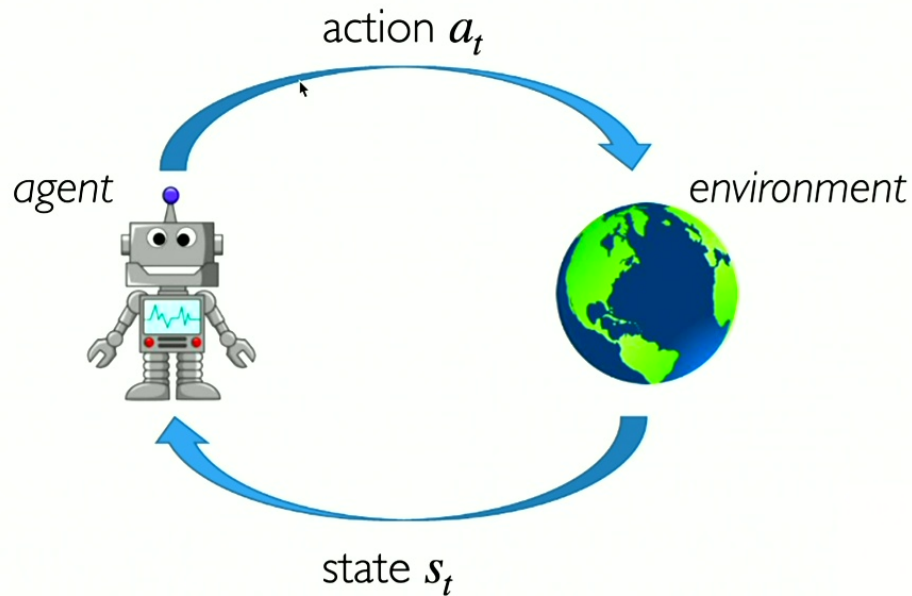
Explain reinforcement learning in three short bullet points

- **Interaction-based Learning:** Agents learn by interacting with an environment, receiving rewards or penalties for actions.
- **Trial and Error:** Agents improve strategies over time by trying actions and learning from outcomes.
- **Exploration vs. Exploitation:** Balances discovering new actions with using known, rewarding actions.

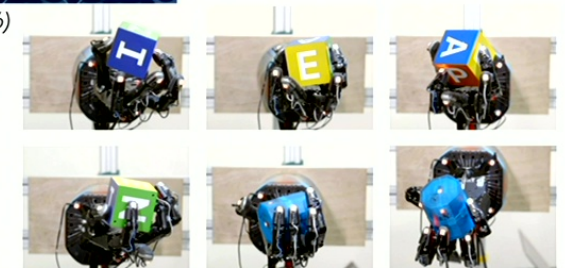
ChatGPT 4o by OpenAI

R. S. Sutton, A. G. Barto, Reinforcement learning: An introduction. MIT press

REINFORCEMENT LEARNING (RL)



D. Silver et al. Nature 529, 484 (2016)



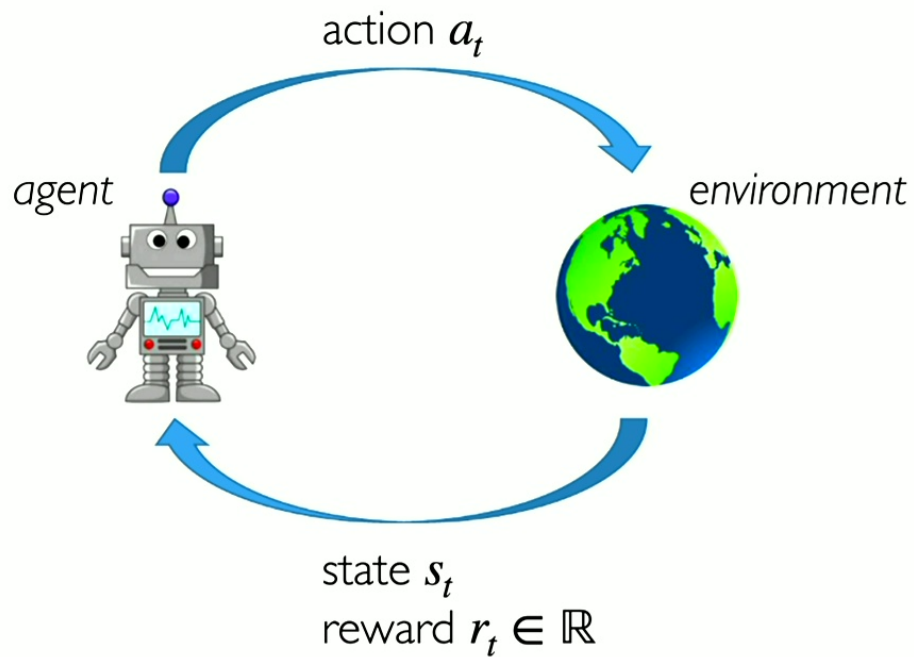
OpenAI et al. arXiv:1808.00177 (2019)

Explain reinforcement learning in three short bullet points

- **Interaction-based Learning:** Agents learn by interacting with an environment, receiving rewards or penalties for actions.
- **Trial and Error:** Agents improve strategies over time by trying actions and learning from outcomes.
- **Exploration vs. Exploitation:** Balances discovering new actions with using known, rewarding actions.

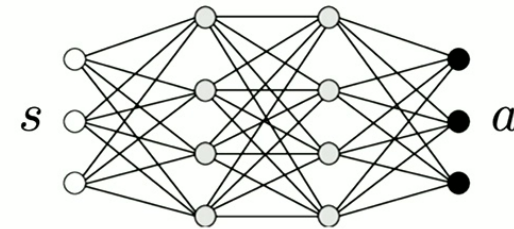
ChatGPT 4o by OpenAI

REINFORCEMENT LEARNING (RL)



Agent chooses actions according to a **policy** (i.e. strategy):

$$\pi(s) = a$$



Goal: Maximize expected cumulative reward by finding an optimal policy

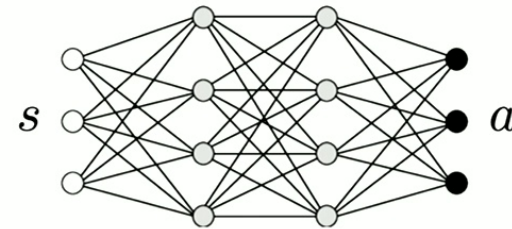
REINFORCEMENT LEARNING (RL)

RL agents can

- learn w/o knowing the physical laws of the environment
- produce protocols from different initial states w/o further optimization
- adapt their protocols in dynamically changing or stochastic environments

Agent chooses actions according to a **policy** (i.e. strategy):

$$\pi(s) = a$$



Goal: Maximize expected cumulative reward by finding an optimal policy

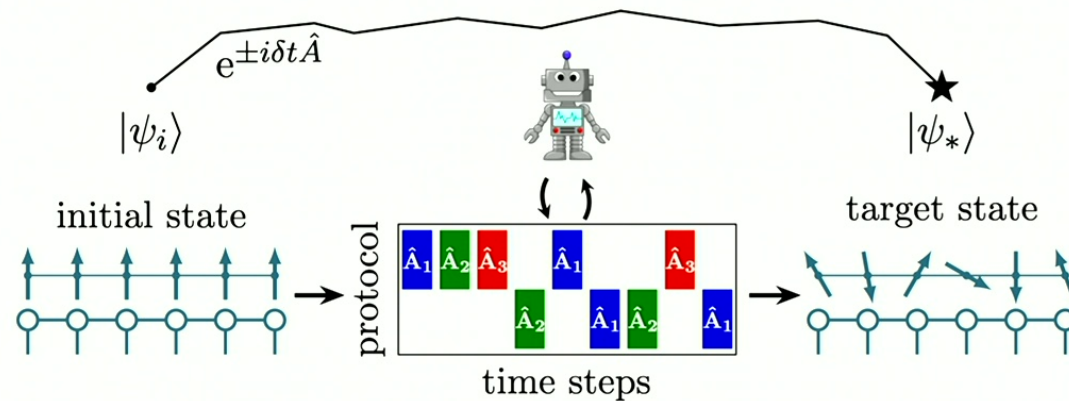
RL FOR QUANTUM MANY-BODY CONTROL

Challenge: **Optimization is expensive**

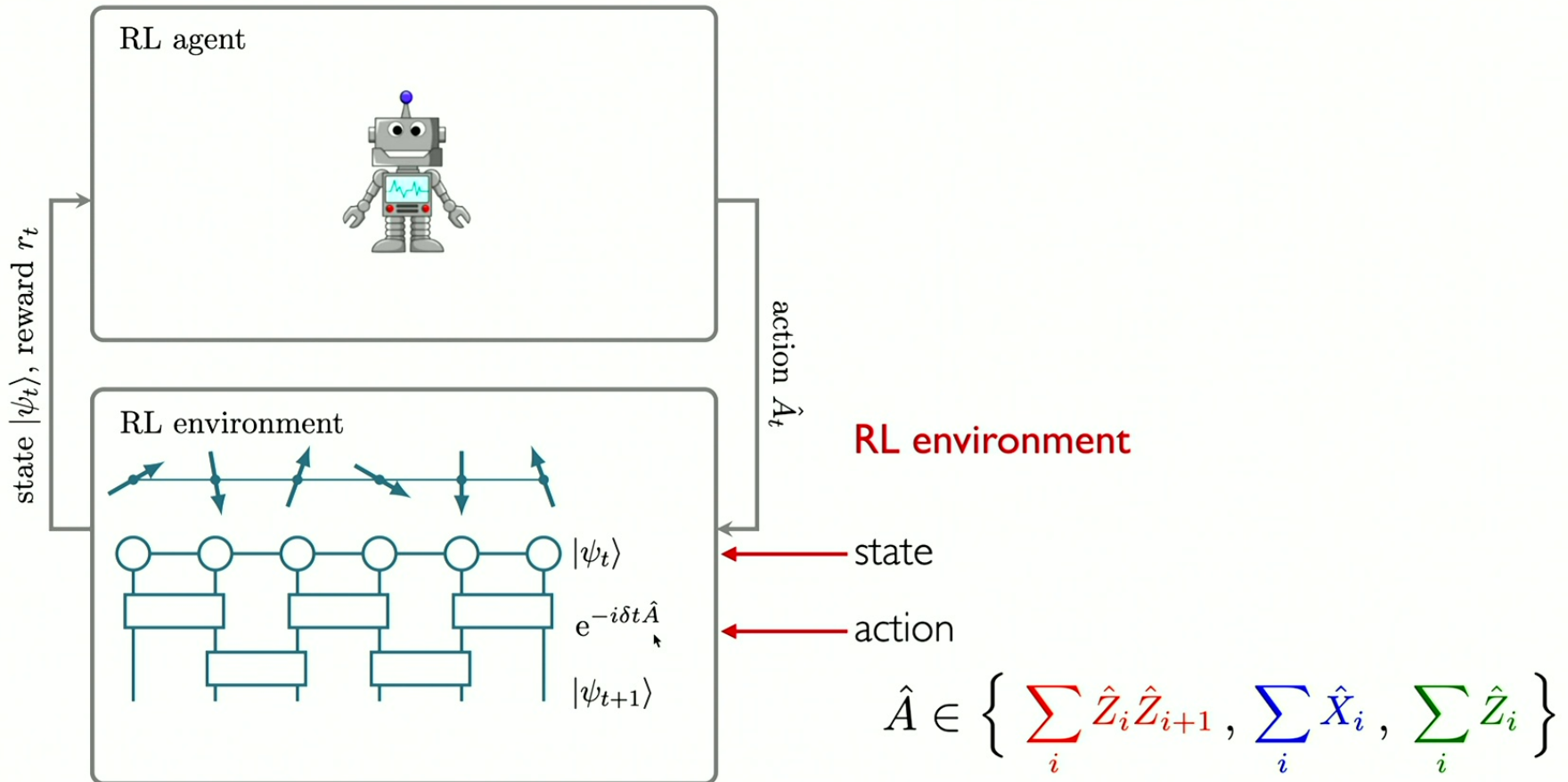
→ Perform numerical optimization in advance on classical computer

→ But: curse of dimensionality of quantum many-body systems

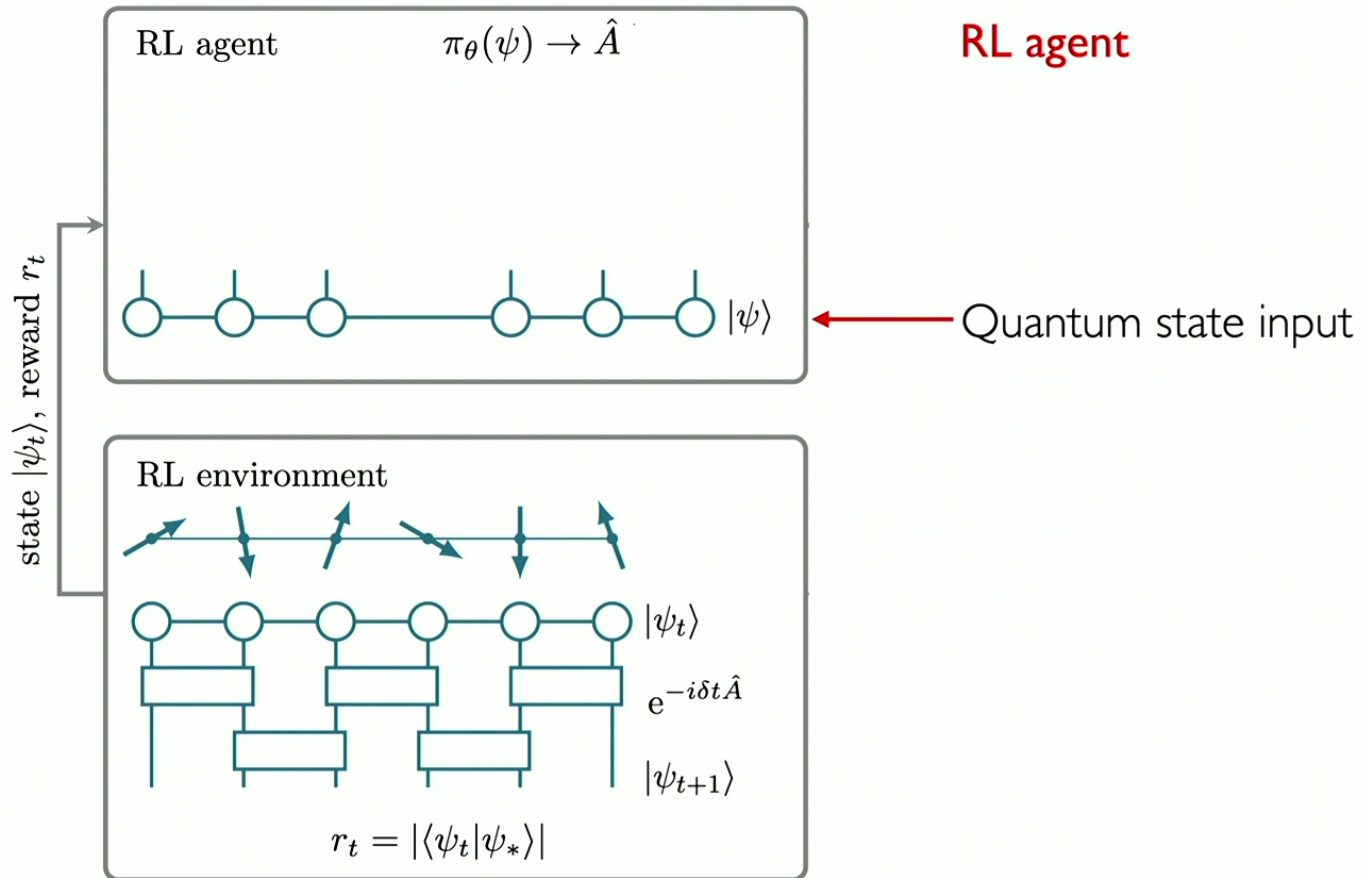
Our control framework: Deep **reinforcement learning** (RL) with **matrix product states** (MPS)



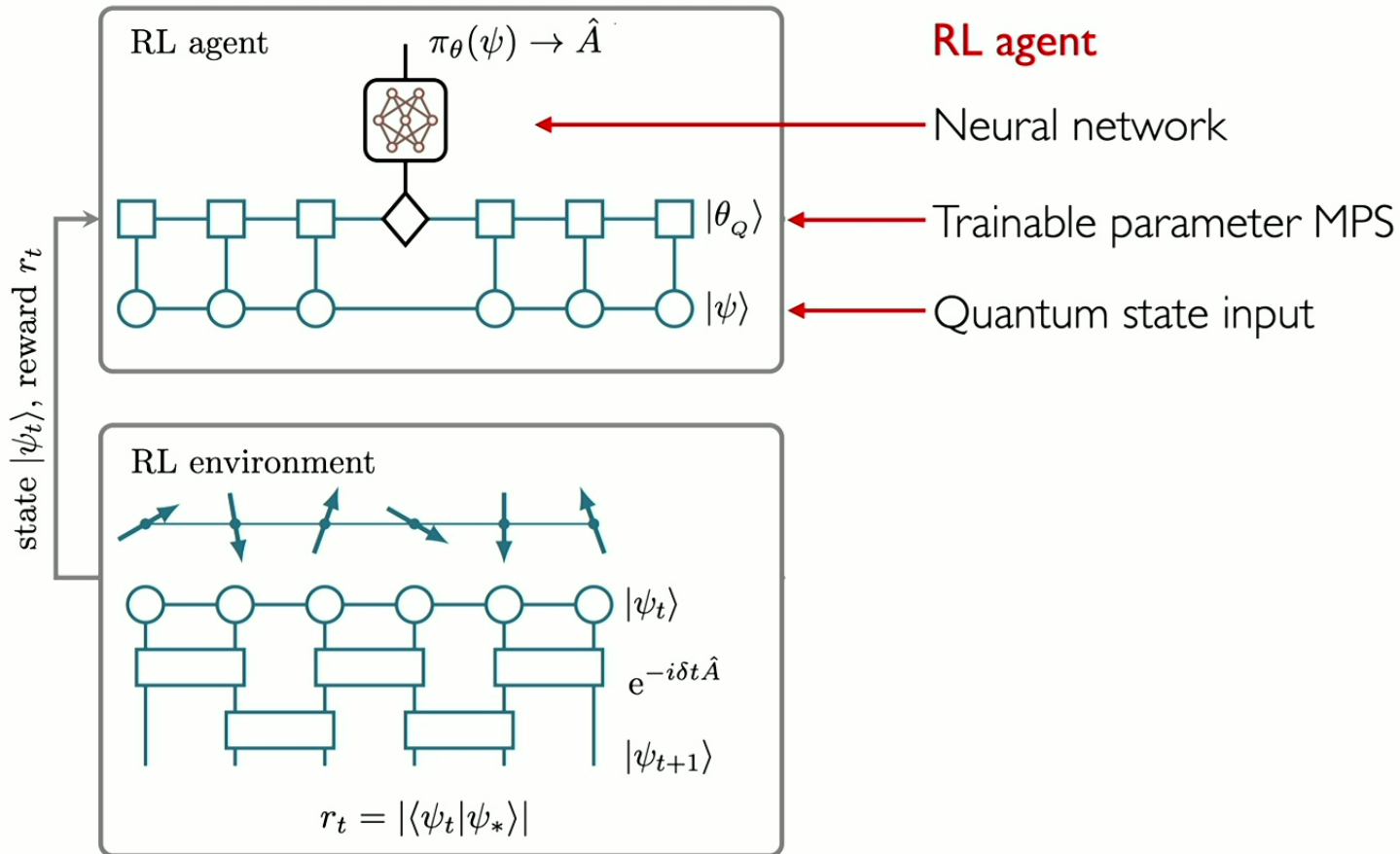
RL FRAMEWORK



RL FRAMEWORK

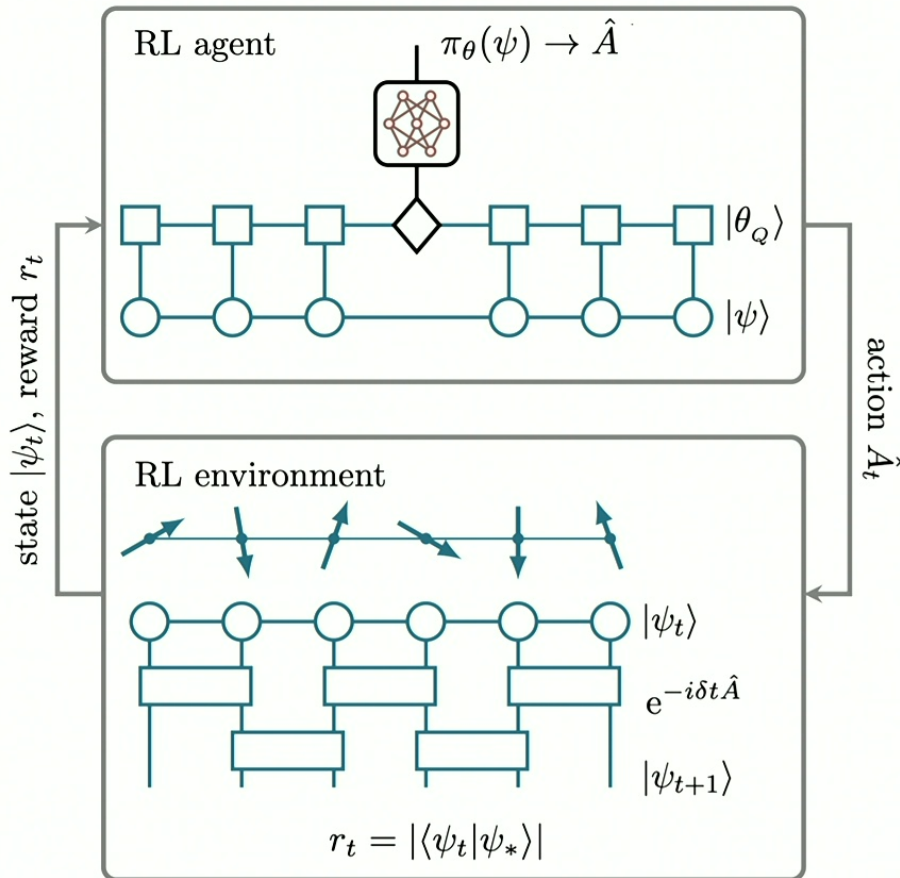


RL FRAMEWORK

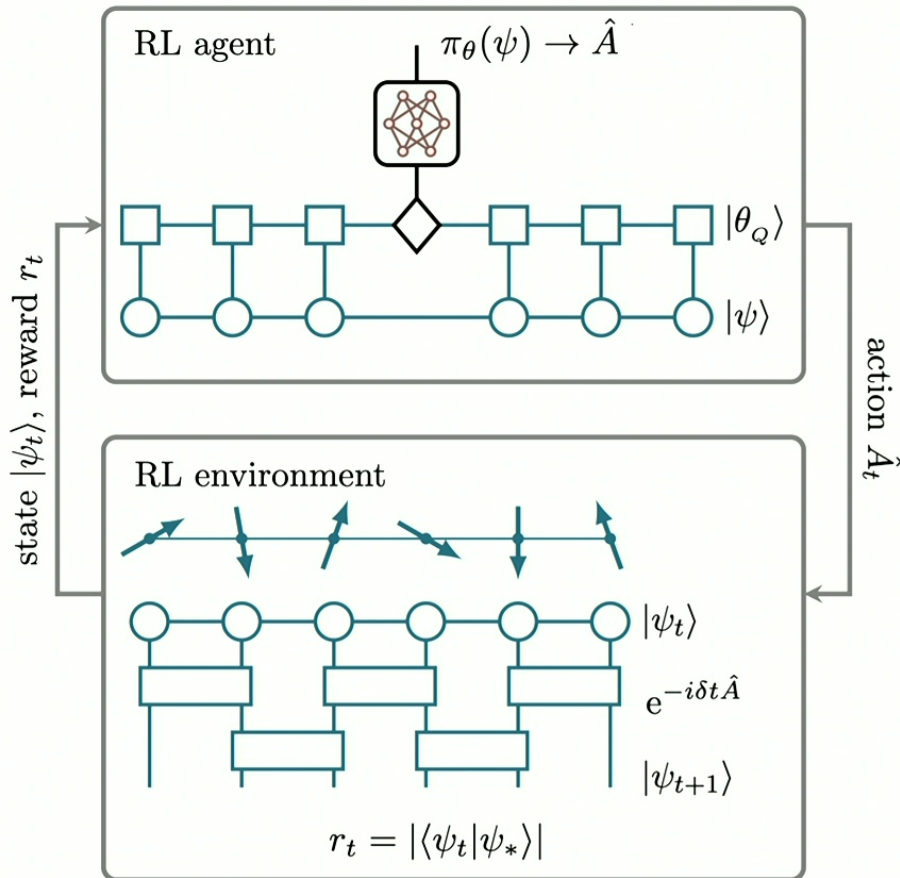


RL FRAMEWORK

Training



RL FRAMEWORK



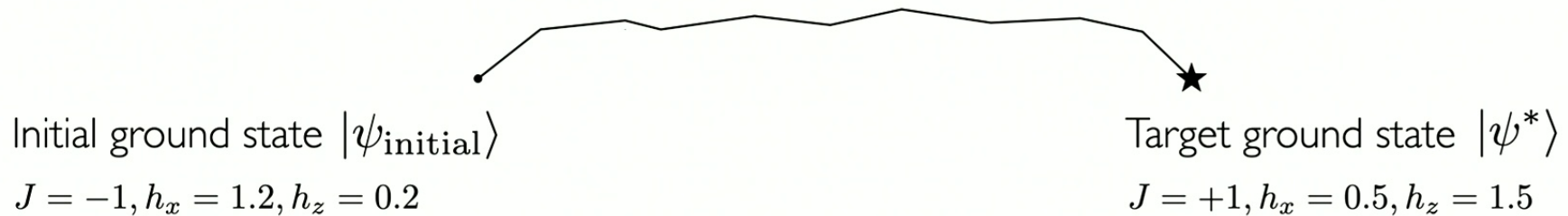
Training

Start each episode from a (random) initial state

Terminate episode when fidelity threshold is reached, e.g. $F = 0.99$

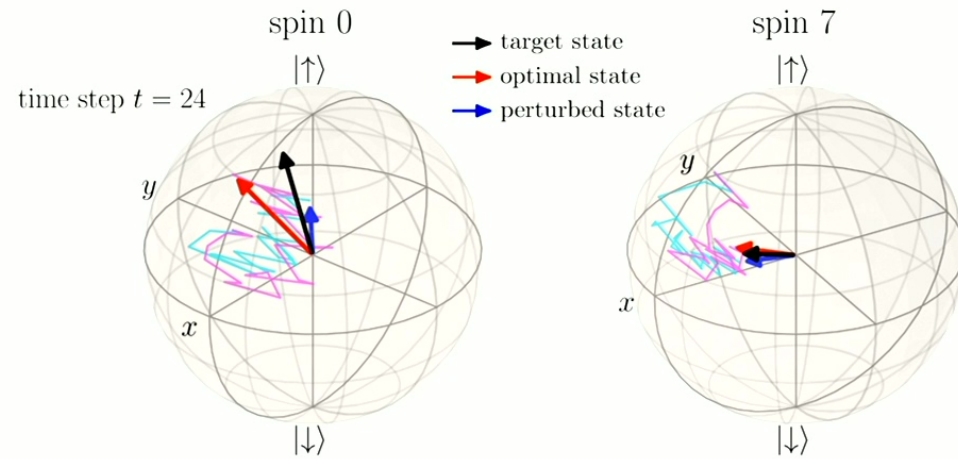
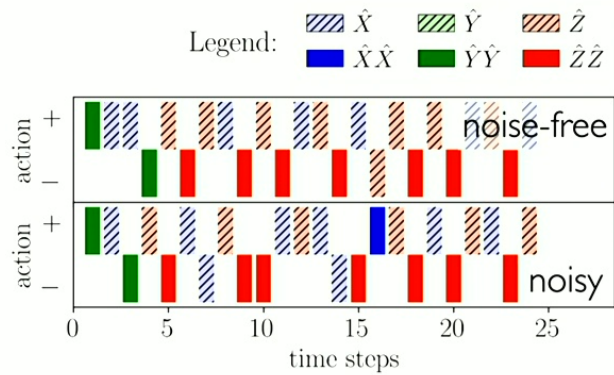
GROUND STATE PREPARATION

$$\hat{H}_{\text{Ising}} = J \sum_{i=1}^{N-1} \hat{Z}_i \hat{Z}_{i+1} - h_x \sum_{i=1}^N \hat{X}_i - h_z \sum_{i=1}^N \hat{Z}_i$$



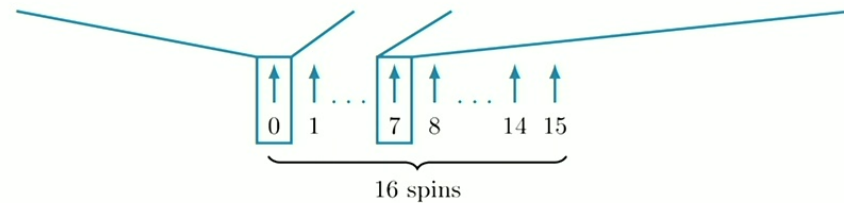
The agent can prepare the target state from (nearly) any Ising ground state

GROUND STATE PREPARATION



Make environment noisy

$$A \rightarrow A + \epsilon$$



Fidelity threshold $F_{\text{opt}} = 0.97$

SUMMARY

- **Matrix product states** (MPS): Compressed representations of exponentially large quantum many-body states
- **Reinforcement learning** (RL): An agent dynamically learns optimal controls in a trial-and-error fashion to maximize long term rewards
- RL + MPS → **Efficient quantum many-body control** *Nature Machine Intelligence* **5**, 780-791 (2023)



Marin Bukov

THANK YOU

