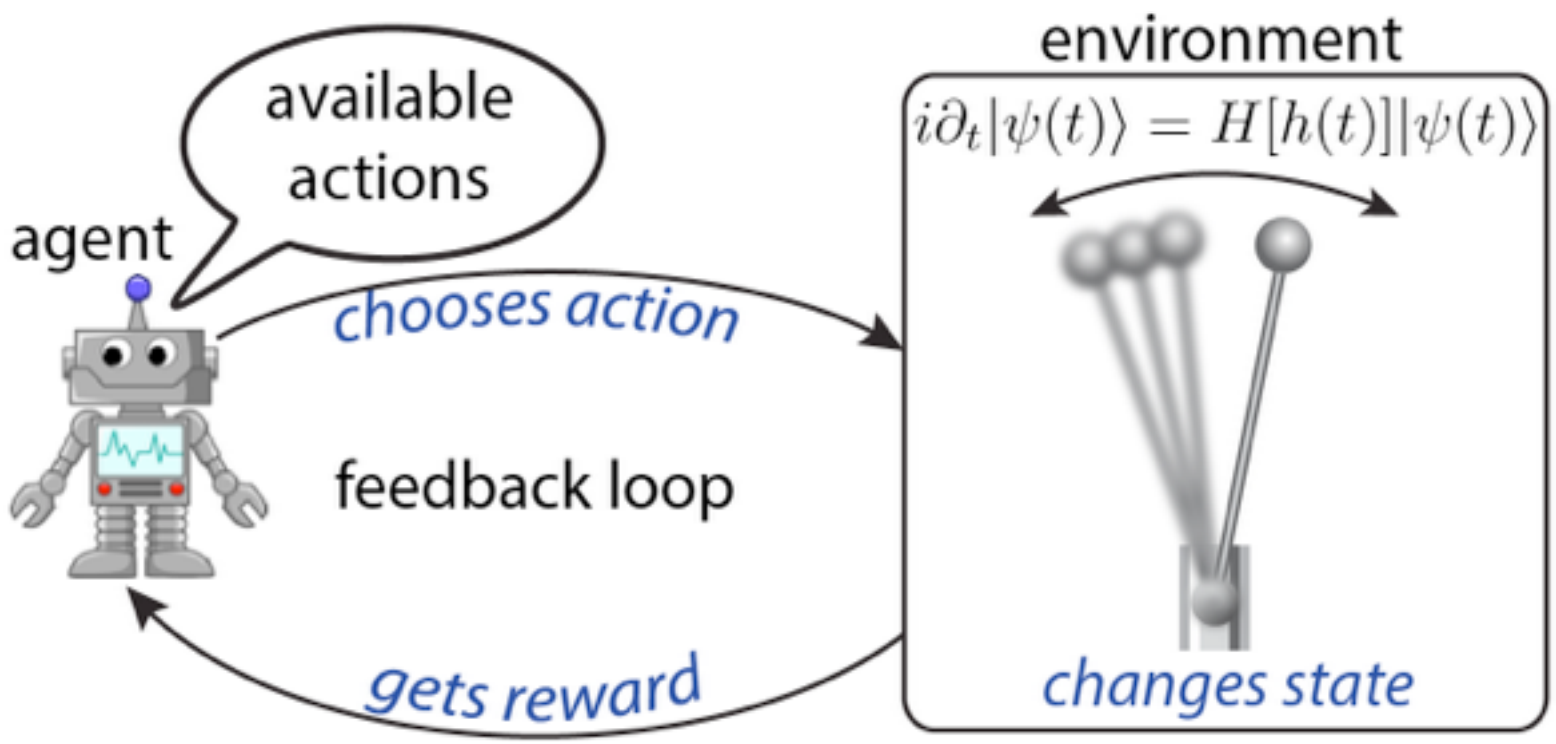
Reinforcement Learning: Introduction and Applications to Nonequilibrium Dynamics



Big Questions: Which problems can we study with ML that we can't do otherwise?
Can ML lead to the discovery of new physics?
What's ML's most appropriate physics application as a toolbox?

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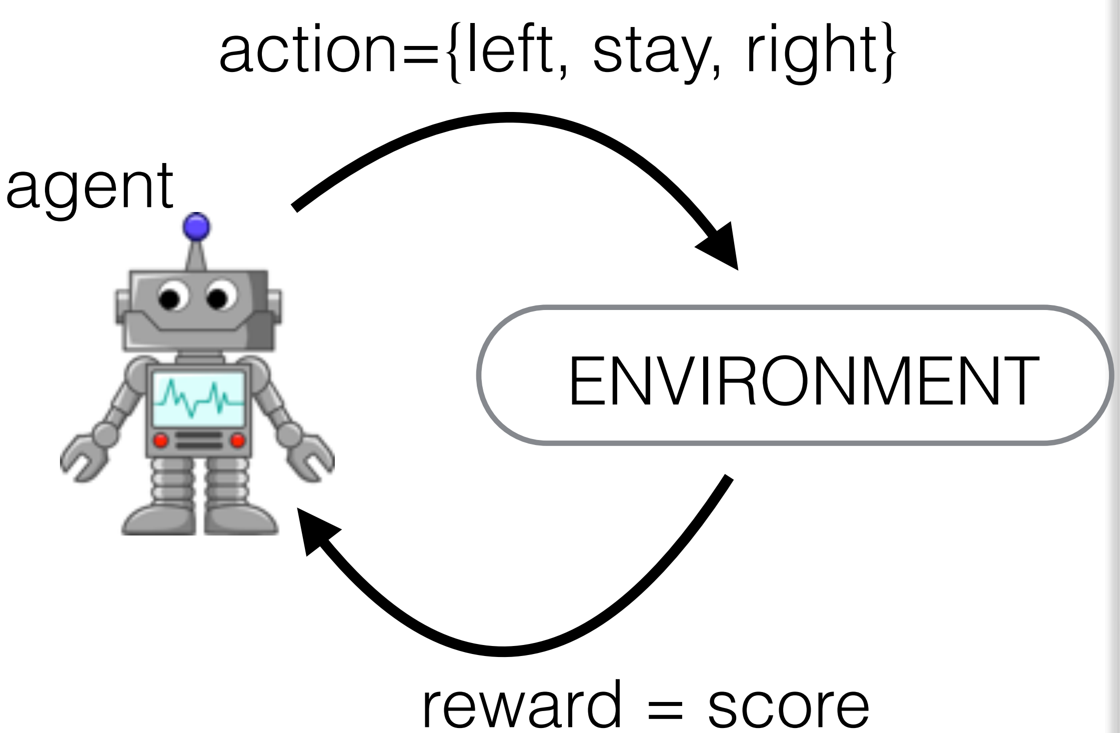
What is Reinforcement Learning?



Silver et al., Nature 529 (2016) [Google DeepMind]

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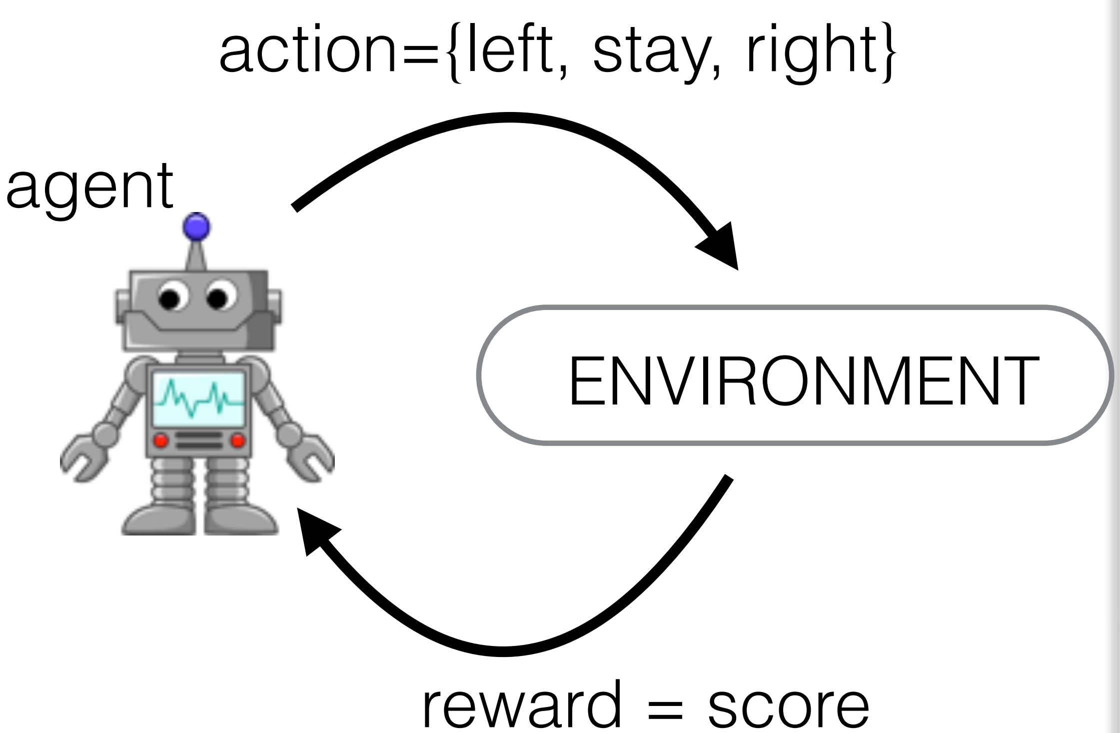

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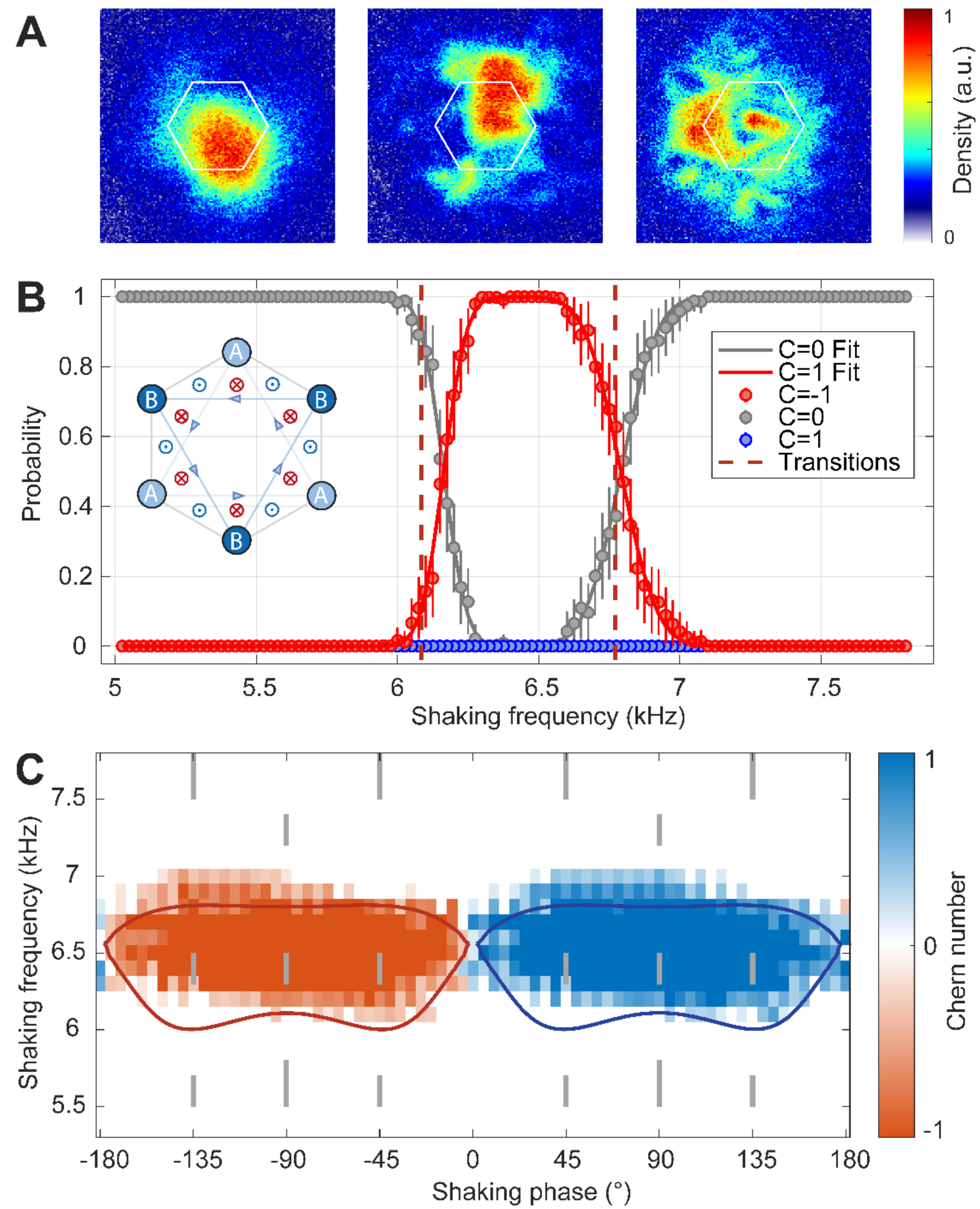
Machine Learning

→ Supervised Learning

- labelled data $\{(x,y)\}$
- find approx. model for the mapping $x \mapsto y$

learning topological phases in experiment



train set: 10,436 raw ToF images
test set: 15,963 images
validation set: 3,992 images

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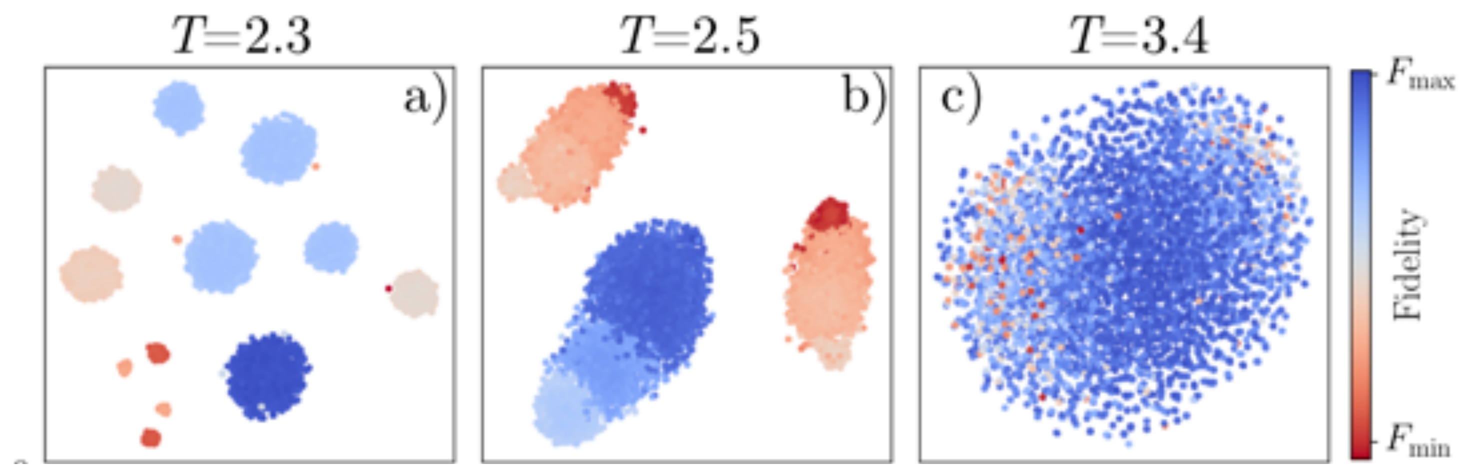
Machine Learning

→ Supervised Learning

- labelled data
- find approx. model which generalizes beyond fitting

visualize glassy (control) transitions



→ **Unsupervised Learning**

A. Day, M.B., et al, arXiv:1803:10856

- **un**labelled data $\{x\}$
- find approx. probability distr. which generates the data

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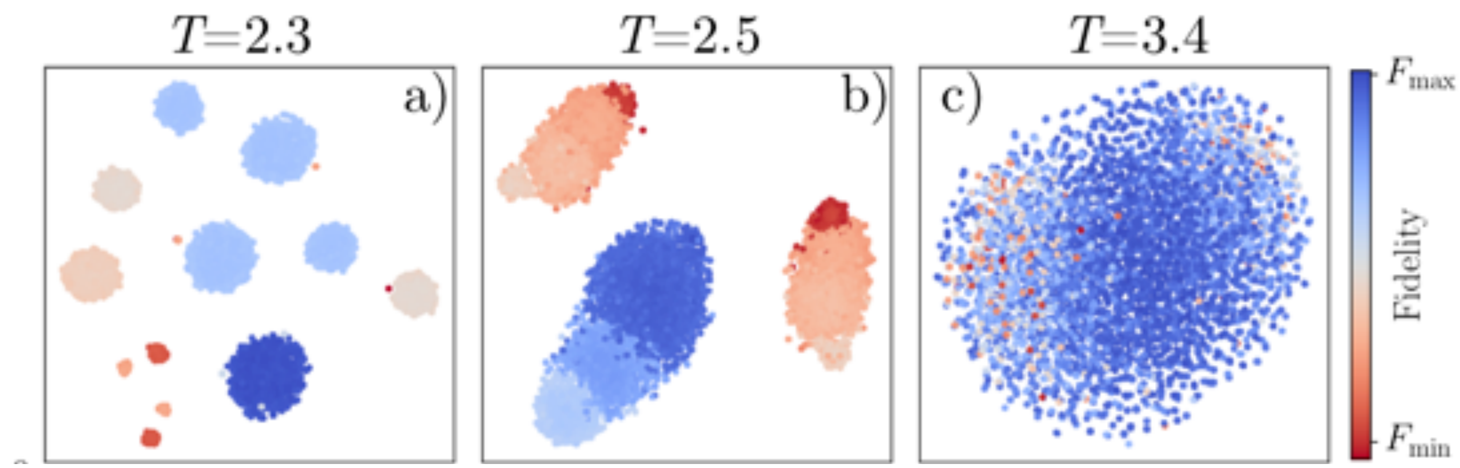

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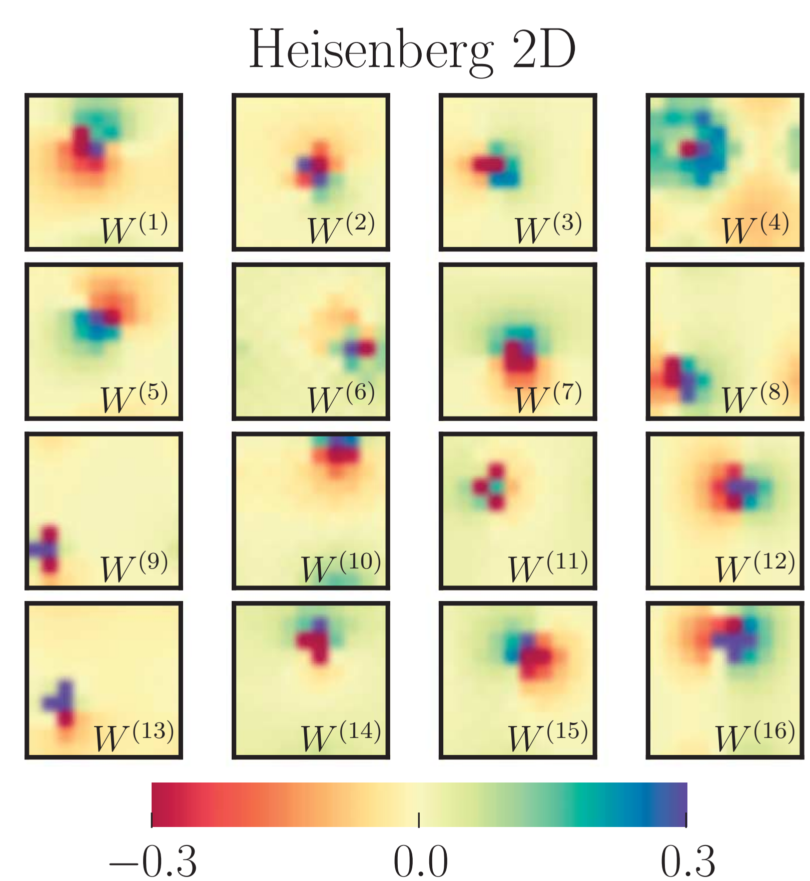
variational quantum states



Carleo and Troyer, Science (2017)

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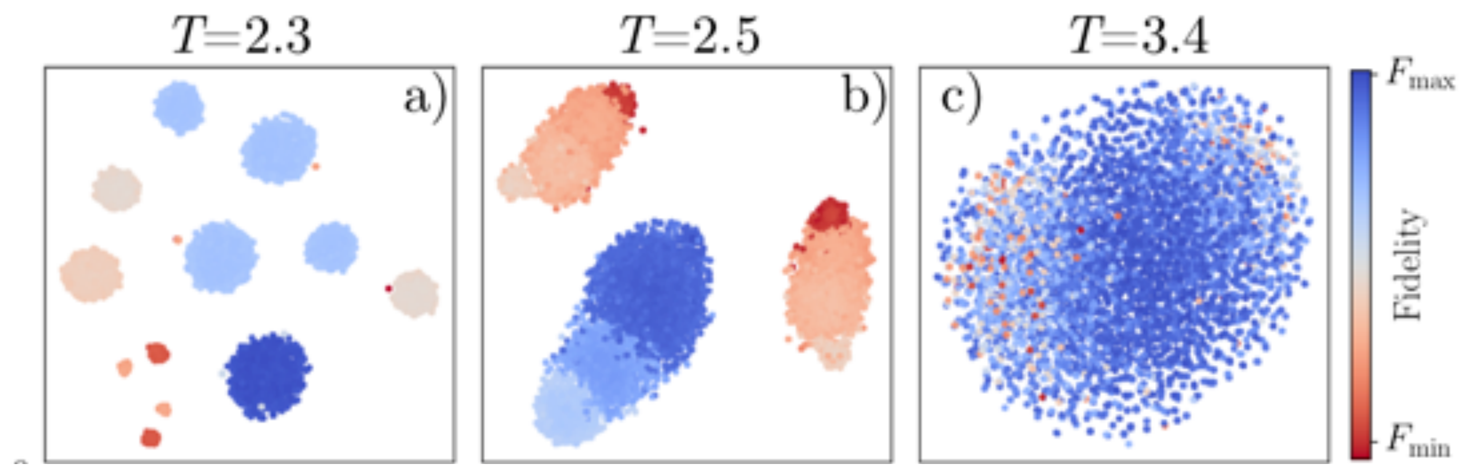

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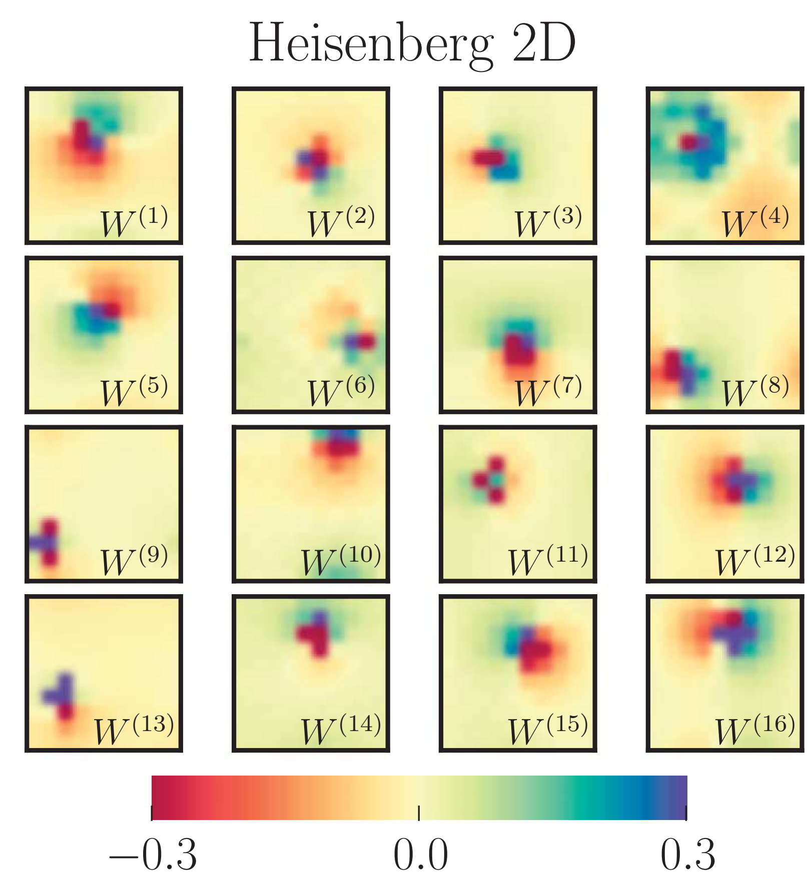

Carleo and Troyer, Science (2017)

reviews: ML in physics

Dunjko and Briegel: *ML & AI in the Quantum Domain, Rep Prog Phys 81 074001 (2018)*

P. Mehta, M.B., et al: *High Bias, Low-Variance Intro to ML for Physicists,* arXiv: 1803:08823 (2018)

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Machine Learning

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→ Supervised Learning

- labelled data
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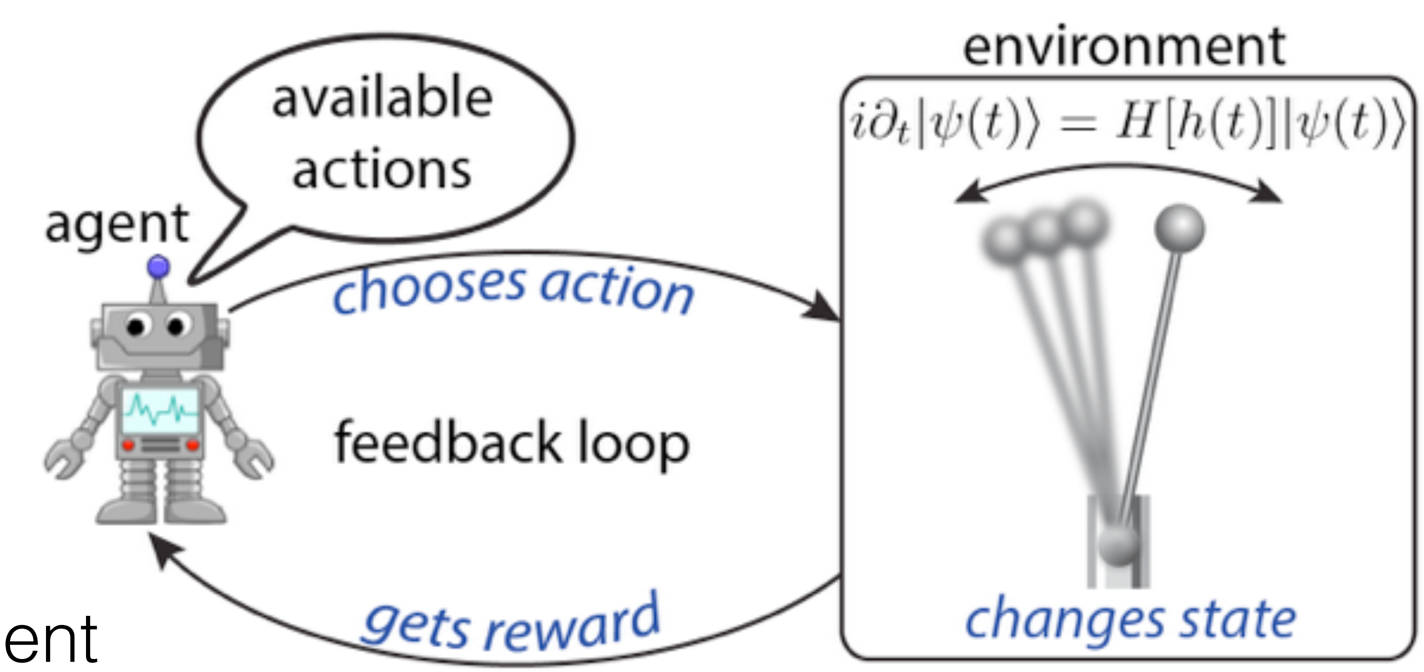
→ **Reinforcement Learning**

- agent learns strategy by interactions with its environment
- probability which generates the learning data changes with time due to interaction with the environment



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Examples of RL Applications

outside physics

video games

Mnih et al, Nature (2015)

board games

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locomotion

Lillicrap et al, arXiv:1509:02971

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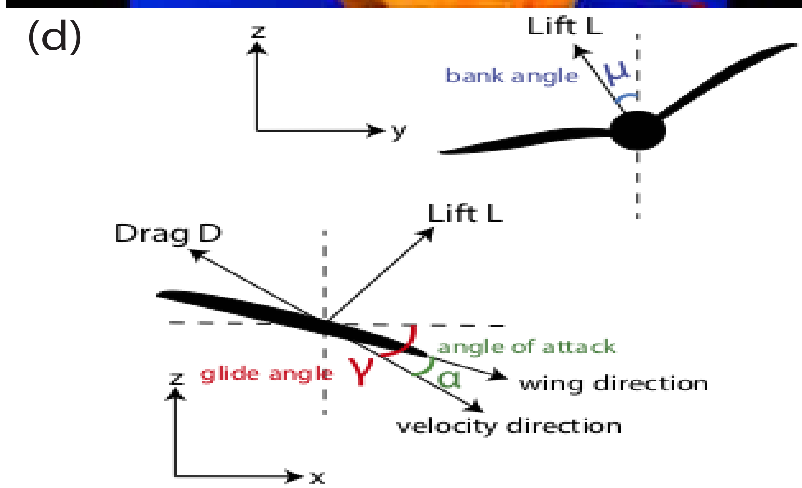

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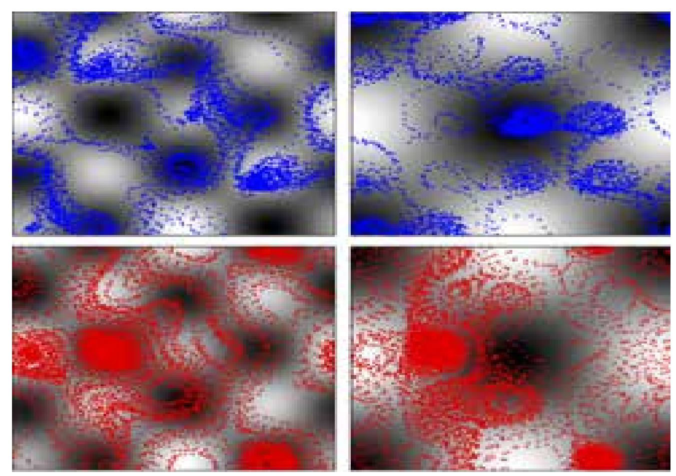

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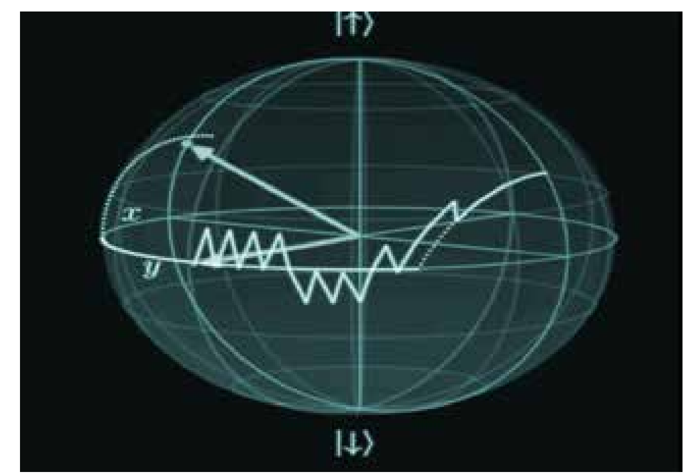


Reddy et al, PNAS 113 4877 (2016)

Colabrese et al, PRL 118 15004 (2018)

M.B. et al, PRX 8 0311086 (2018)

Fossil et al, PRX 8 031084 (2018)

August et al, arXiv:1802.04063

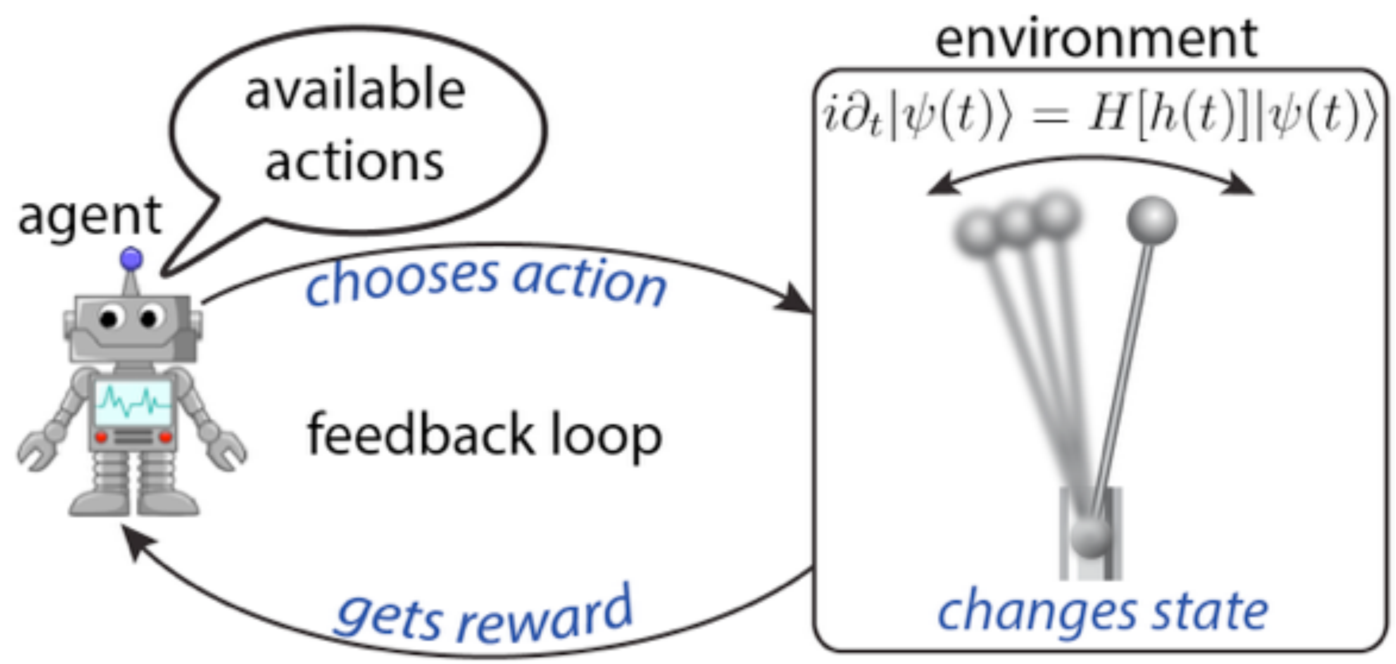
in physics

and more: design of molecular properties, quantum optics experiment design, etc.

The RL Formalism

→ RL formalism

- state space $\mathcal{S}$
- action space $\mathcal{A}$
- reward space $\mathcal{R}$



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Sutton and Barto, *Reinforcement Learning: an Introduction*, MIT press

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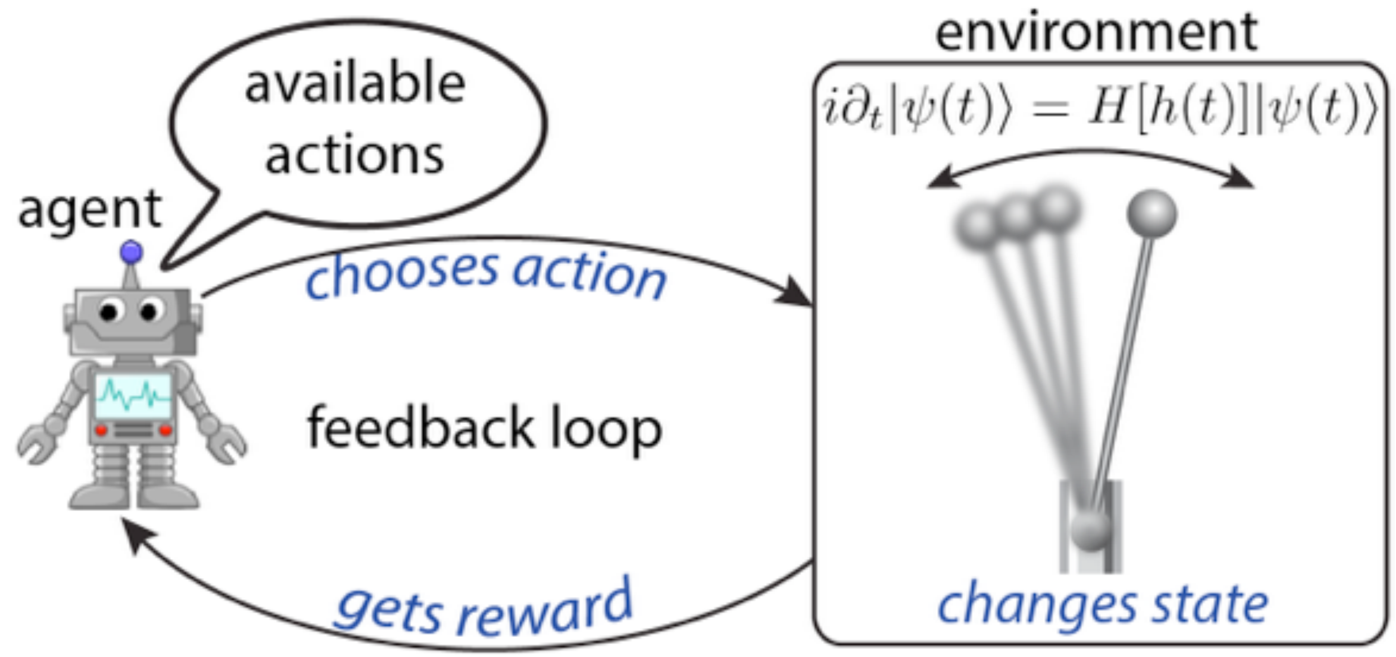
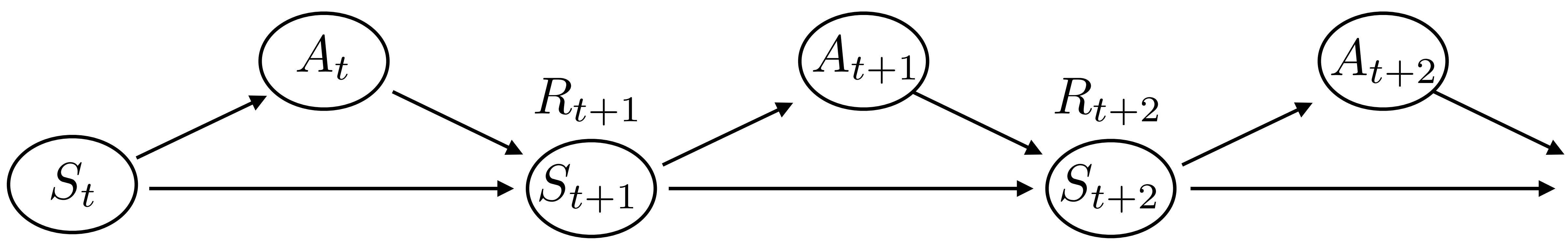


→ RL as Markov decision process



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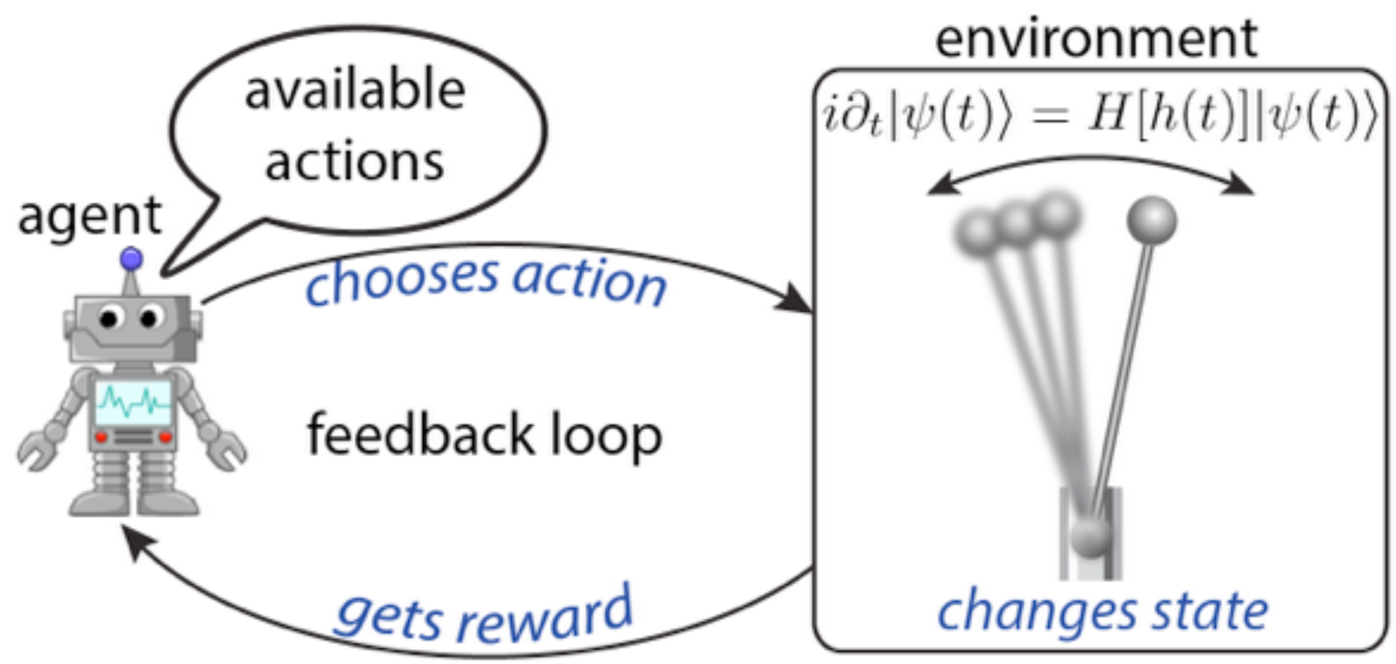

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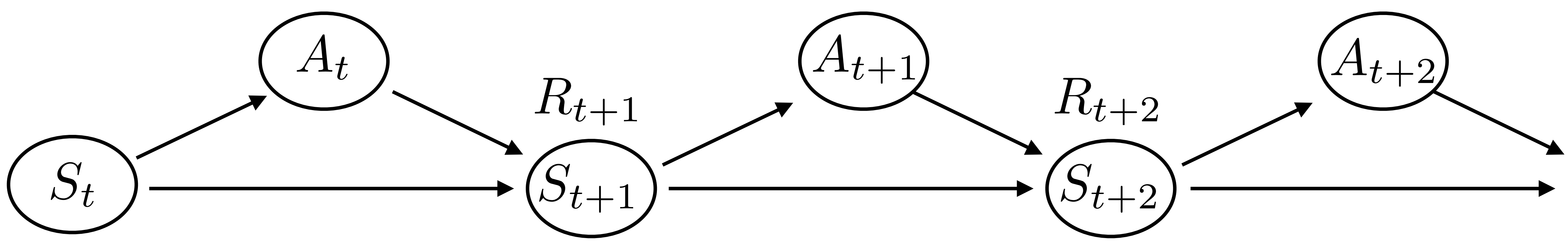

→ episodic learning

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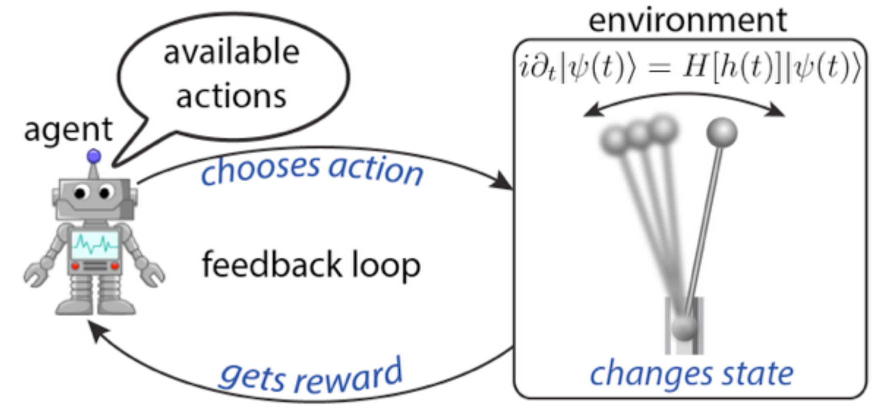
The RL Problem



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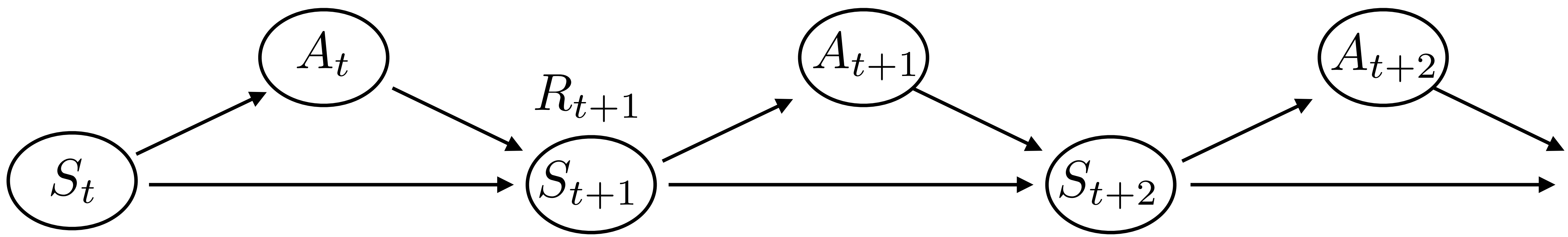

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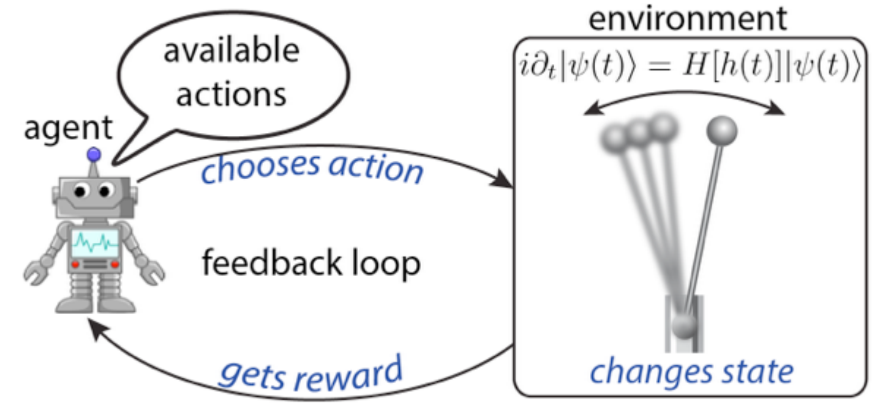

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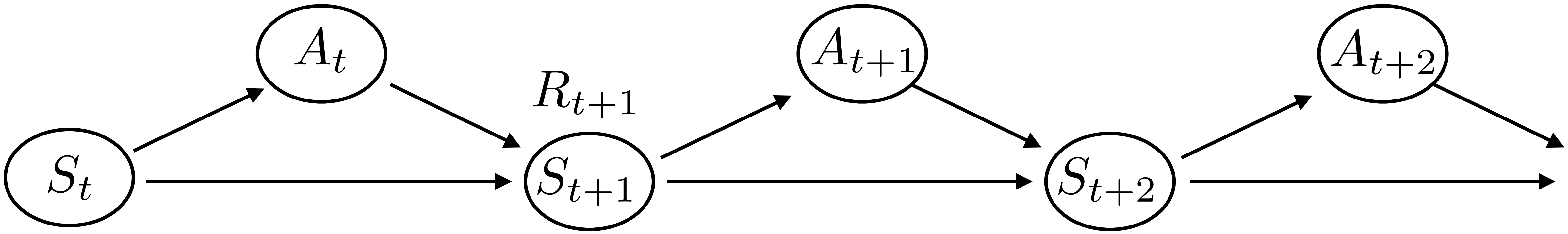

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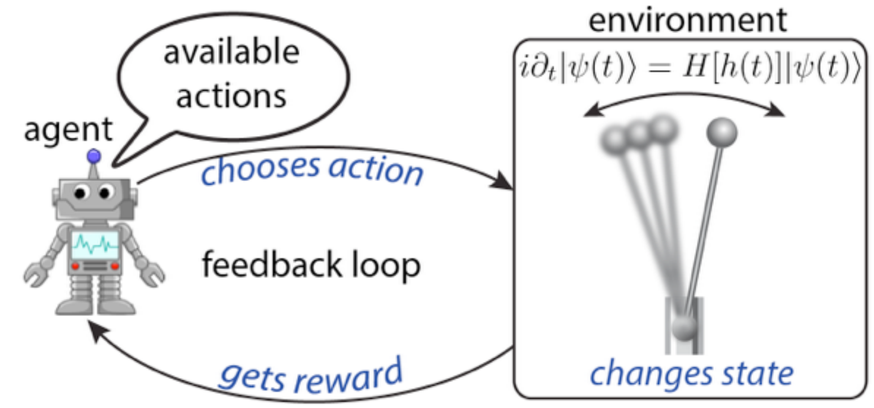

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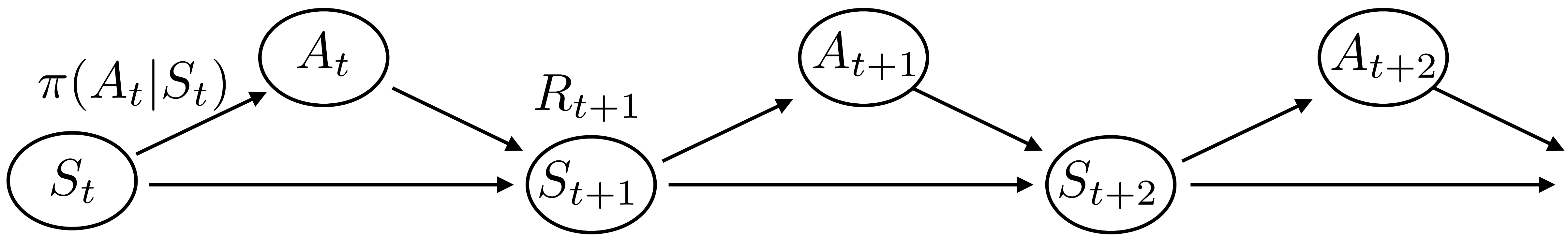

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  - **RL agent**: decision-making algorithm to learn & improve the ***policy***

    $\pi(a|s)$ probability distribution $\mathcal{A} \times \mathcal{S} \to [0,1]$

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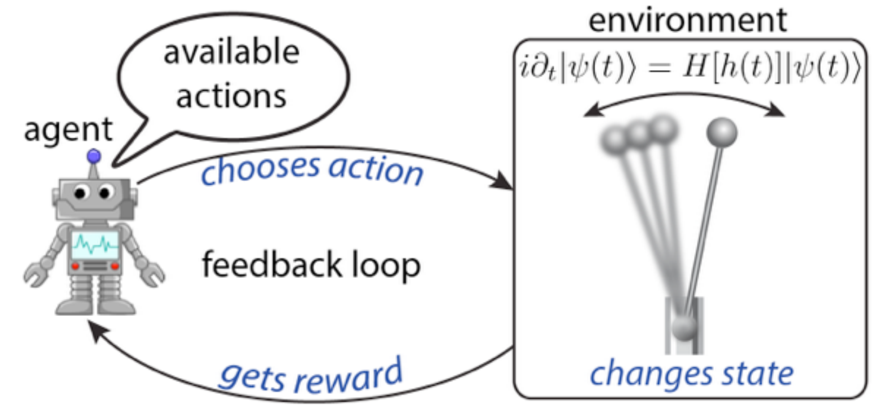

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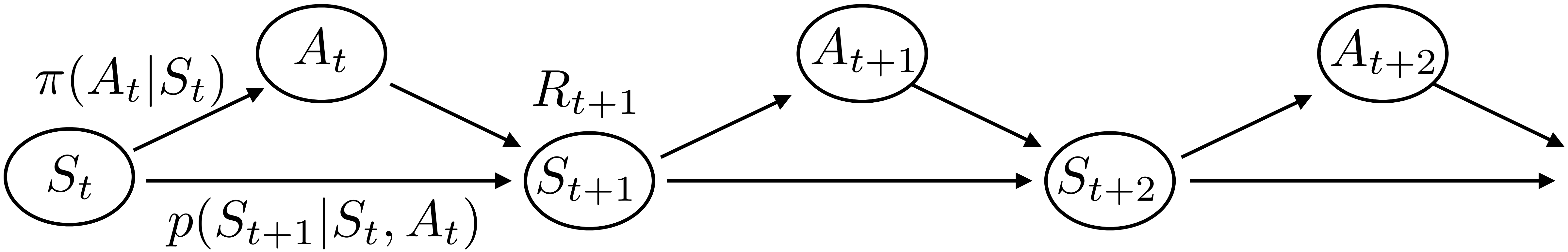

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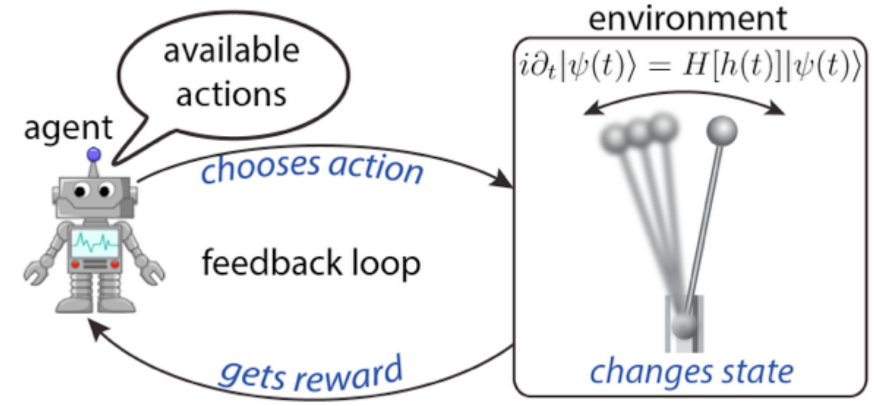

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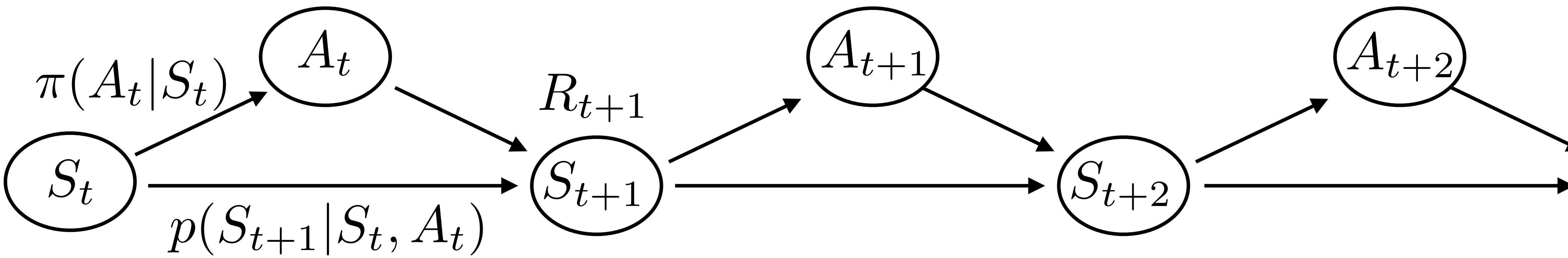

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→ RL **objective**: find policy which maximizes the total *expected return* from step t onwards $G_t = R_{t+1} + \cdots + R_T$

$$R_{t+1} = \sum_{s'} p(s'|S_t, A_t)\, r(s', S_t, A_t)$$

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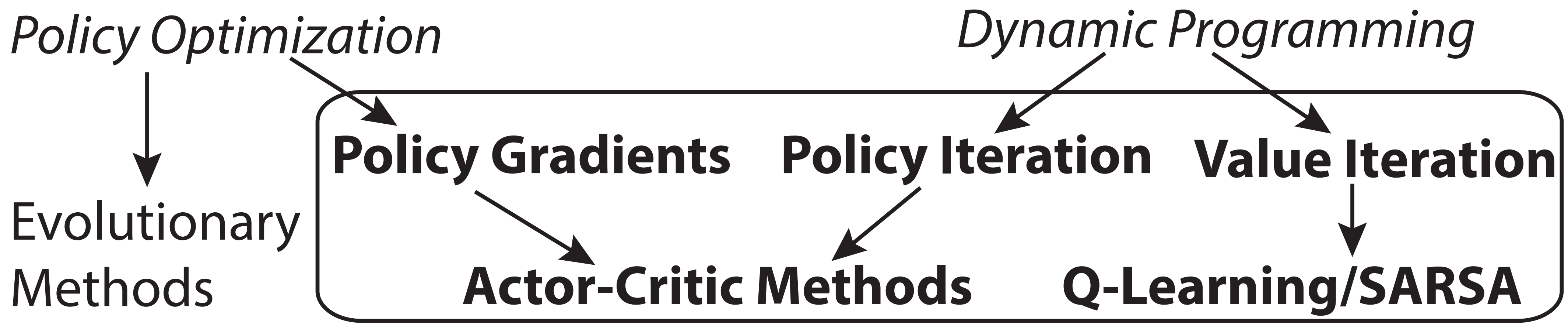
Sutton and Barto, *Reinforcement Learning: an Introduction*, MIT press

Overview of RL Algorithms



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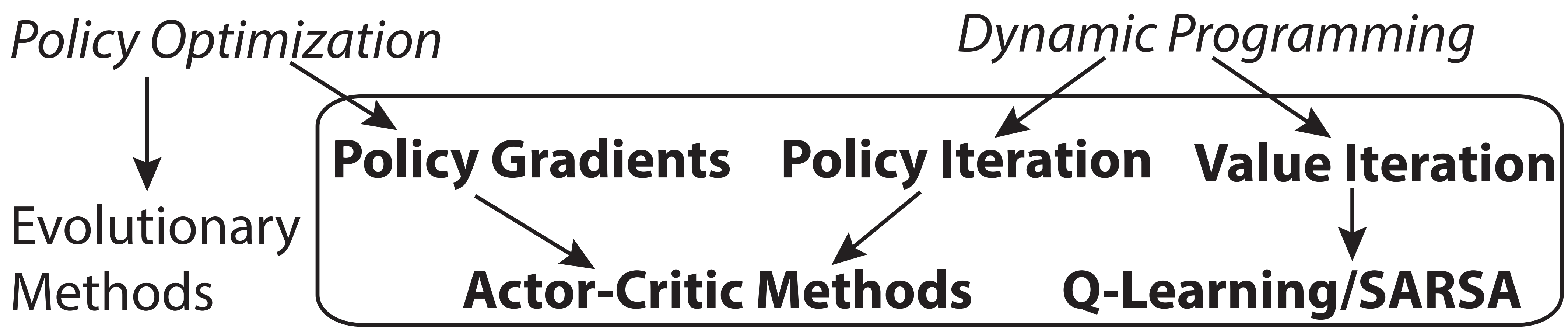

→ Value Iteration methods

- value function: ***expected*** total return under the policy $\pi(a|s)$ from state s

$$v_\pi(s) = \mathbb{E}_{a\sim\pi(a|s)}[G_t|S_t = s]$$

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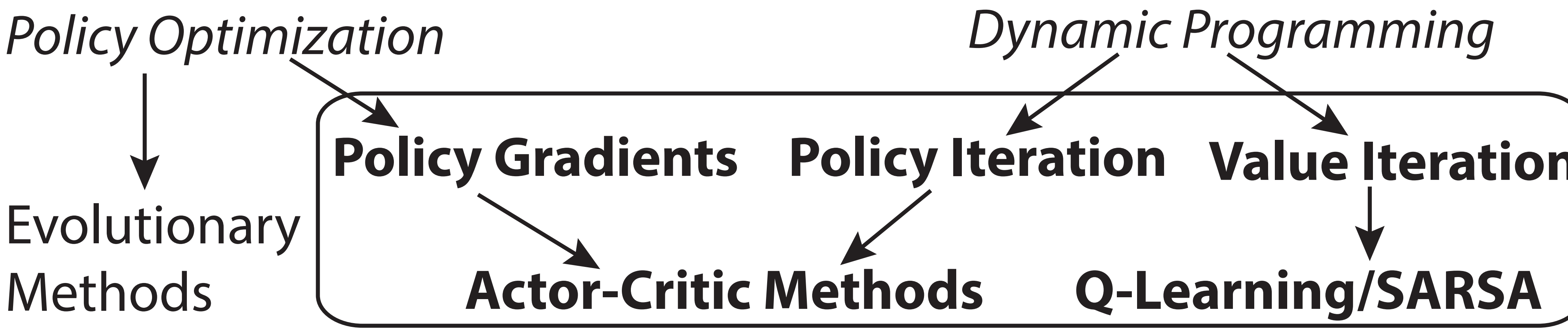

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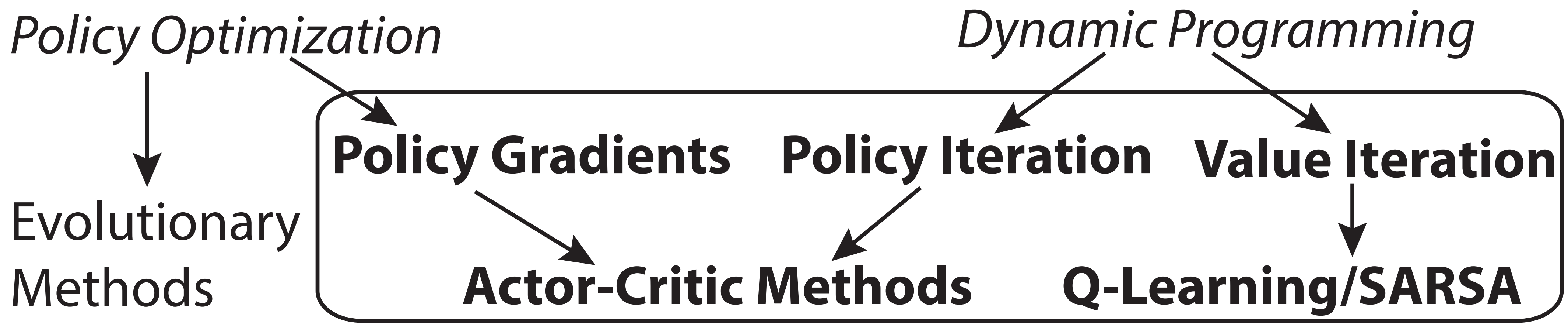

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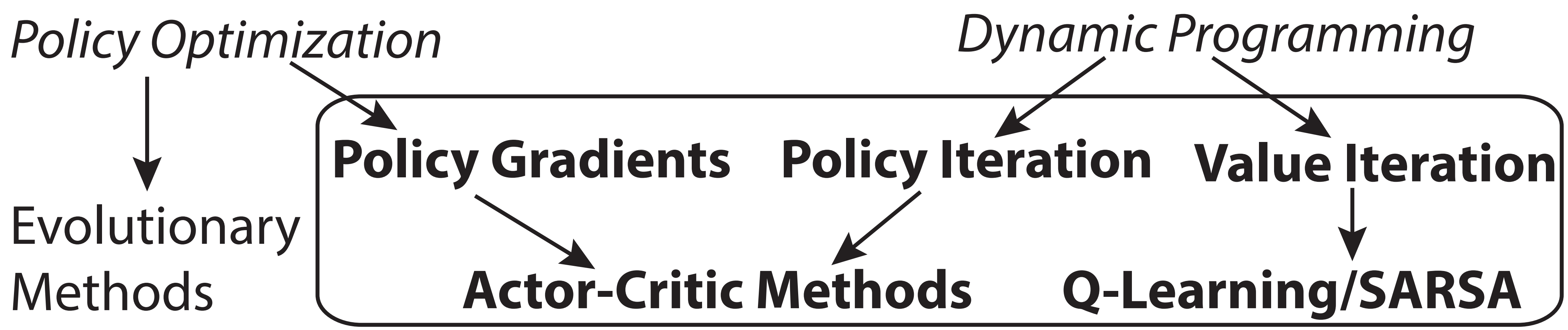

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Bellman's equation: $q_*(s,a) = \sum_{s'} p(s'|s,a)\left[r(s,s',a) + \max_{a'} q_*(s',a')\right]$

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RL with Function Approximation

→ problem: state space has exponentially many configurations

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- caveat: RL algorithms have convergence guarantees only for linear function approximators
- lots of empirical tricks to combine Deep Learning and RL

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→ examples of Deep RL:

- Tesauro's Backgammon RL player (1992)
- DeepMind: Atari games, AlphaGo, etc.
- self-driving cars, autonomous drone/helicopter hovering, etc.

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RL and Optimal Control (OC)

→ different sides of the same medal

- RL: appeared first in behavioral psychology: decision making
- OC: appeared in optimization problem solving: variational calculus

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OC ← *closely related* → **RL**

OC	**RL**
based on: ***variational calculus***	***Markov decision processes***
• needs model for environment to express cost function in.	• no model of controlled system, adaptive, autonomous.
• best suited for deterministic environments.	• stochastic/uncertain environments.
• differentiable cost function C_h uses gradient descent.	• reward function can be discontinuous, noisy.
• advantage: if we can compute analytically derivative of C_h.	• figures out effective degrees of freedom without a model.

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Why RL in Nonequilibrium Dynamics?

→ **model-free:** find effective control degrees of freedom (dof)

- microscopic descriptions have extensively many dof
- cannot solve equations of motion
- use (deep) RL to find guiding principles away from equilibrium?
- RL can handle uncertain environments and learn policies in the presence of various (correlated) sources of noise?

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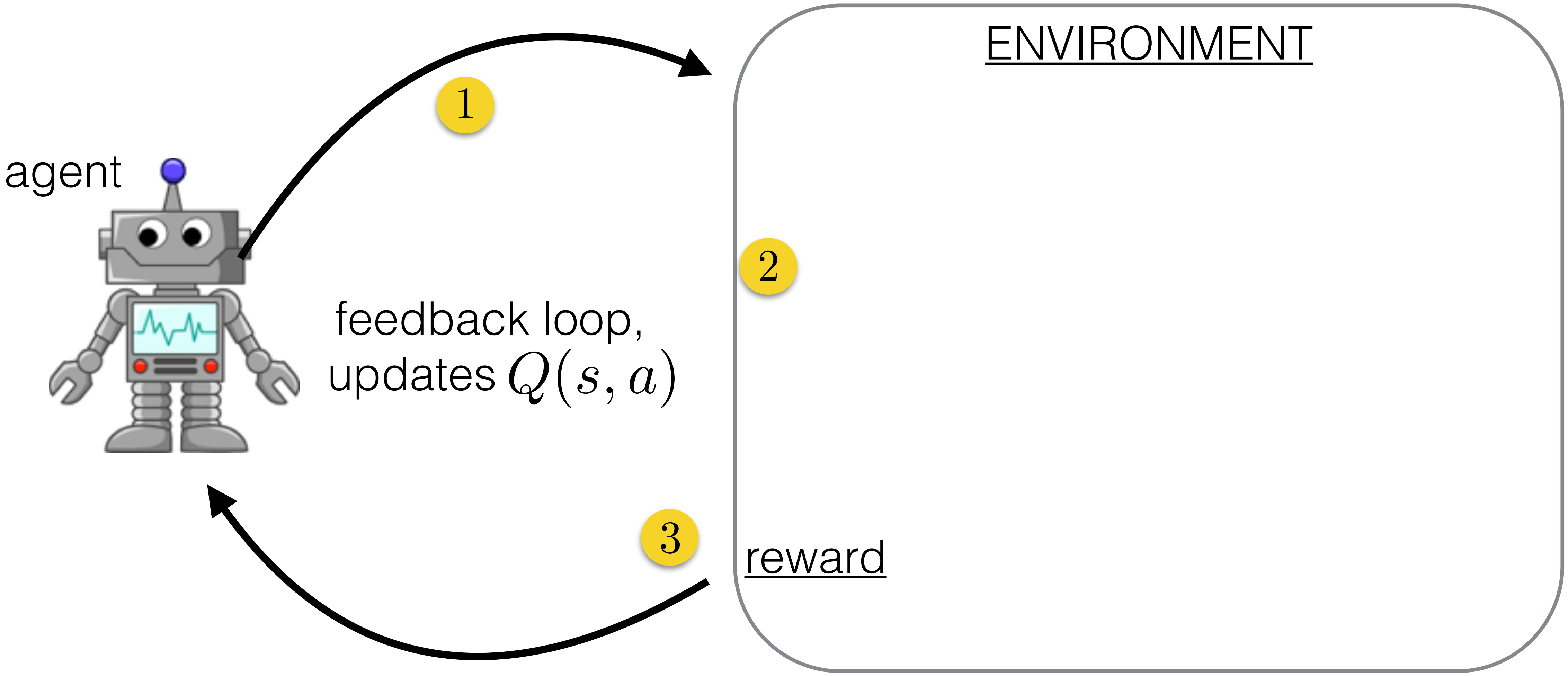
→ **autonomous:** does not require supervision

- RL can automate experimental setups?
- **on-line:** improve policy on-the-fly, i.e. before episode is over

RL Applied to Quantum State Preparation



t_f

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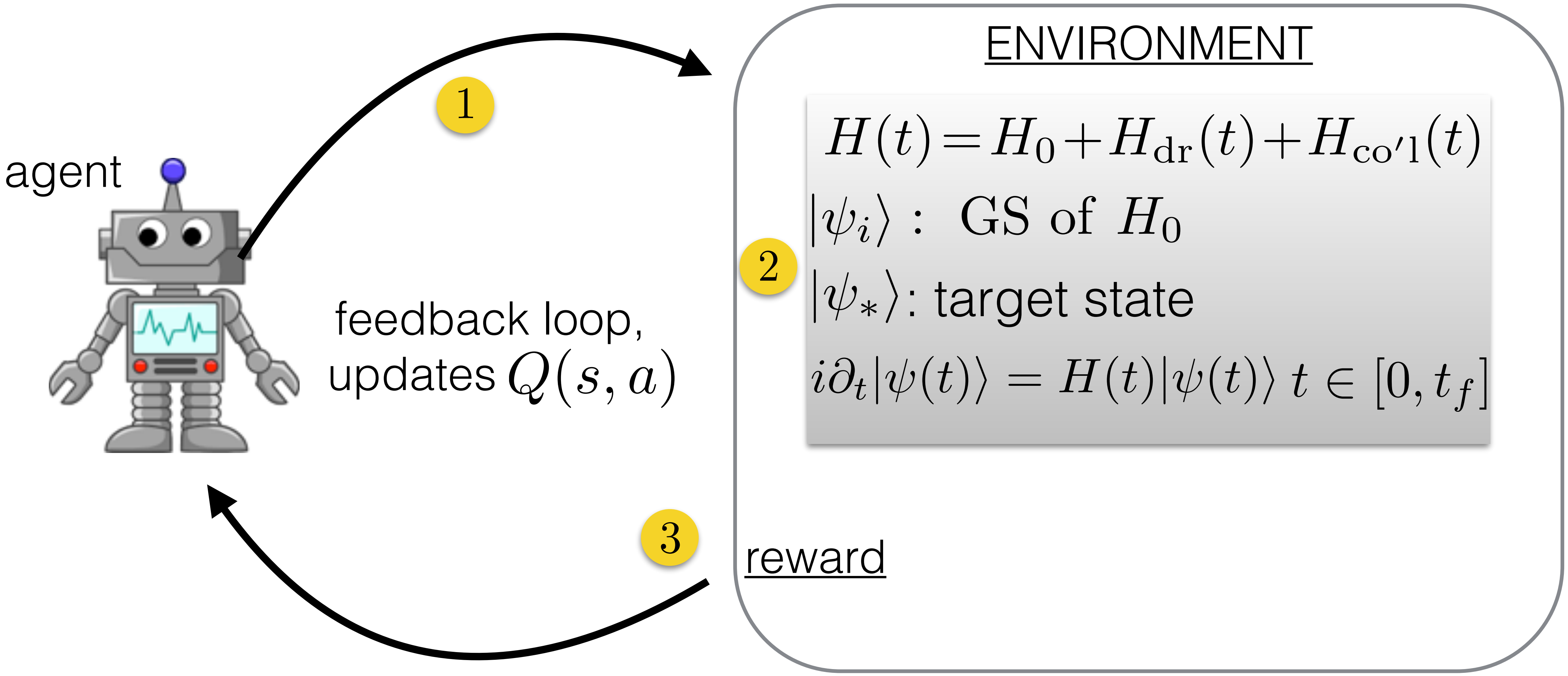

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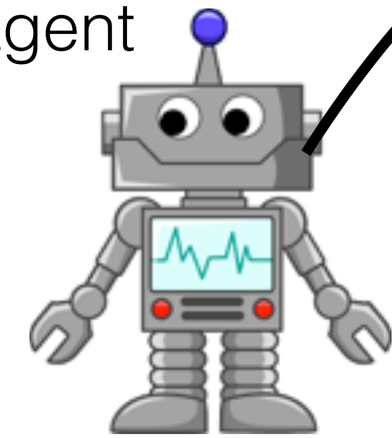
RL Applied to Quantum State Preparation

agent



1

feedback loop, updates $Q(s,a)$

ENVIRONMENT

2

$$H(t) = H_0 + H_{\rm dr}(t) + H_{\rm co'l}(t)$$

$|\psi_i\rangle$: GS of H_0

$|\psi_*\rangle$: target state

$$i\partial_t|\psi(t)\rangle = H(t)|\psi(t)\rangle \; t\in[0,t_f]$$

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reward $r = \begin{cases} 0 & , 0 \le t < t_f \\ |\langle\psi_*|\psi(t=t_f)\rangle|^2 & , t = t_f \end{cases}$

t_f

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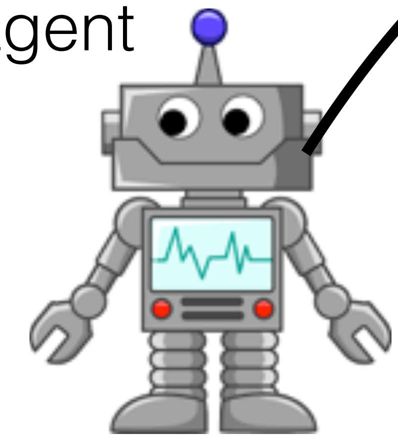

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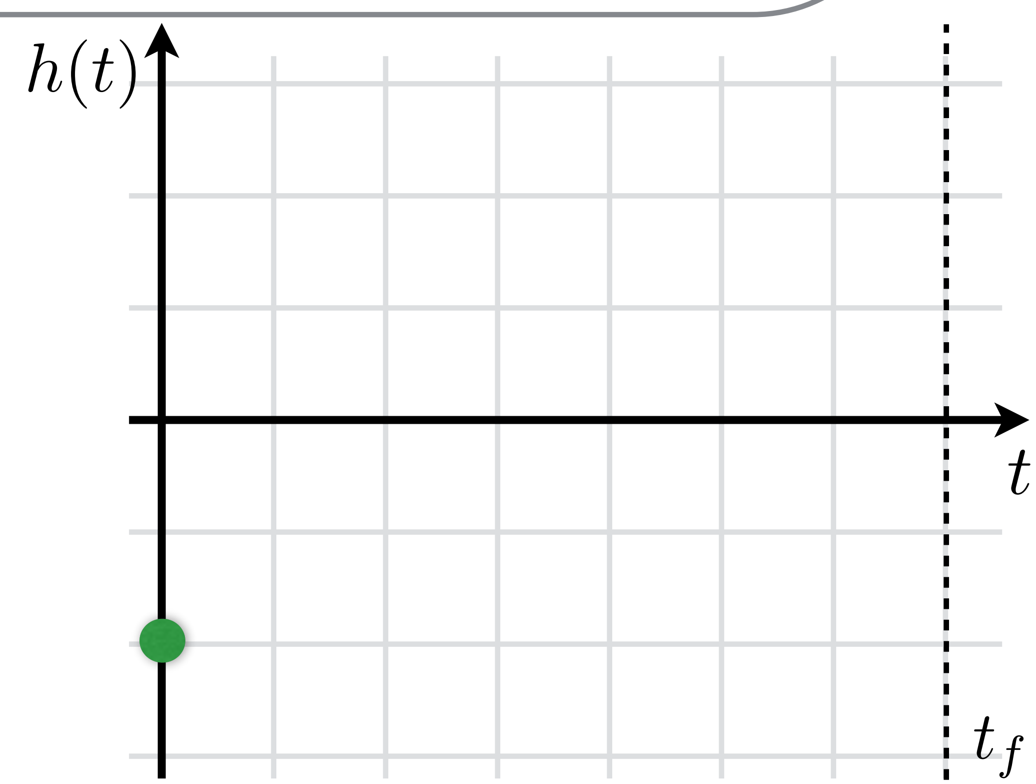

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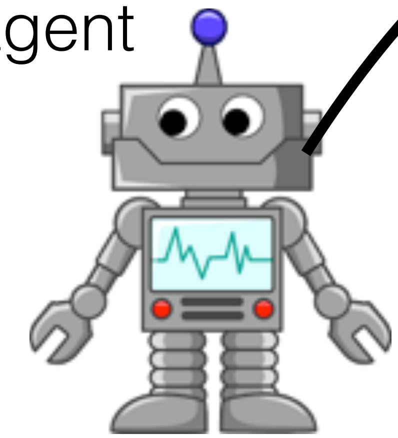

feedback loop, updates $Q(s,a)$

ENVIRONMENT

$$H(t) = H_0 + H_{\mathrm{dr}}(t) + H_{\mathrm{co'l}}(t)$$

$|\psi_i\rangle$: GS of H_0

$|\psi_*\rangle$: target state

$$i\partial_t|\psi(t)\rangle = H(t)|\psi(t)\rangle \quad t\in[0,t_f]$$

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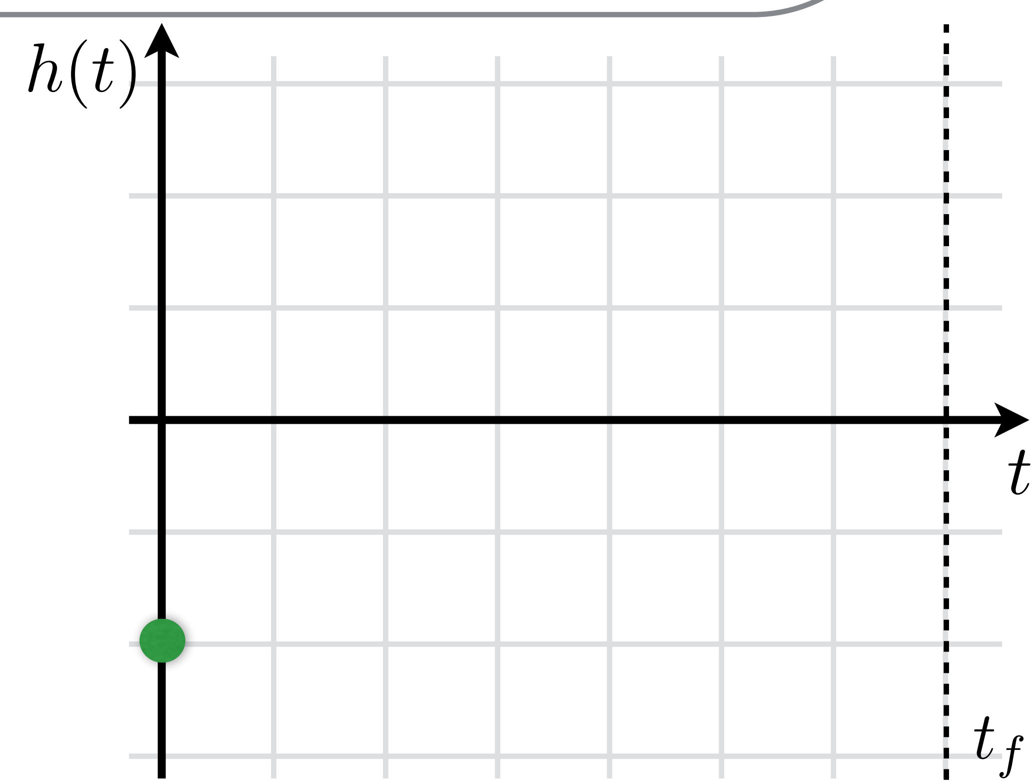

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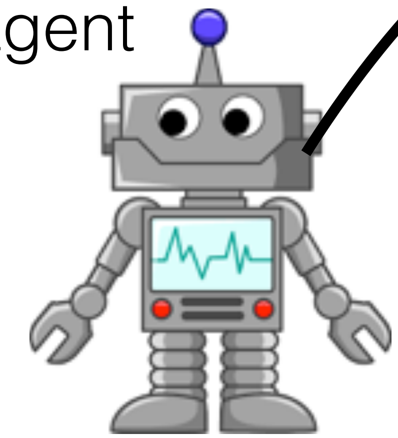

feedback loop,
updates $Q(s,a)$

1

ENVIRONMENT

2

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$$i\partial_t|\psi(t)\rangle = H(t)|\psi(t)\rangle \; t\in[0,t_f]$$

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reward $r = \begin{cases} 0 & , 0\leq t < t_f \\ |\langle\psi_*|\psi(t=t_f)\rangle|^2 & , t=t_f \end{cases}$

1

start from state $s_0=[h(0)]=[-4]$

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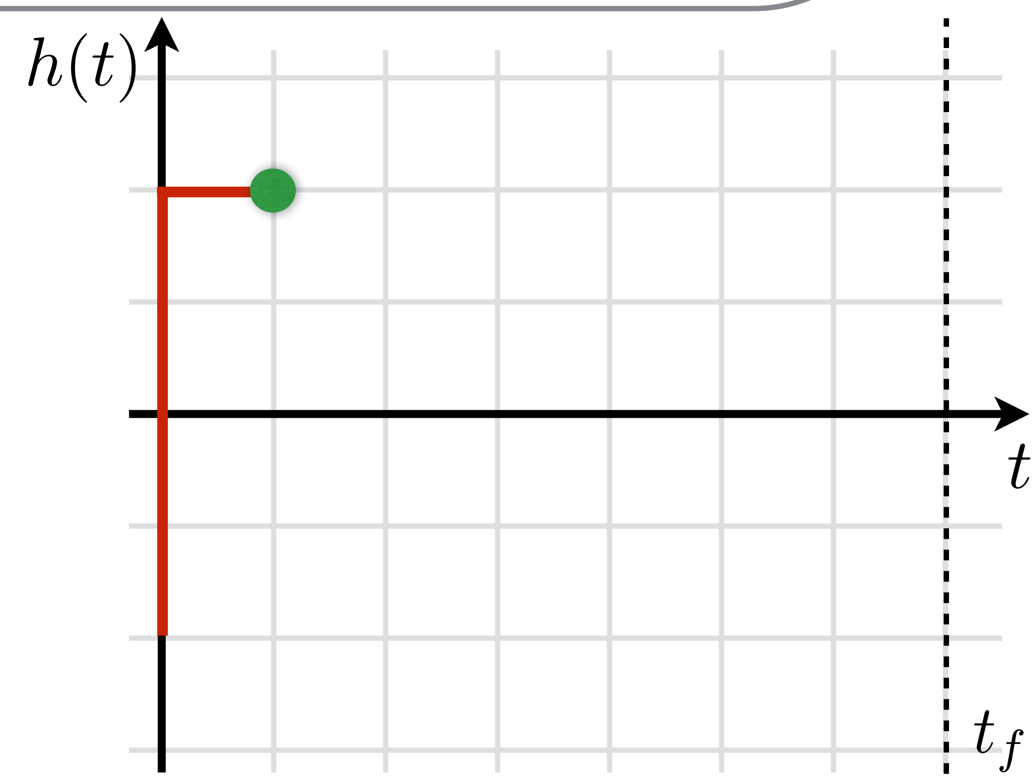

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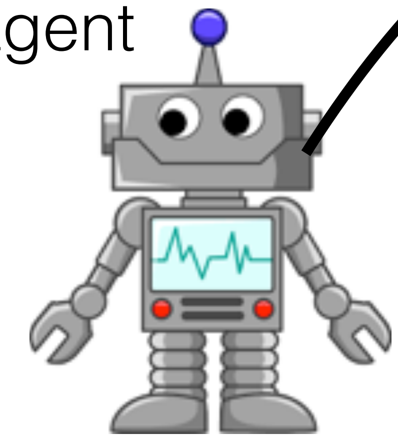

feedback loop, updates $Q(s,a)$

1

ENVIRONMENT

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2

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3

reward $r = \begin{cases} 0 & , 0 \leq t < t_f \\ |\langle\psi_*|\psi(t=t_f)\rangle|^2 & , t = t_f \end{cases}$

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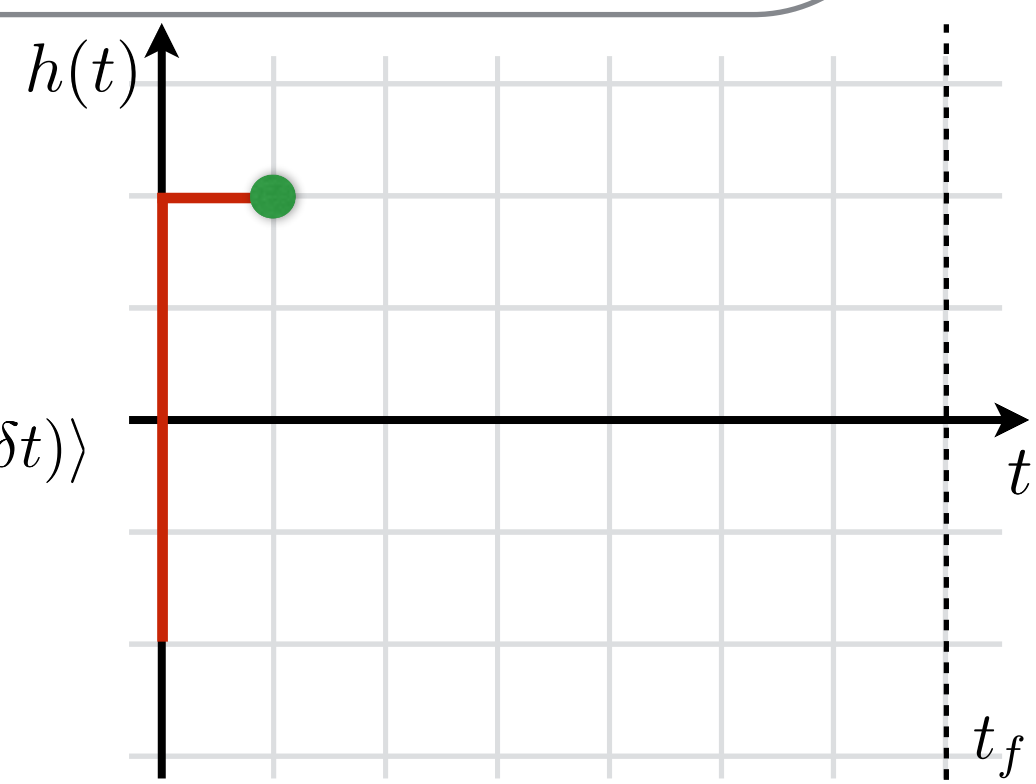

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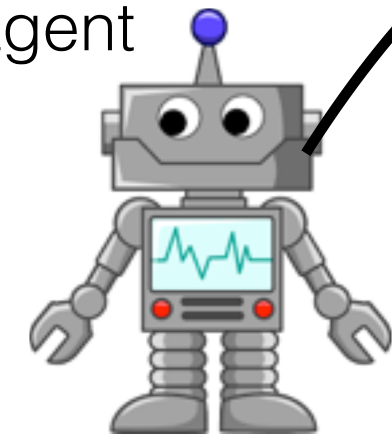

feedback loop, updates $Q(s, a)$

1

ENVIRONMENT

$$H(t) = H_0 + H_{\mathrm{dr}}(t) + H_{\mathrm{co'l}}(t)$$

2

$|\psi_i\rangle$: GS of H_0

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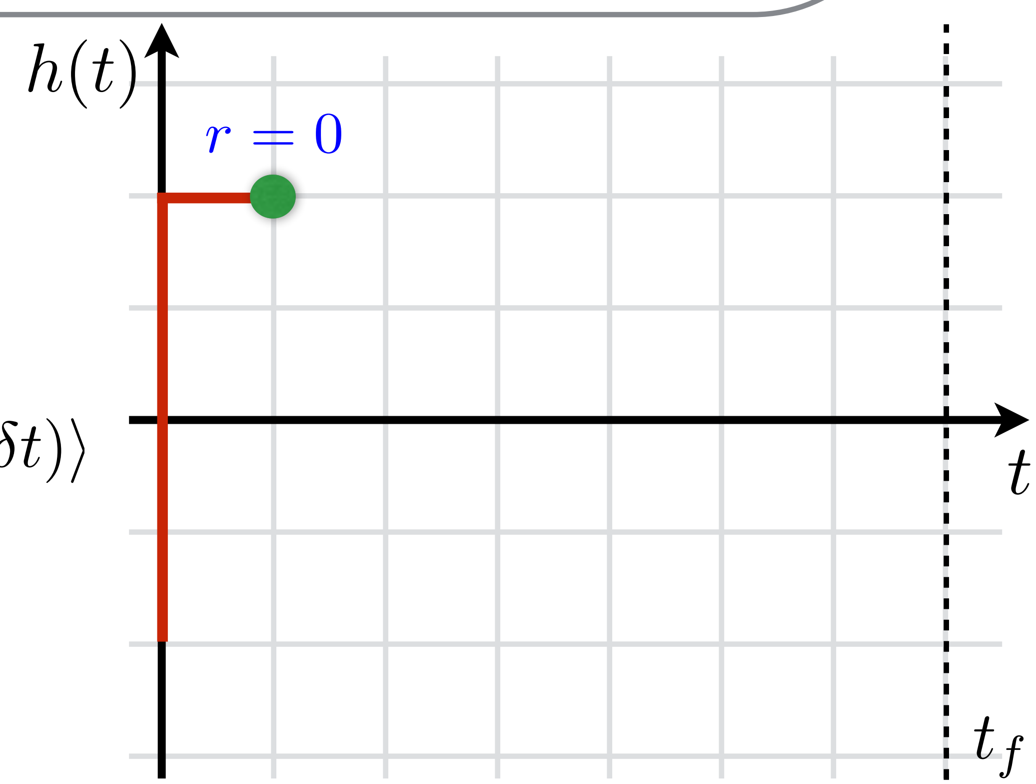

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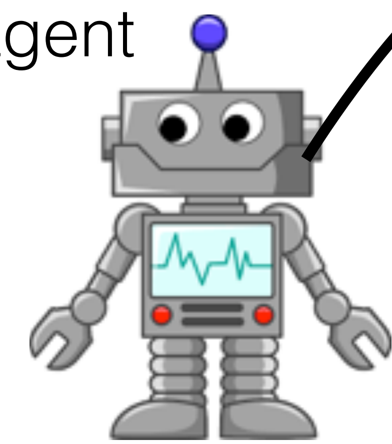

(1)

feedback loop,
updates $Q(s,a)$

(3)

ENVIRONMENT

$$H(t) = H_0 + H_{dr}(t) + H_{co'l}(t)$$

(2)

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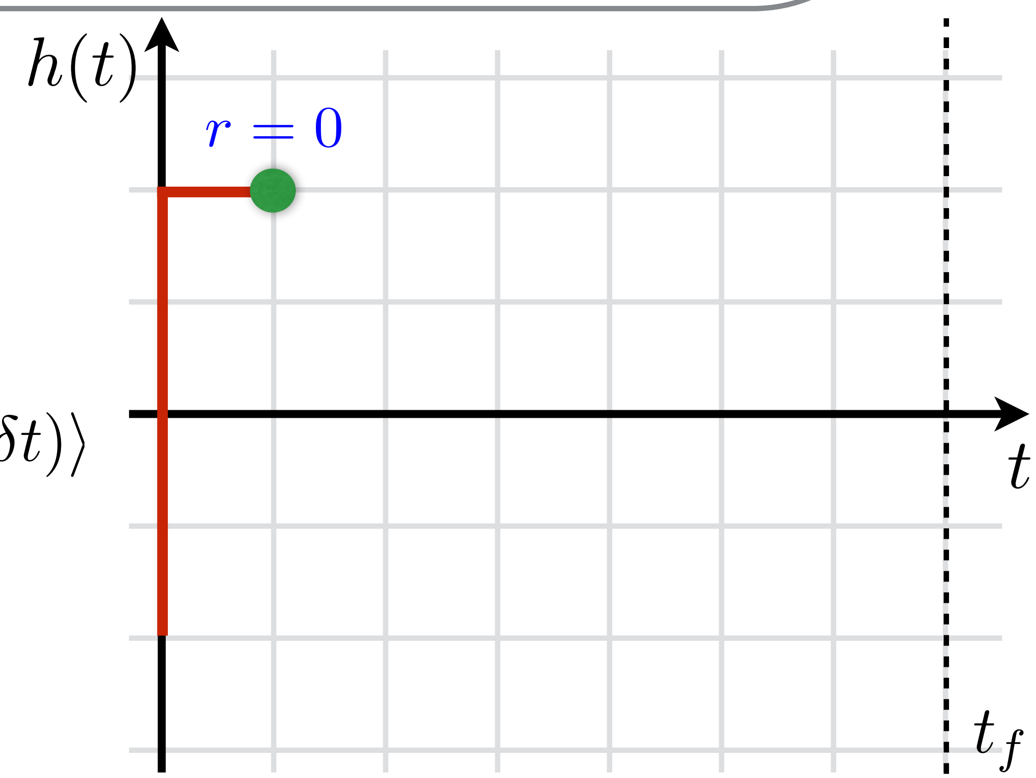

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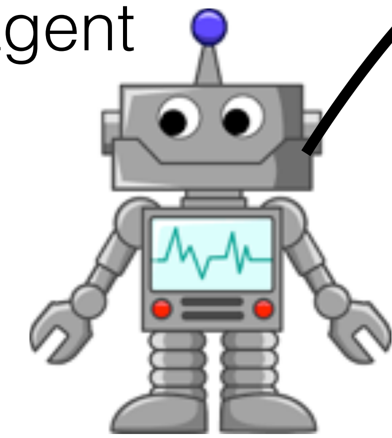

feedback loop, updates $Q(s, a)$

1 → **ENVIRONMENT**

2

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$$i\partial_t|\psi(t)\rangle = H(t)|\psi(t)\rangle \; t \in [0, t_f]$$

3 ← reward $r = \begin{cases} 0 & , 0 \leq t < t_f \\ |\langle\psi_*|\psi(t = t_f)\rangle|^2 & , t = t_f \end{cases}$

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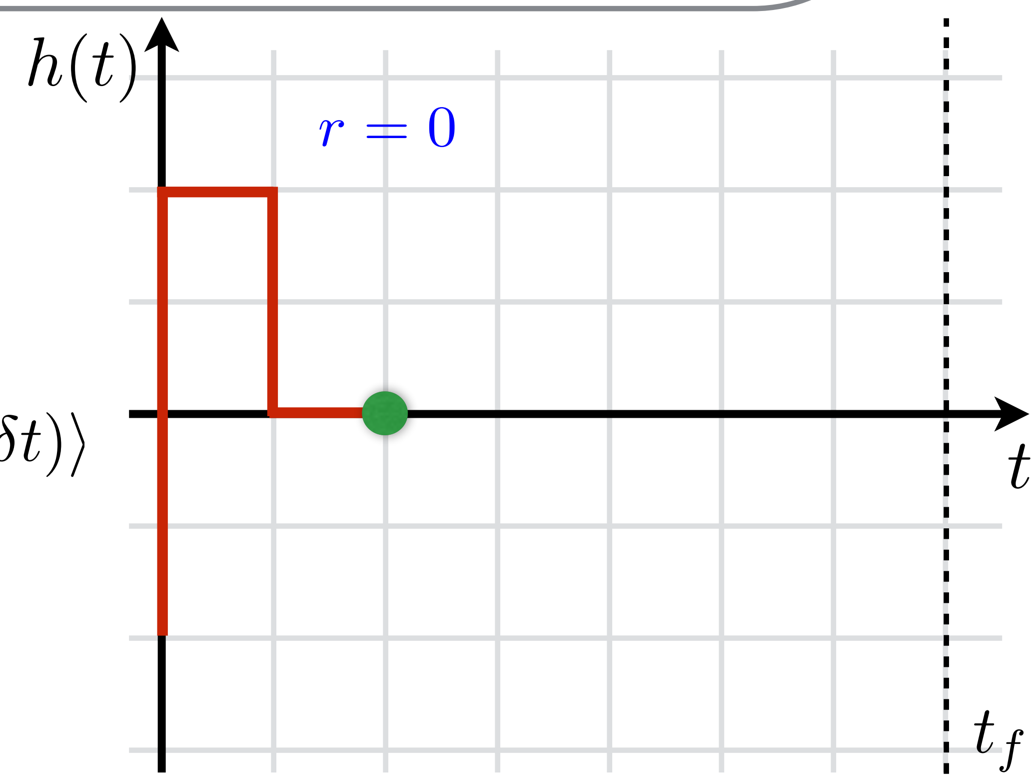

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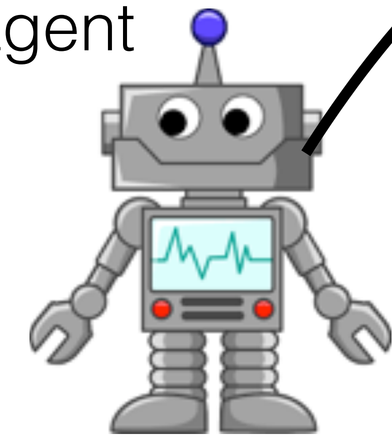

1

feedback loop,
updates $Q(s,a)$

3

ENVIRONMENT

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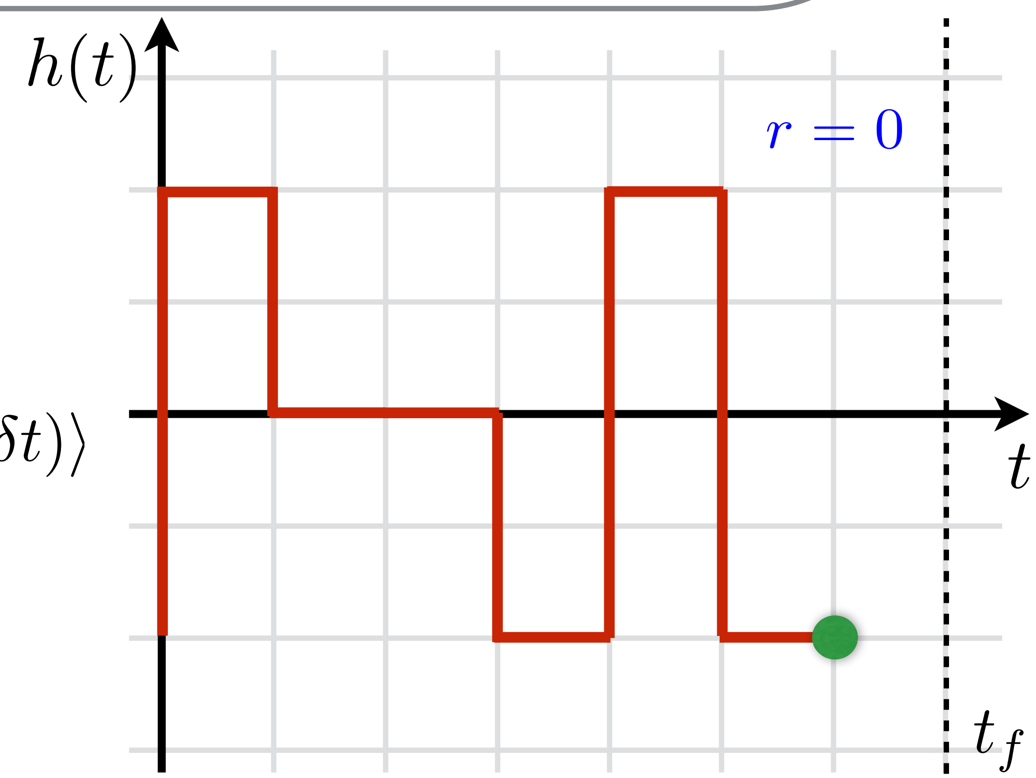

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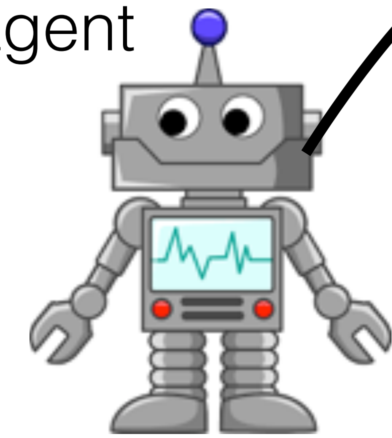

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feedback loop, updates $Q(s,a)$

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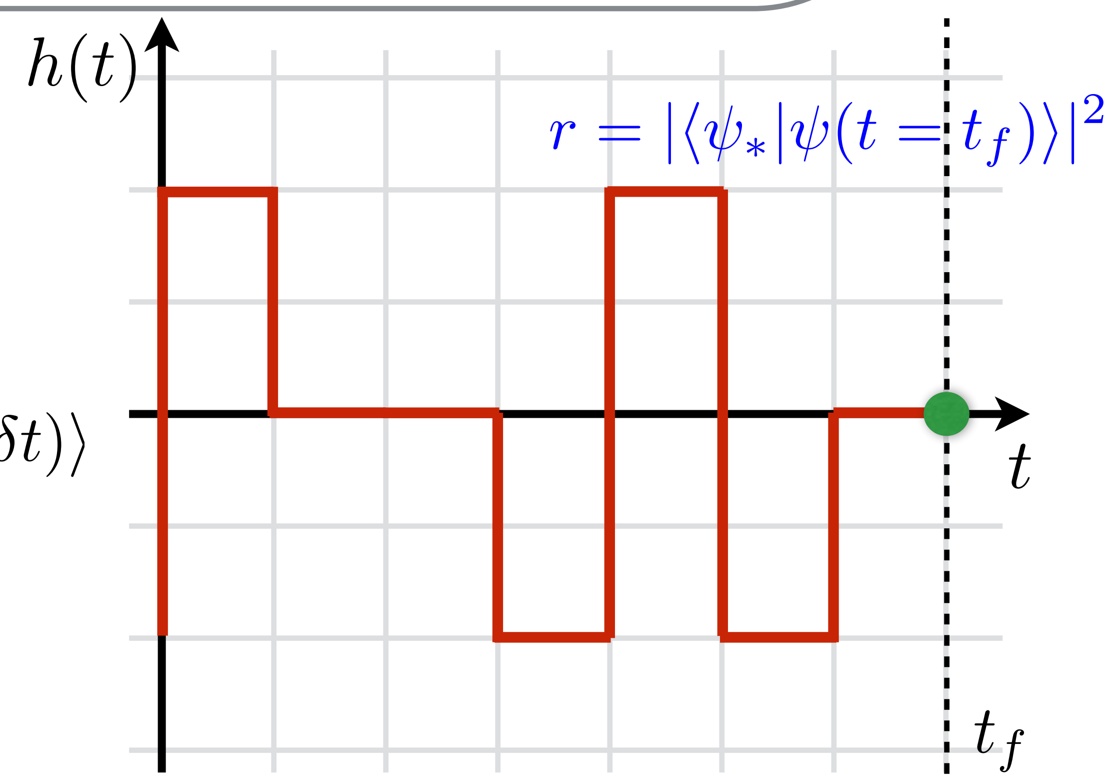

episode completed

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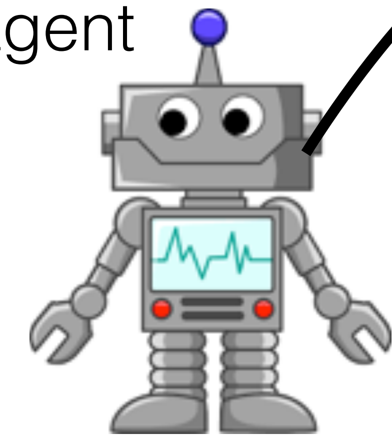

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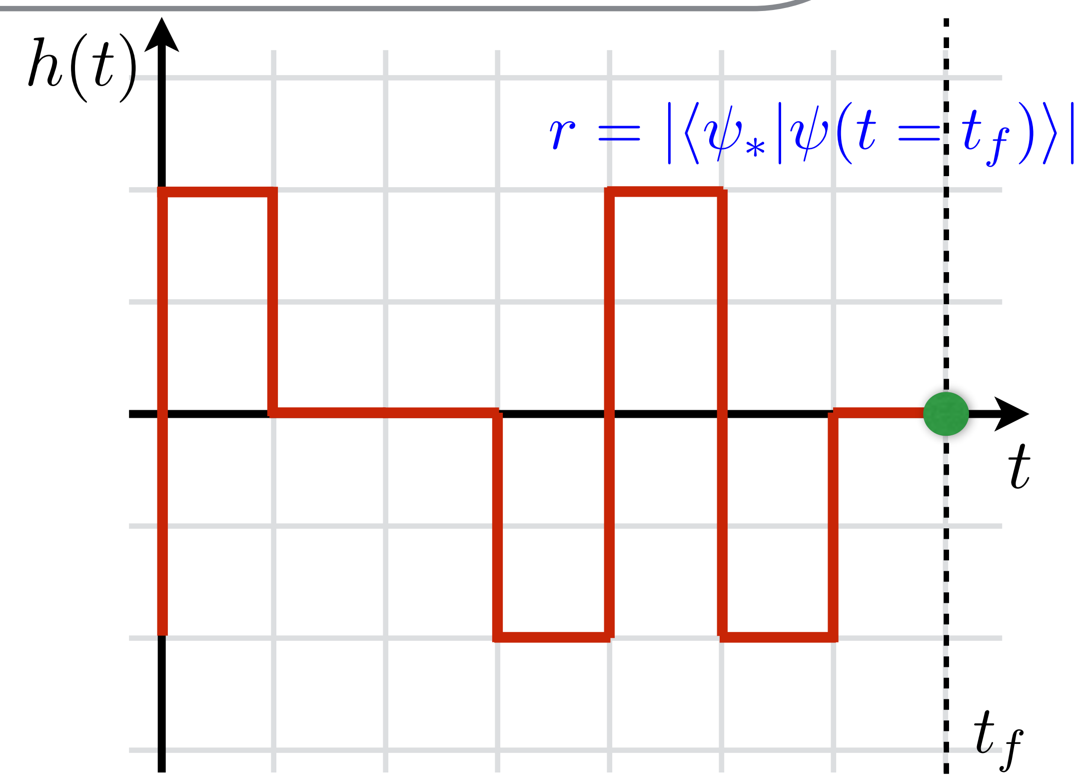

problems:

→ state space *exponentially* big

→ how do we choose actions?

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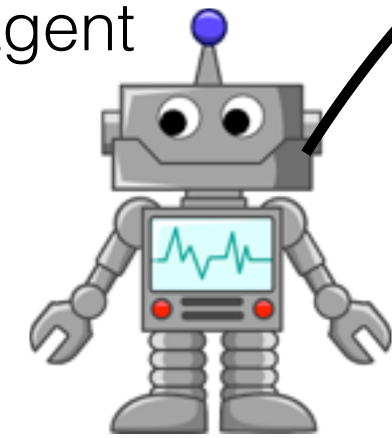

1

feedback loop, updates $Q(s,a)$

ENVIRONMENT

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$$H(t) = H_0 + H_{\rm dr}(t) + H_{\rm co'l}(t)$$

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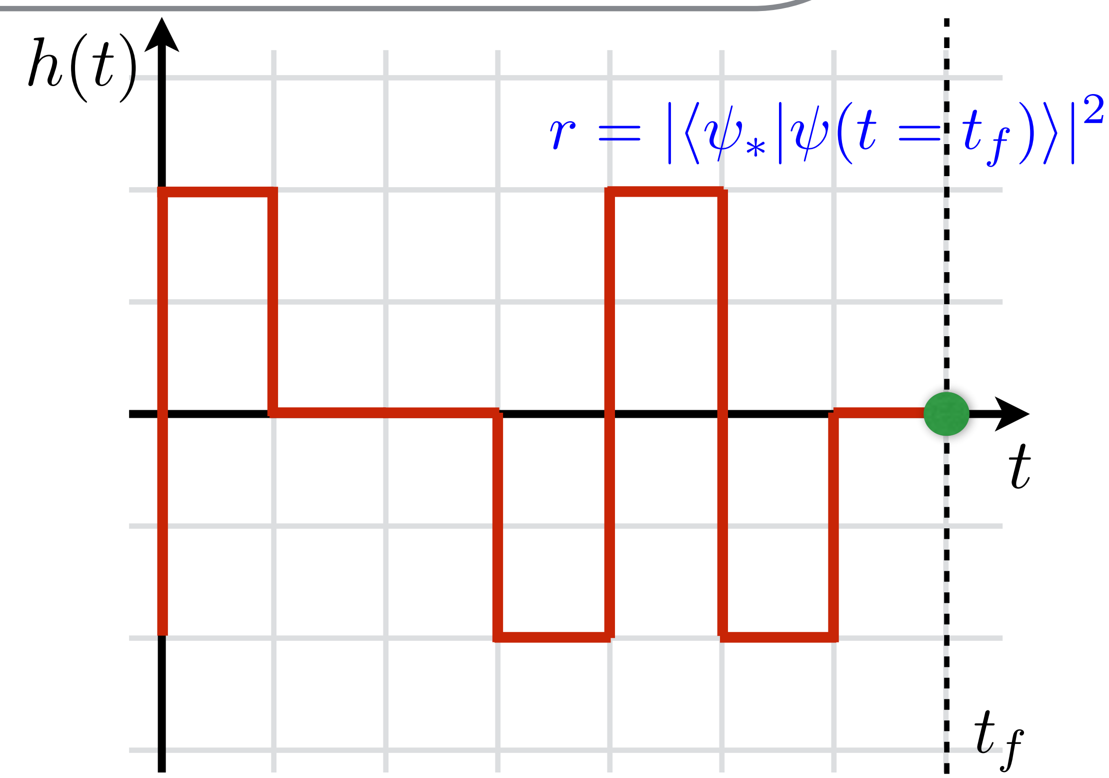

problems:

→ state space *exponentially* big

RL ~ biased MC sampling

→ how do we choose actions?

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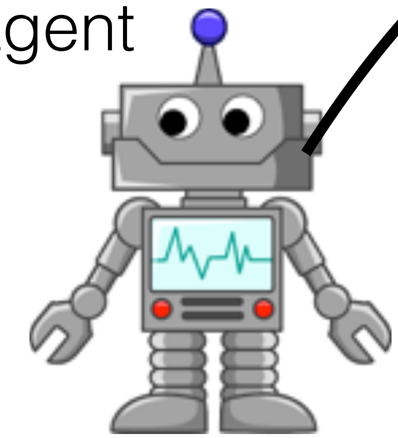

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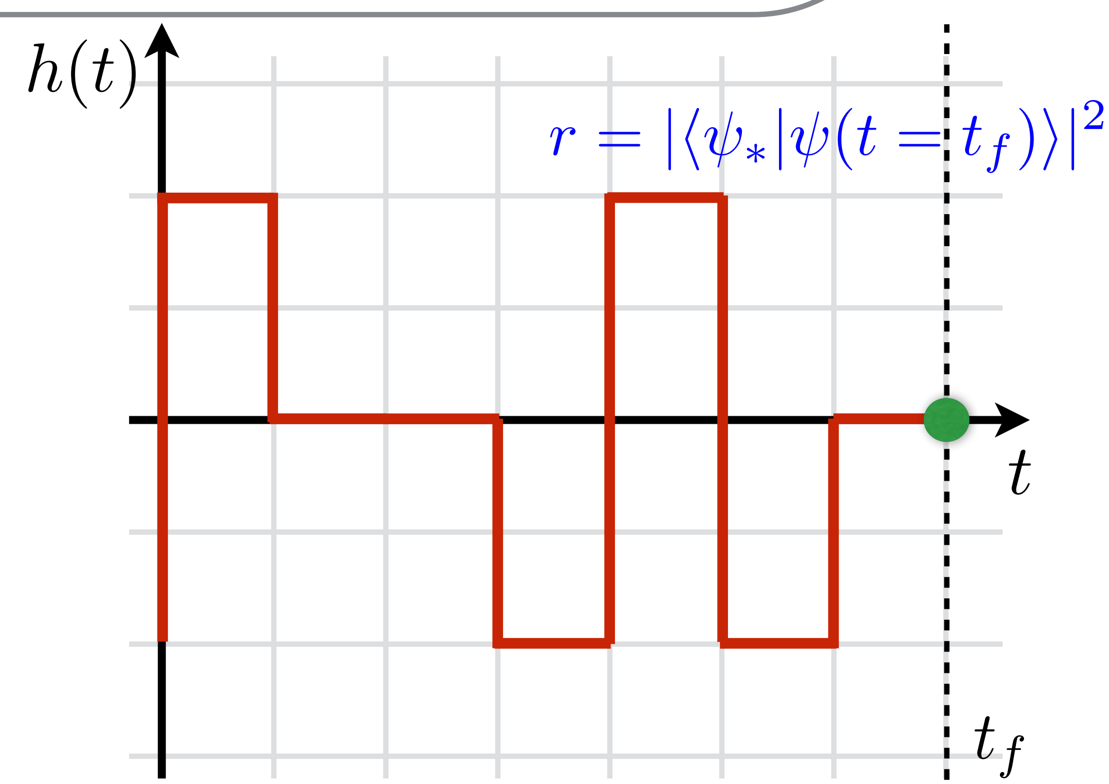

problems:

→ state space *exponentially* big

RL ~ biased MC sampling

→ how do we choose actions?

exploration exploitation dilemma

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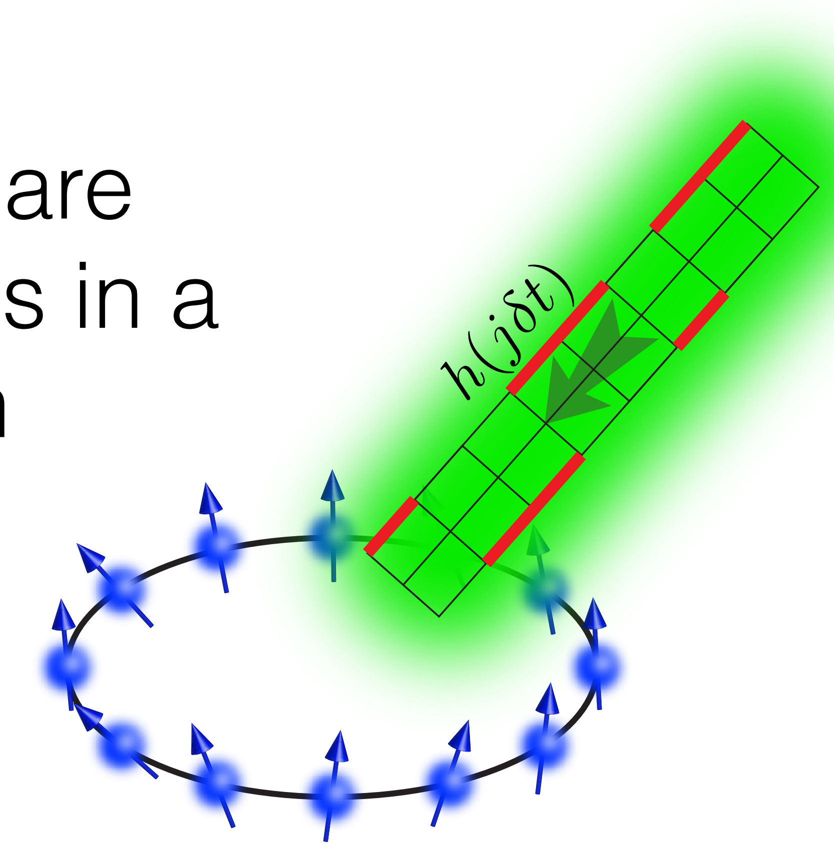
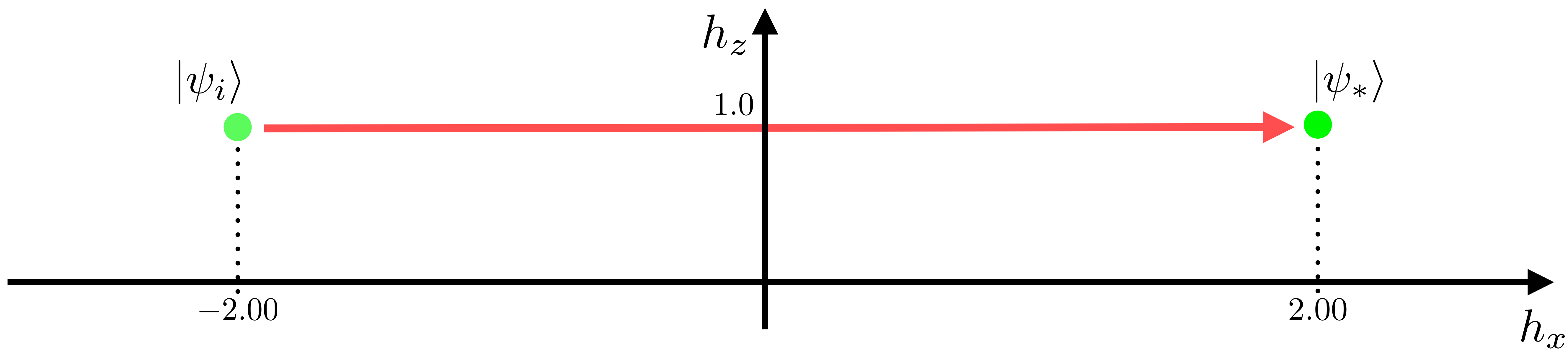
Example 1:

use RL to autonomously prepare paramagnetic many-body states in a **nonintegrable spin chain**



$$H(t) = -\sum_{j=1}^{L} S^z_{j+1}S^z_j + h_z S^z_j + h_x(t) S^x$$

→ initial $|\psi_i\rangle$ and target $|\psi_*\rangle$ states are (paramag) GS at:



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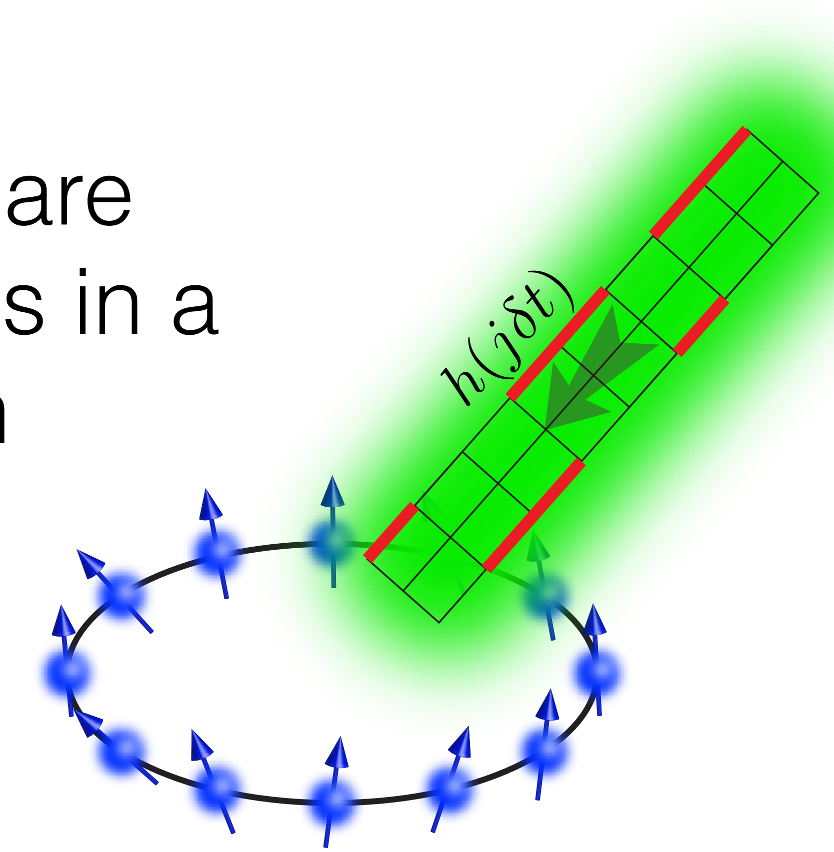

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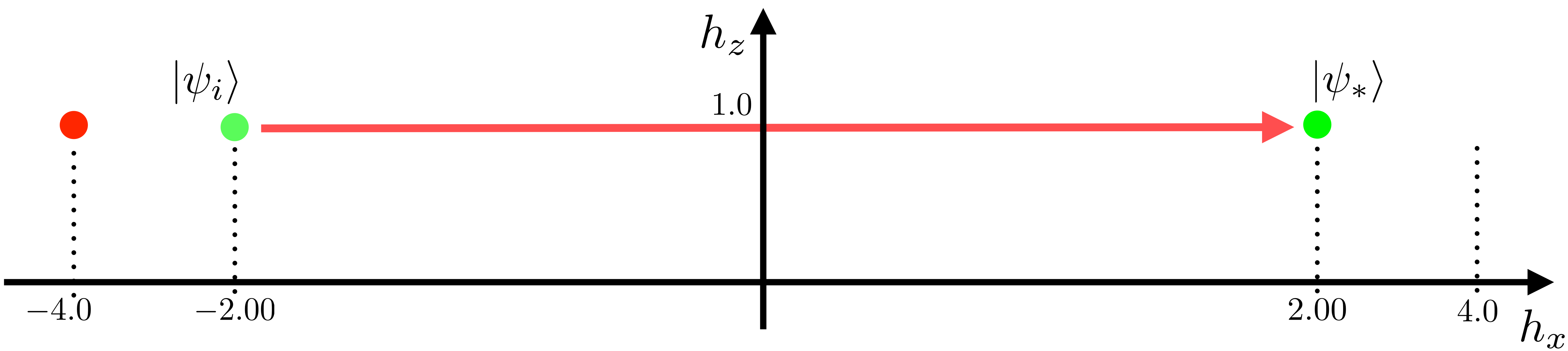

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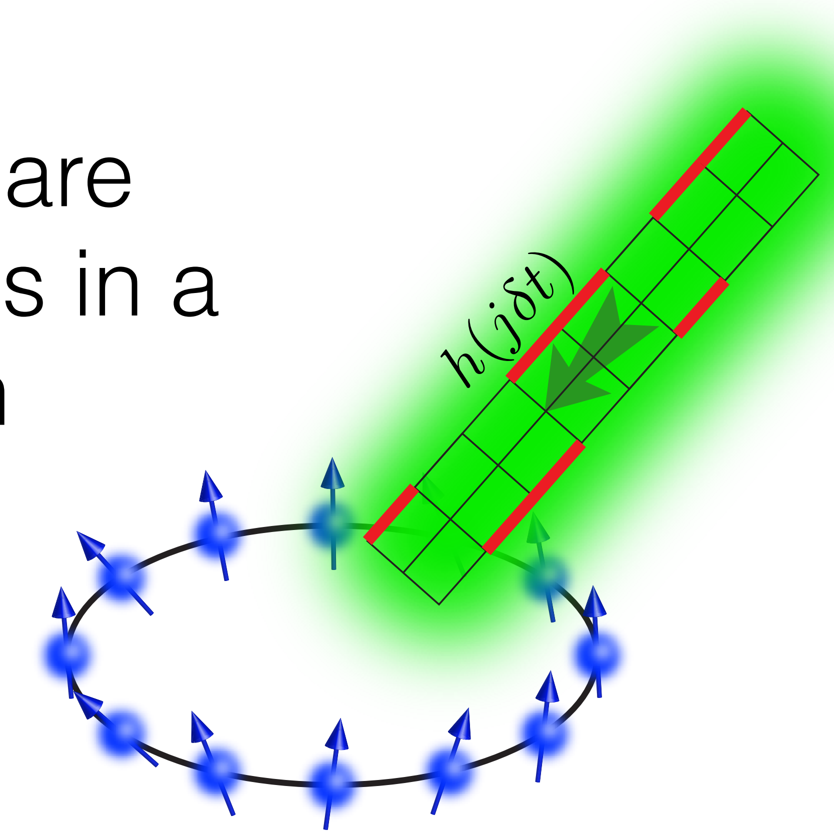

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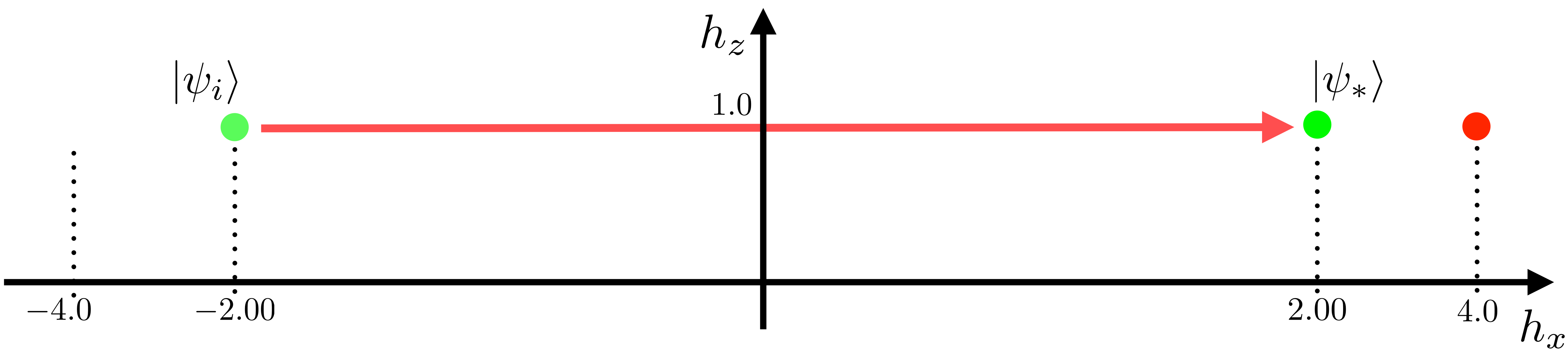

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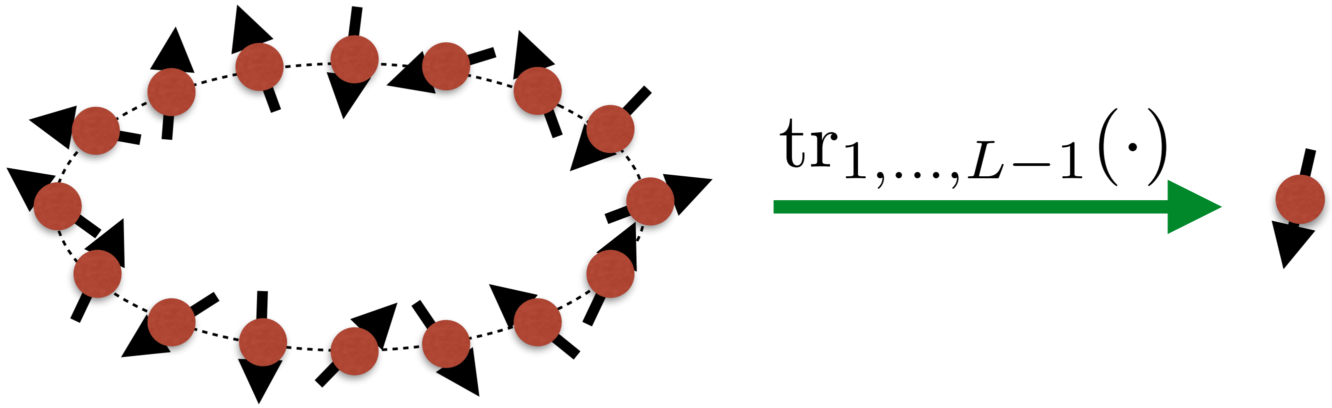
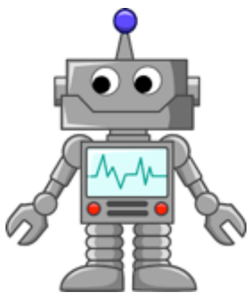
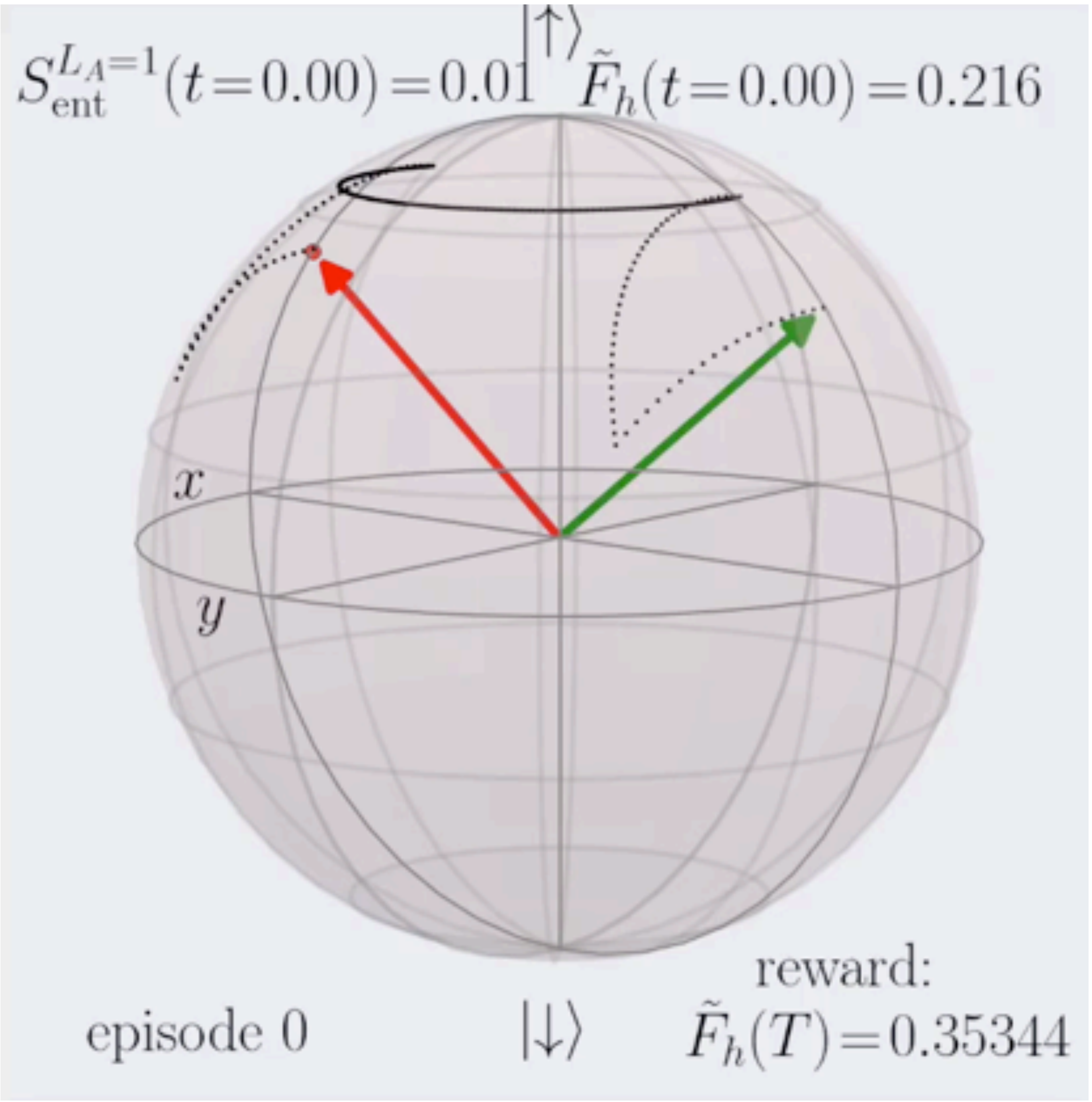
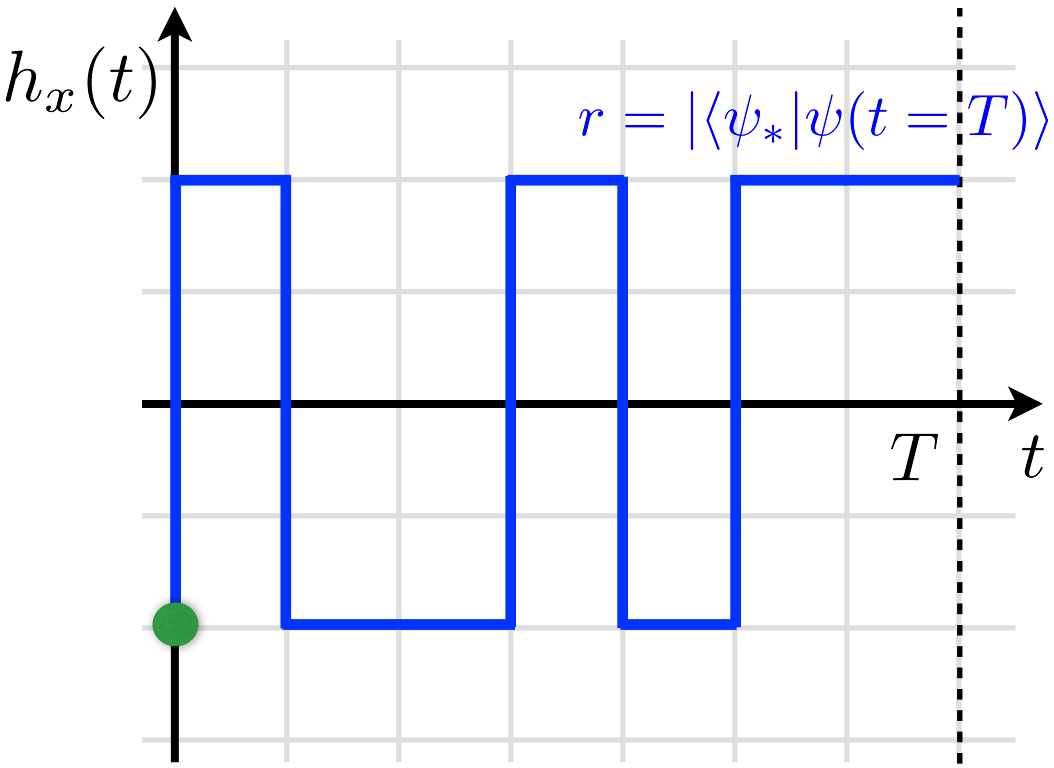
Learning a Many-Body Protocol



$h_x \in \{\pm 4\}$ bang-bang protocols





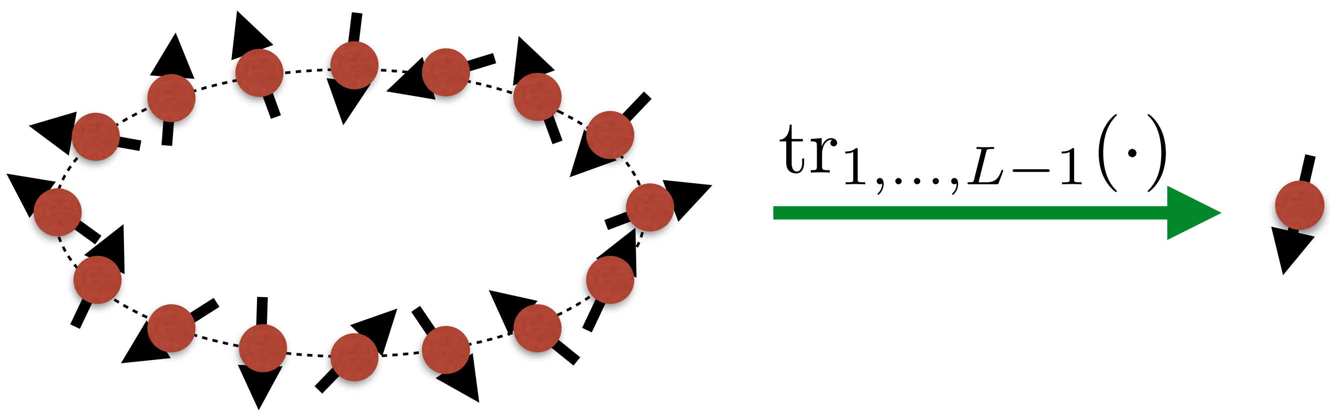


episode completed

$$H = \sum -S^z_{j+1}S^z_j - h_z S^z_j - h_x(t) S^x_j$$

arXiv: *1705.00565* (2017)

Learning a Many-Body Protocol



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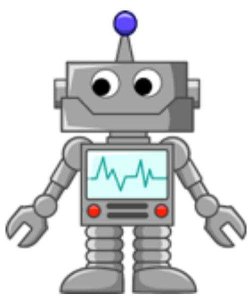

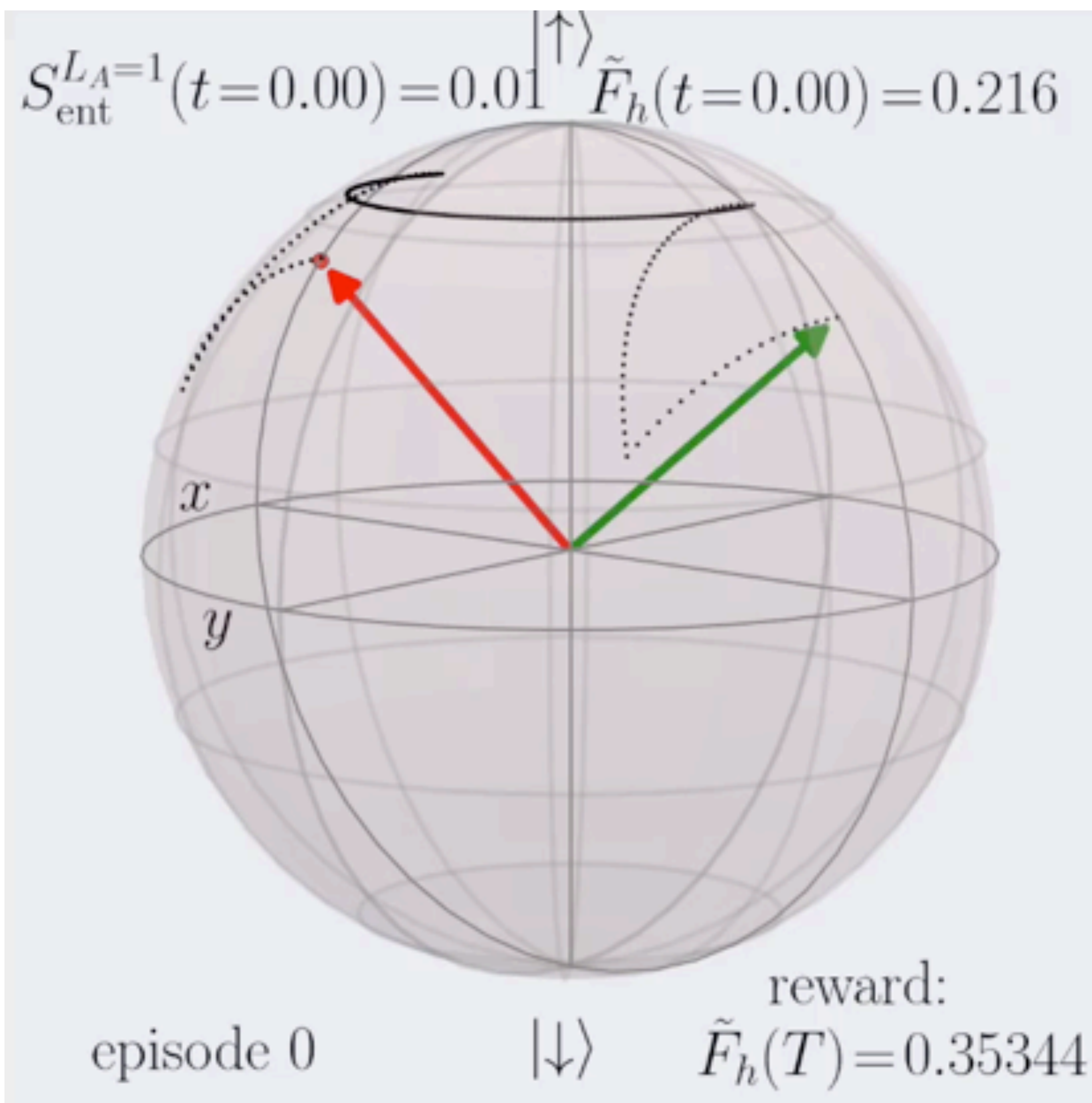

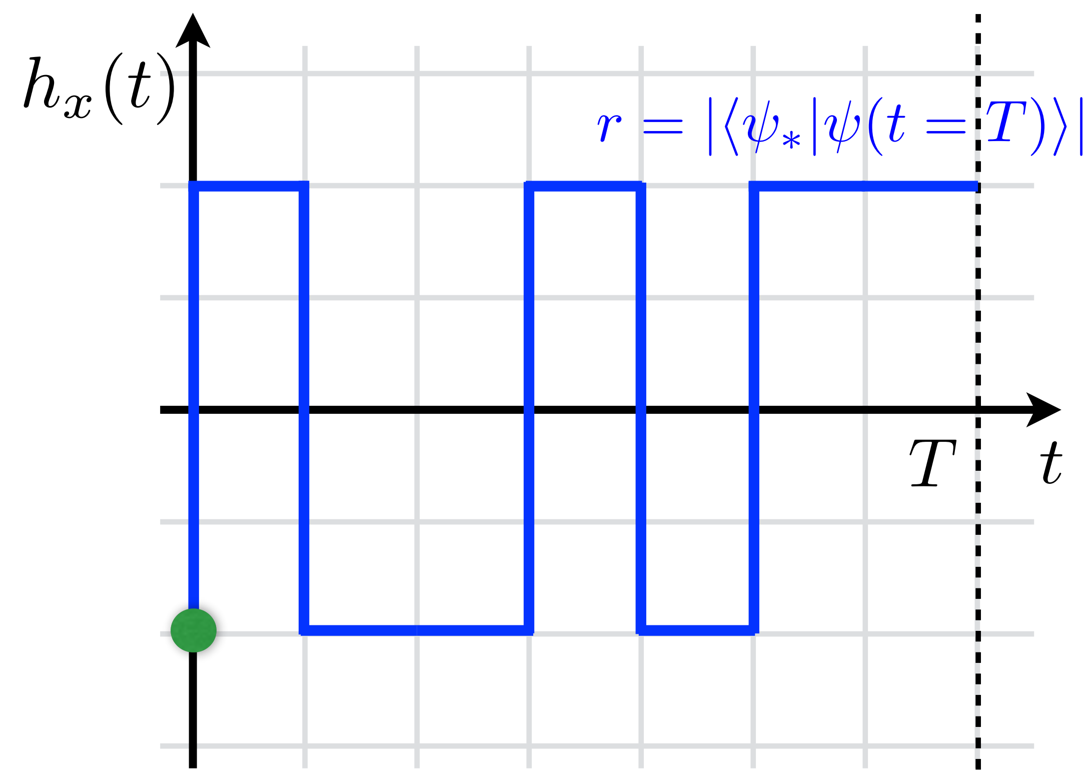

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Learning a Many-Body Protocol

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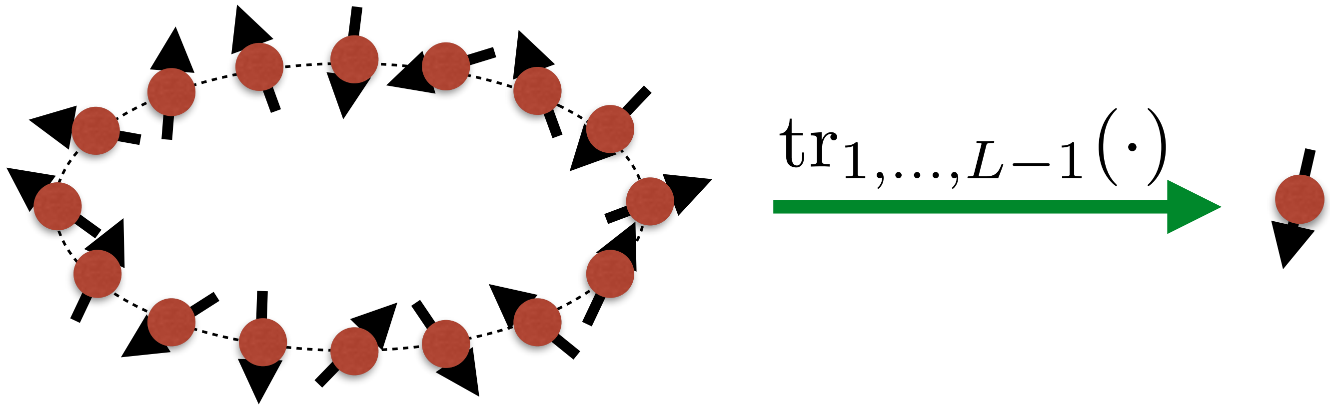

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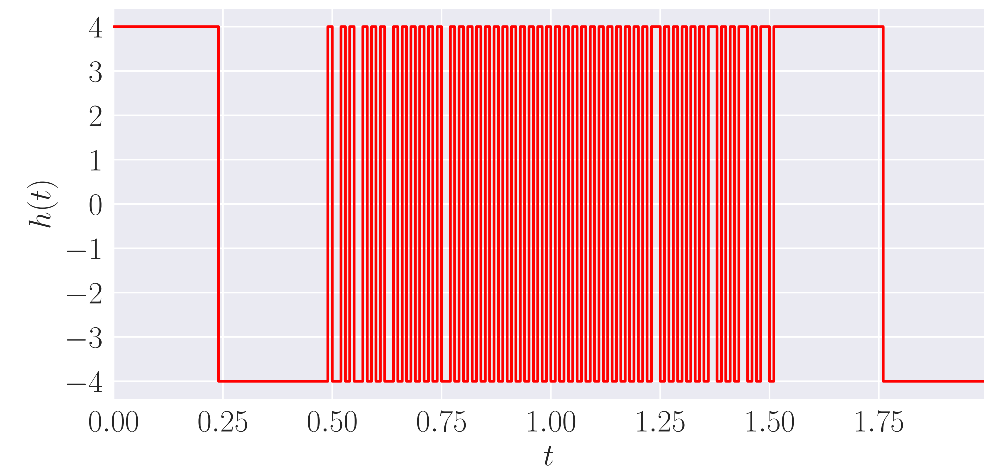

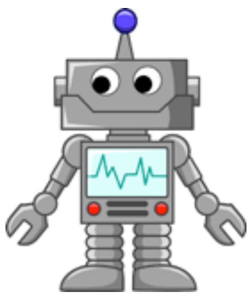

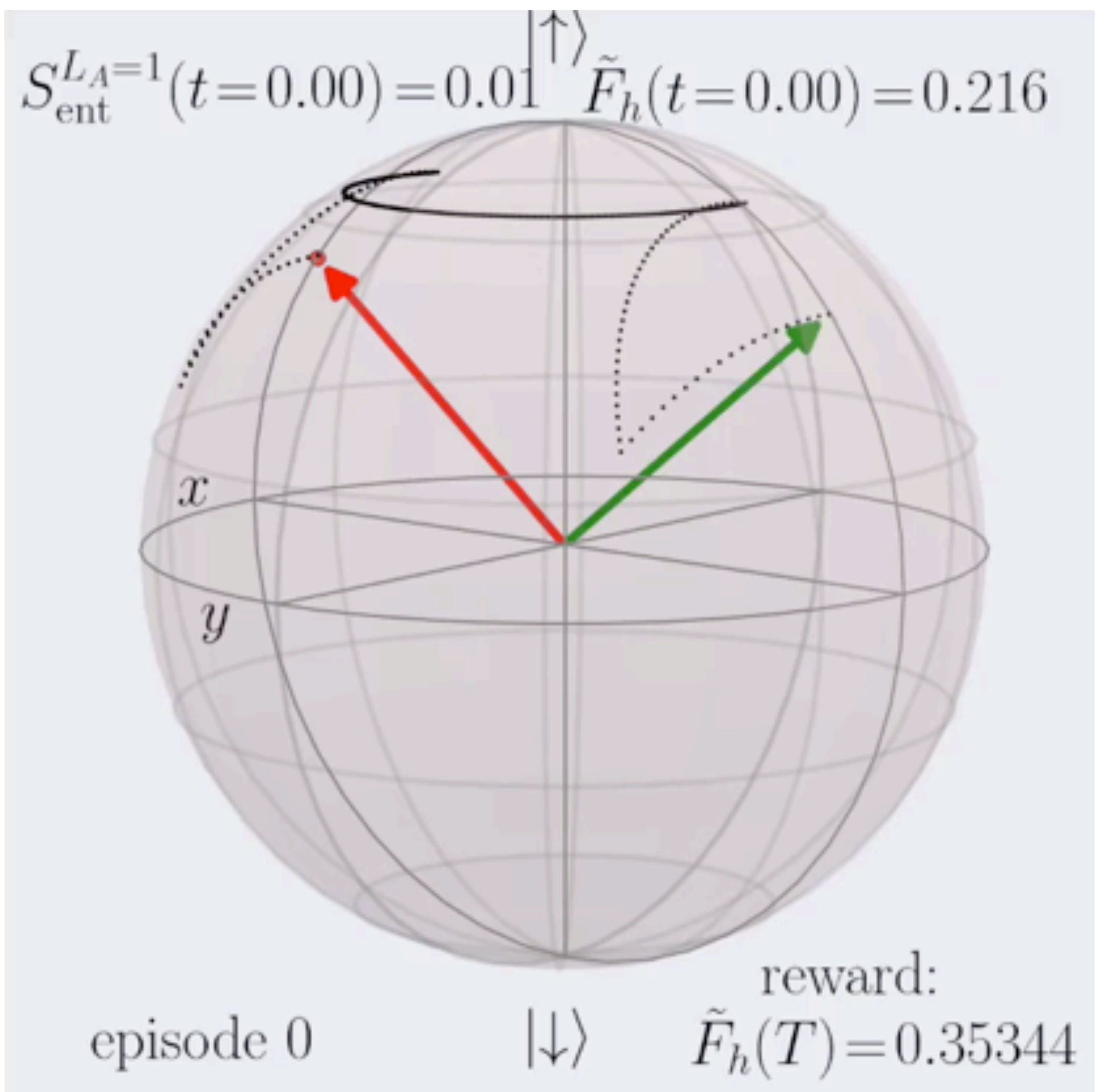

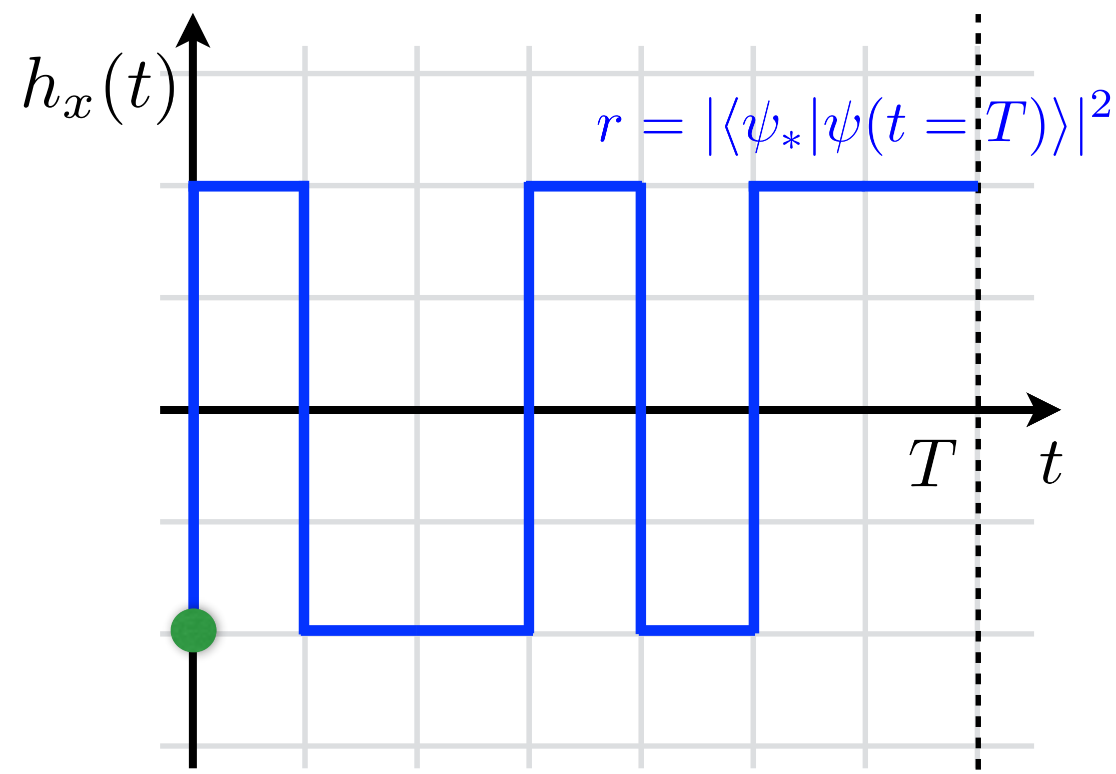

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$$H = \sum -S^z_{j+1}S^z_j - h_z S^z_j - h_x(t)S^x_j$$

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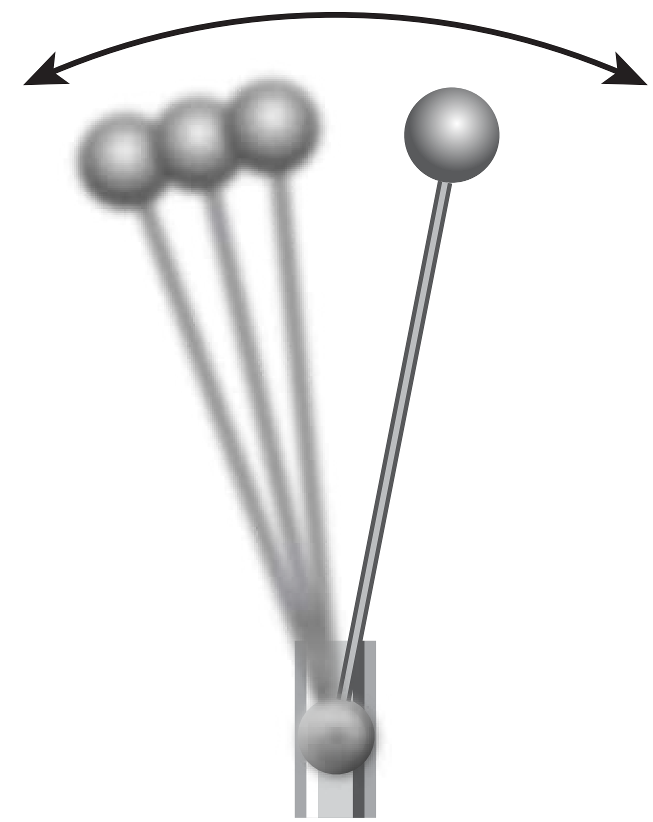
Example 2:

use RL to autonomously prepare
Floquet engineered states in a ***simulation of an "experiment"***

Challenges:



→ **no** direct **access** to quantum state:
play game w/o looking at screen

→ **probabilistic** quantum measurements

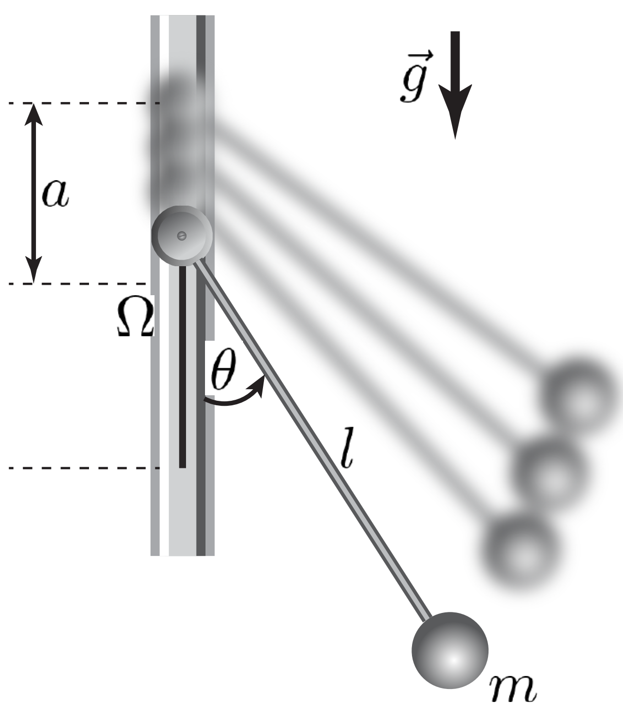
→ **uncertainty** in preparing initial state

→ occasional **failure** of control apparatus

→ additionally: all other problems of how to actually prepare the state if the above were absent and no analytics is known

The Kapitza pendulum

- Kapitza, 1951
- paradigmatic example of Floquet engineering



bluedwarf1127: YouTube (2009)

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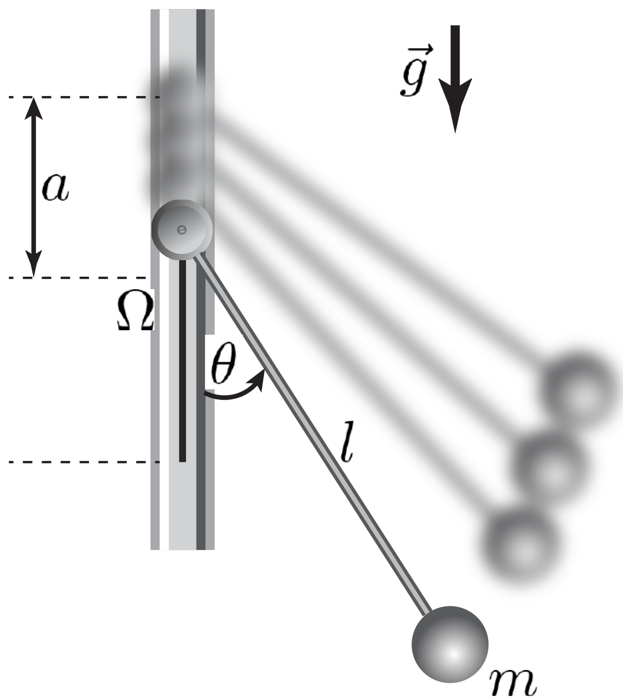

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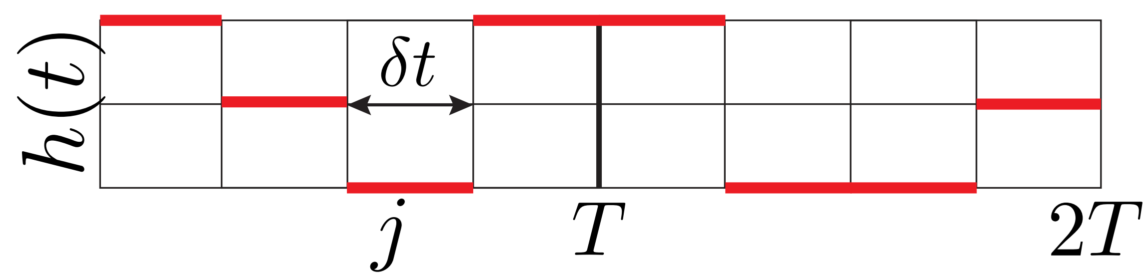
Floquet Engineering Control Problem

→ find optimal control field *on top of periodic drive*

$$H_{\rm rot}(t) = H_0 + H_{\rm drive}(t) + H_{\rm control}(t)$$

$$H_{\rm drive}(t) = -\frac{A}{2m}\mathrm{sign}(\cos\Omega t)[p_\theta, \sin\theta]_+ + \frac{A^2}{4}\left(1-\mathrm{sign}(\sin\Omega t)\right)\cos 2\theta$$

$$H_0 = \frac{p_\theta^2}{2m} - m\omega_0^2\cos\theta \qquad H_{\rm control}(t) = h(t)\sin\theta$$ horizontal kicks



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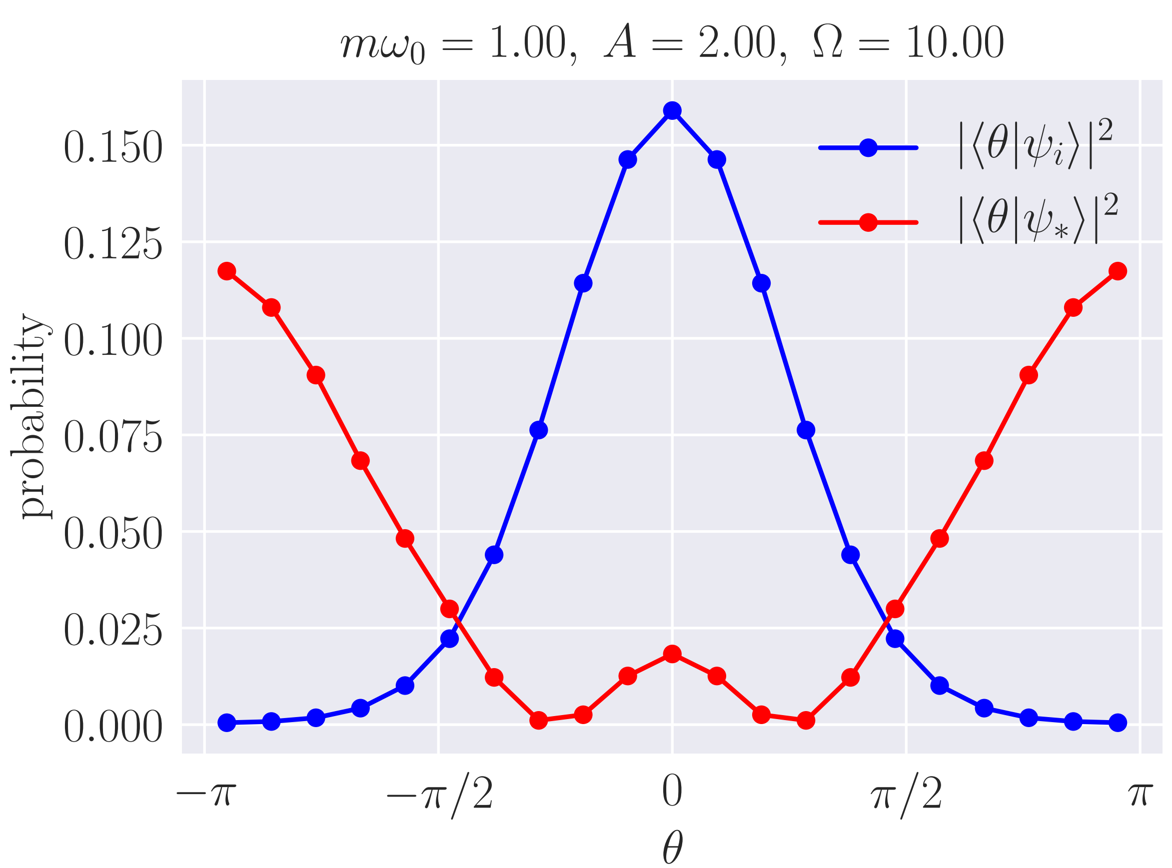
initial state: $|\psi_i\rangle$: GS of H_0

target state: $|\psi_*\rangle$ inverted position eigenstate of $H_F(\Omega)$



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GOAL: find bang-bang protocol $h(t) = h(j\delta t) \in \{-4, 0, +4\}$

such that $|\psi(t=0)\rangle = |\psi_i\rangle, |\psi(t=t_f)\rangle = |\psi_*\rangle$

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Floquet Engineering Control Problem

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$$H_{\rm rot}(t) = H_0 + H_{\rm drive}(t) + H_{\rm control}(t)$$

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measure: quantum measurement of final state $|\psi(t=t_f)\rangle$ along target state $|\psi_*\rangle$

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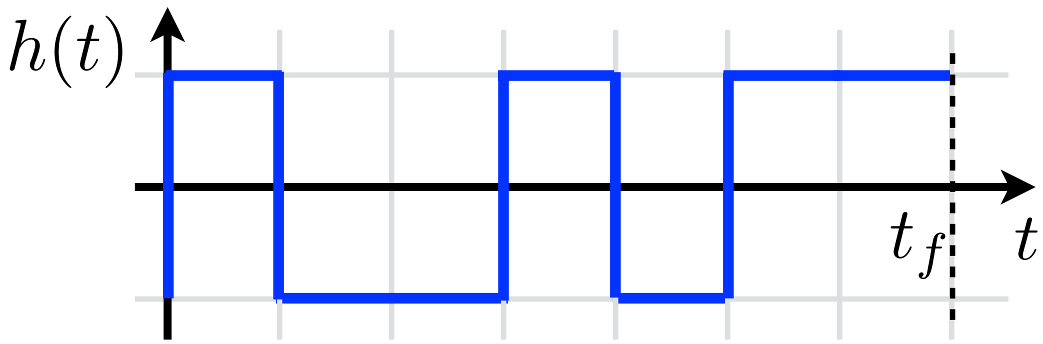
Let's give this game a try!



measurement: -1

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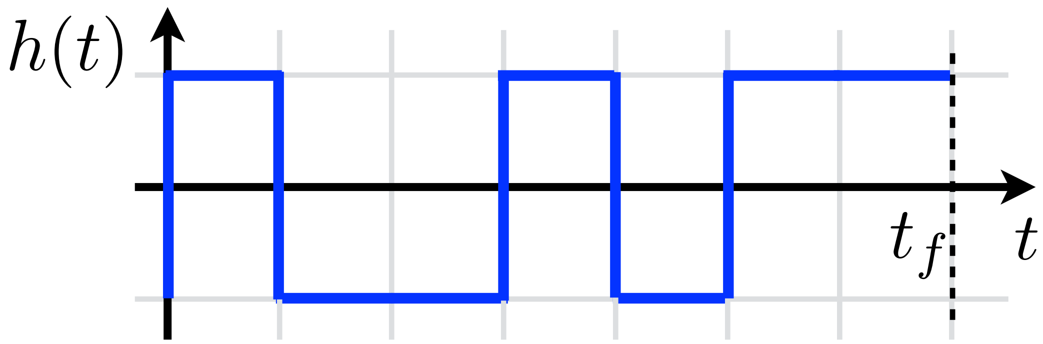

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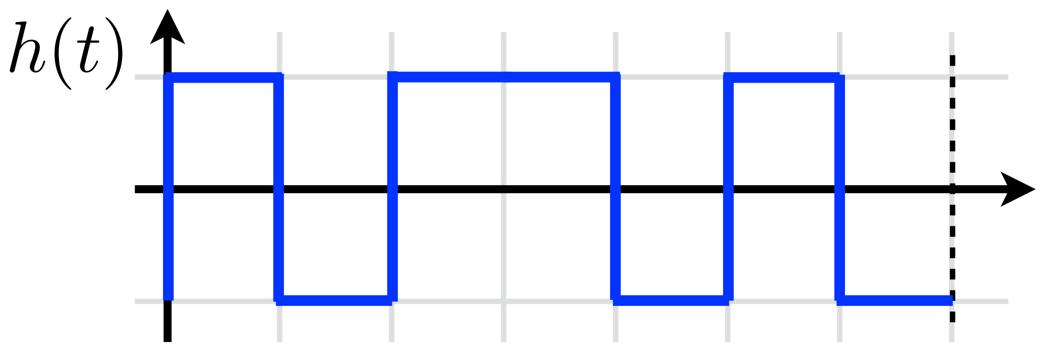

measurement: $+1$

(different final state: different probability to be in the target state)

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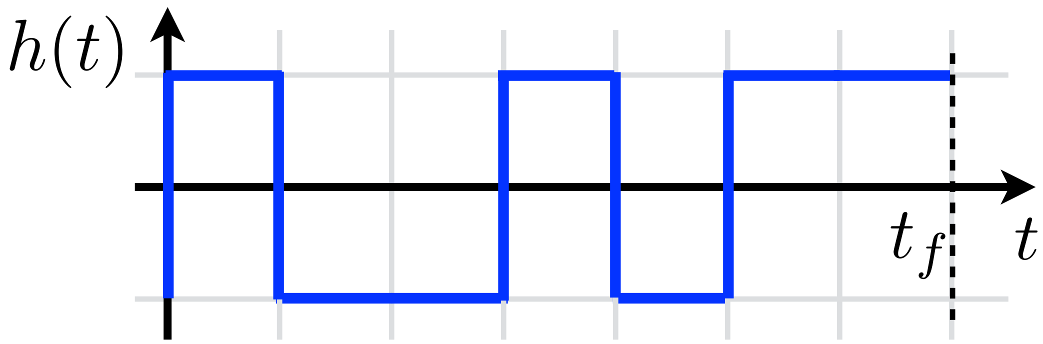
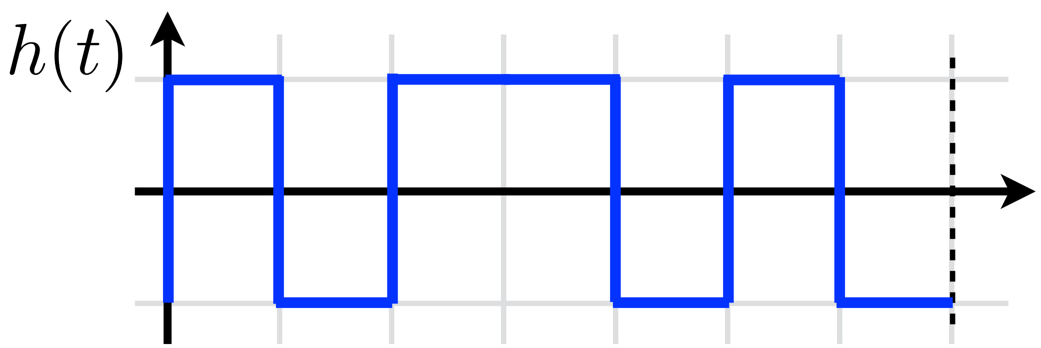


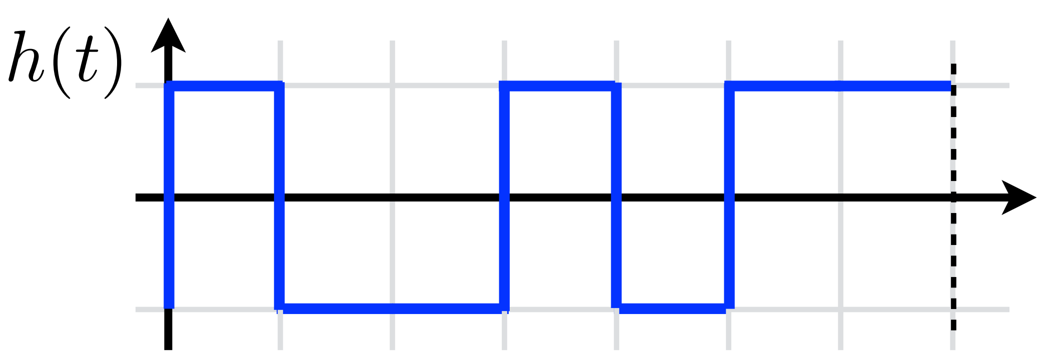
measurement: -1



measurement: $+1$

(different final state: different probability to be in the target state)

→ repeat protocol!



measurement: $+1$

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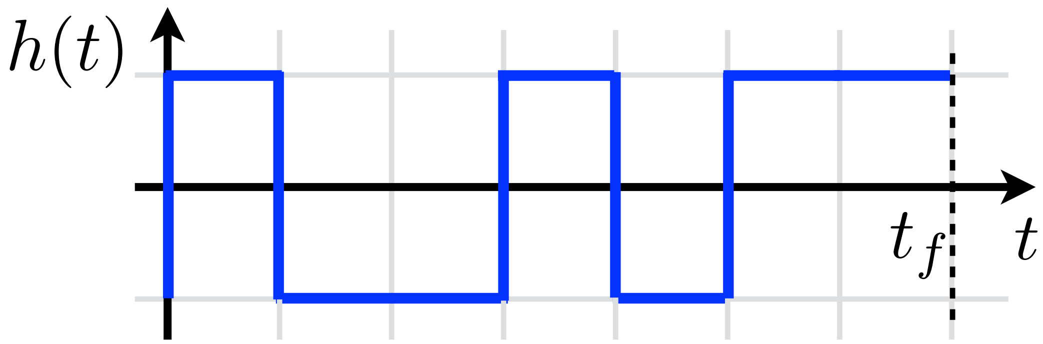
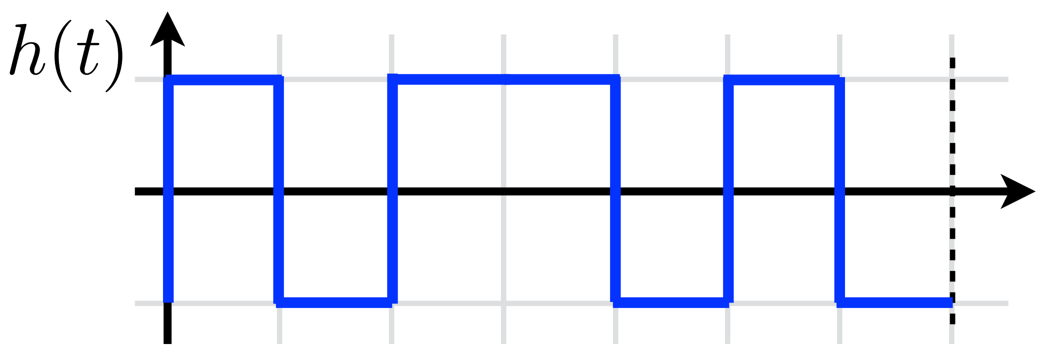


measurement: -1



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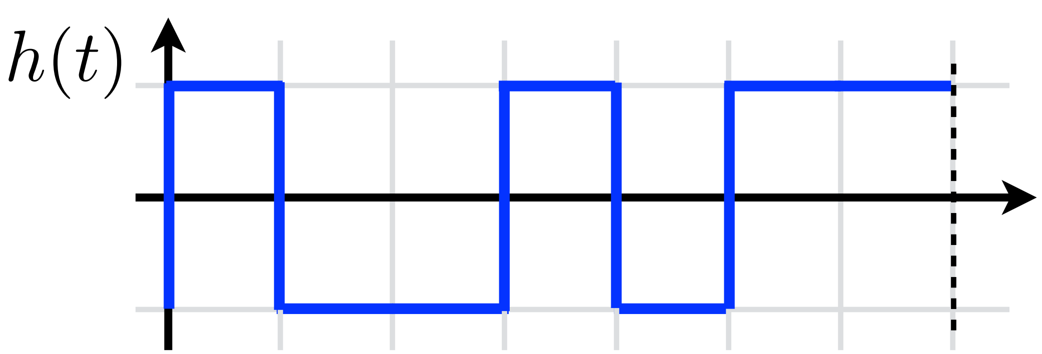
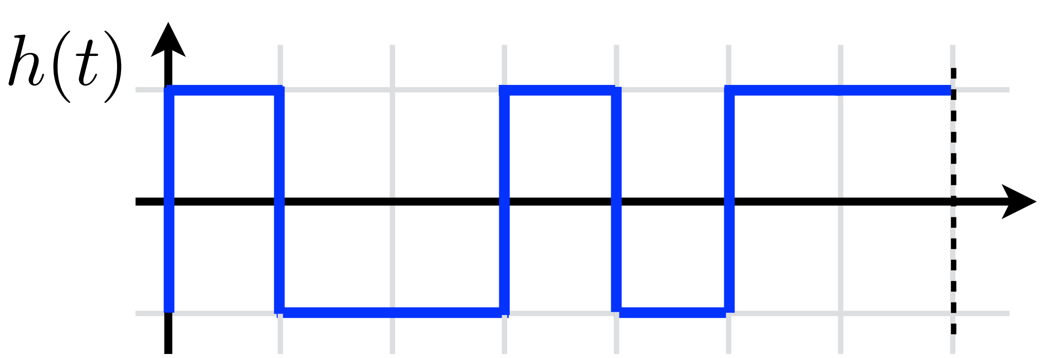


measurement: $+1$



measurement: -1

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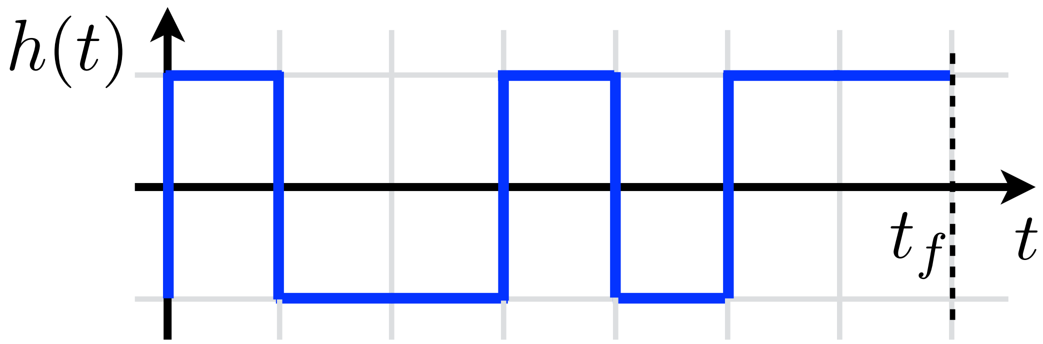

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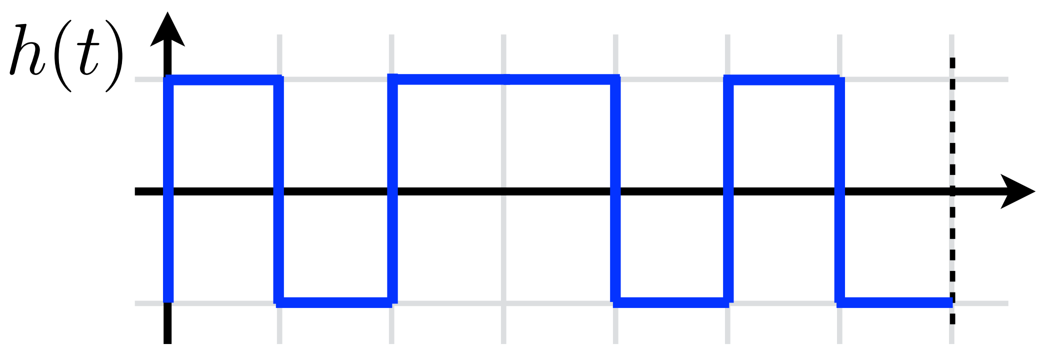

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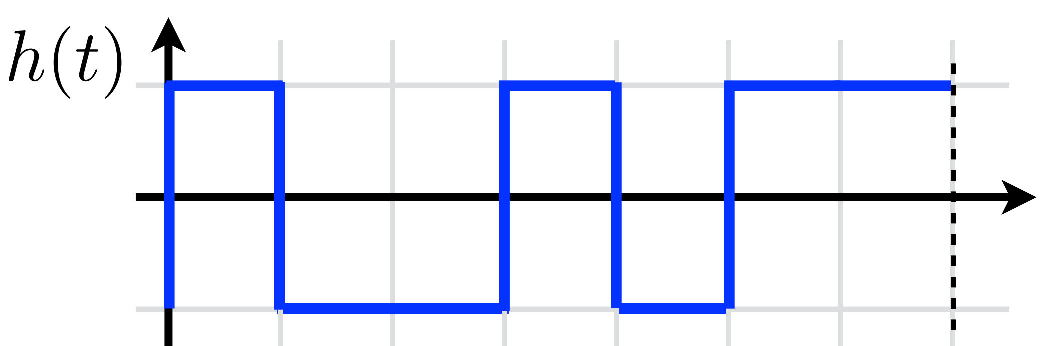
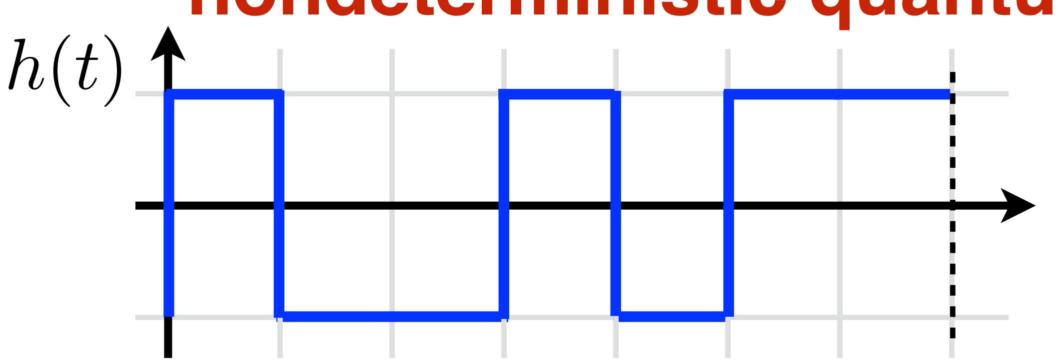


measurement: $+1$

nondeterministic quantum measurements create headache!



measurement: -1

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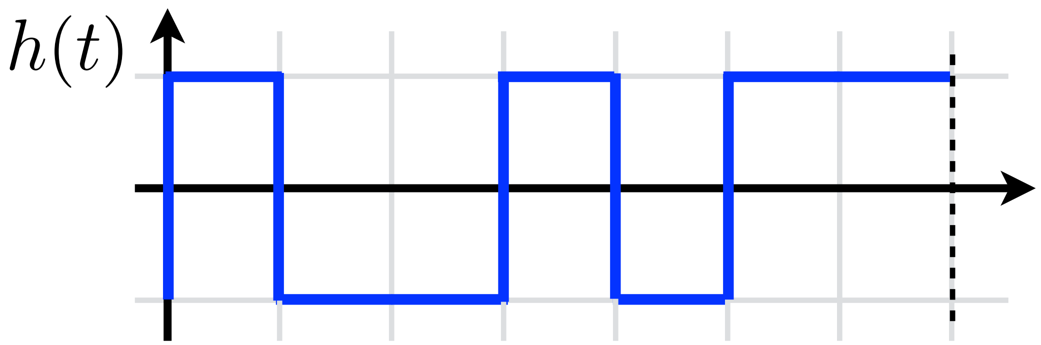
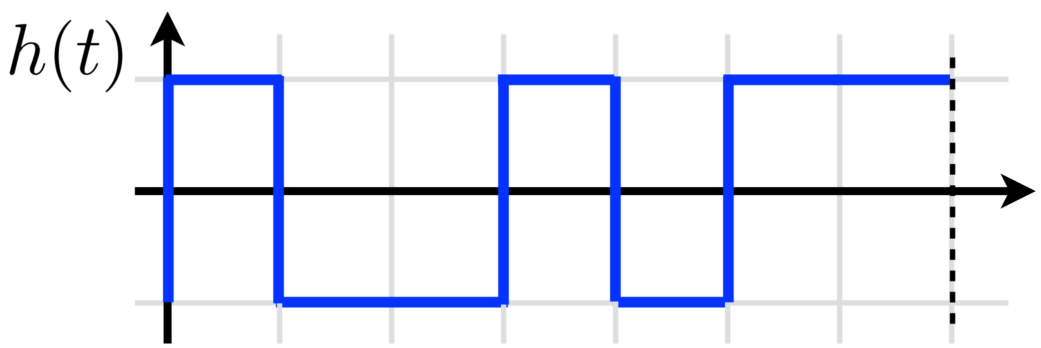
Let's get rid of this 'quantumness' for a sec

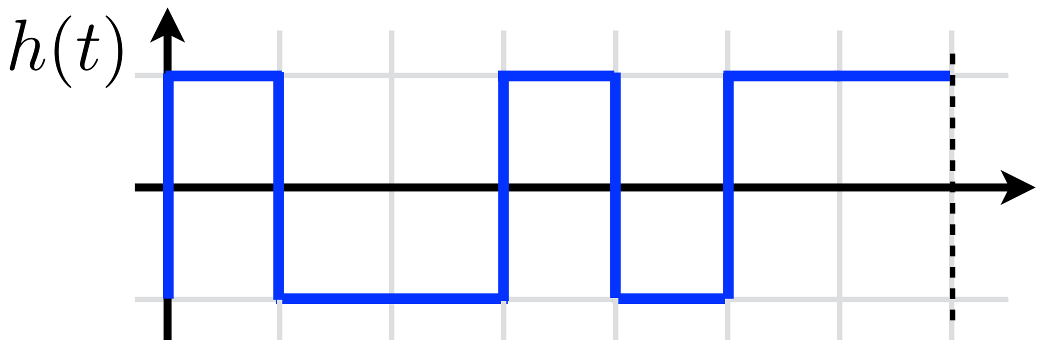
→ repeat protocol again!



measurement:
$F_h = |\langle\psi(T)|\psi_*\rangle|^2 = 0.632$



measurement: $F_h = 0.592$



measurement: $F_h = 0.668$

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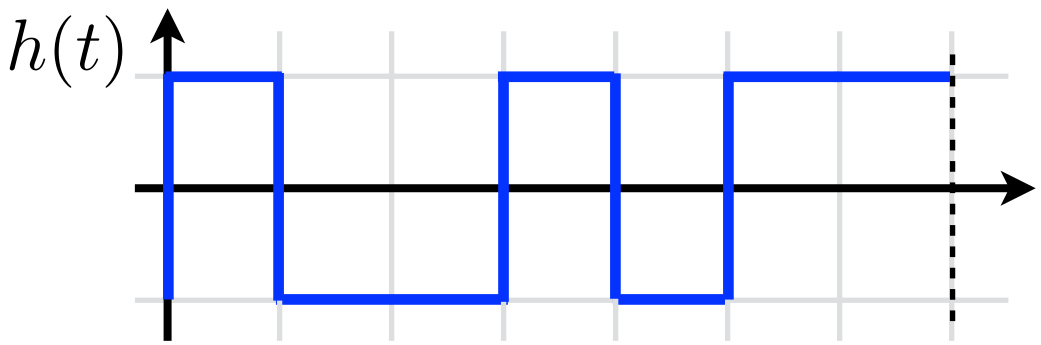
Let's get rid of this 'quantumness' for a sec

→ repeat protocol again!



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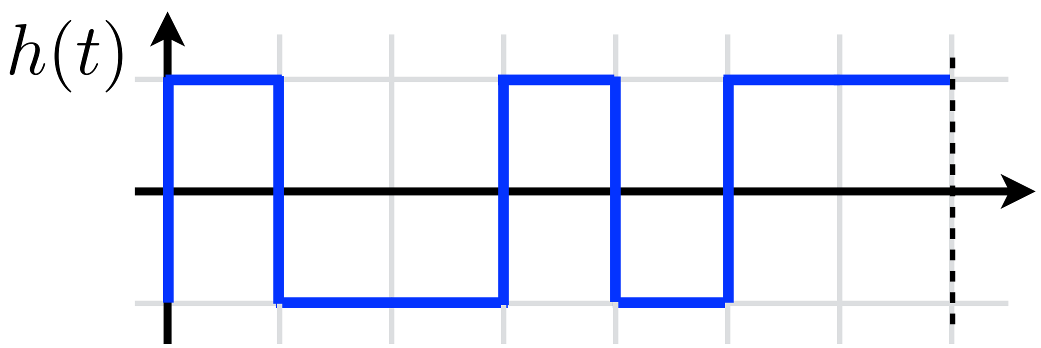
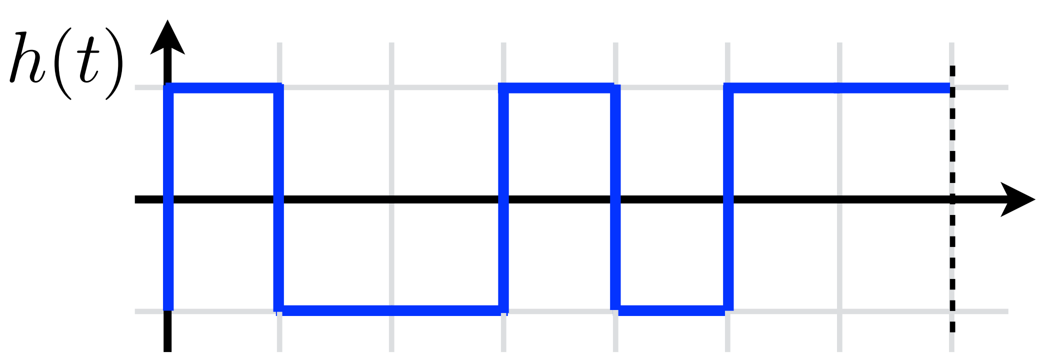
$F_h = |\langle \psi(T) | \psi_* \rangle|^2 = 0.632$



measurement: $F_h = 0.592$

initial state could not be prepared perfectly: more headache!



measurement: $F_h = 0.668$

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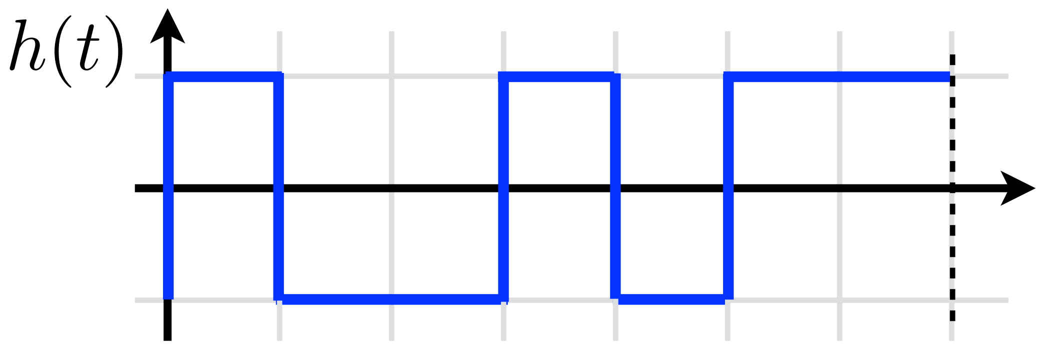
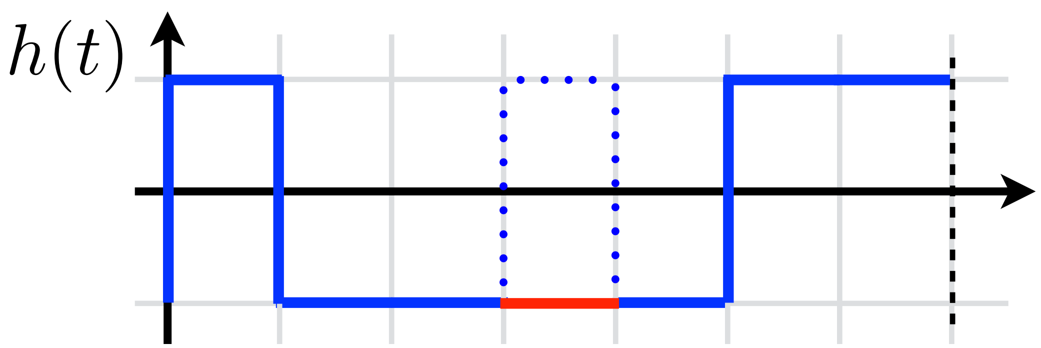
Let's maybe also fix the initial state

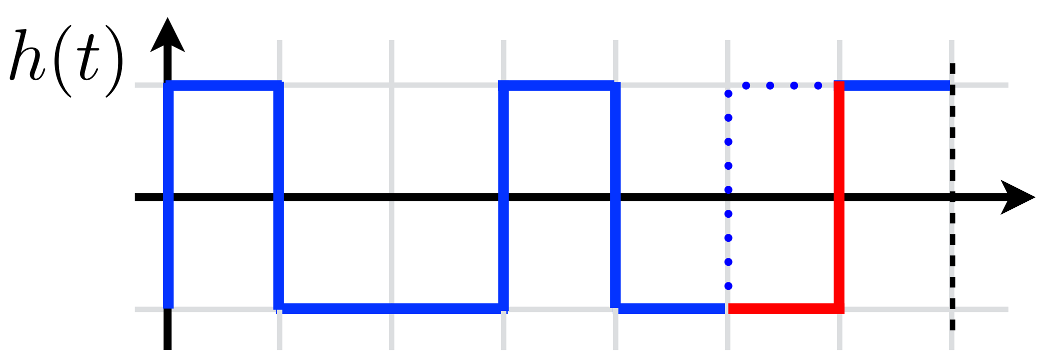
→ repeat protocol again!



measurement: $F_h = 0.627$



measurement: $F_h = 0.572$



measurement: $F_h = 0.657$

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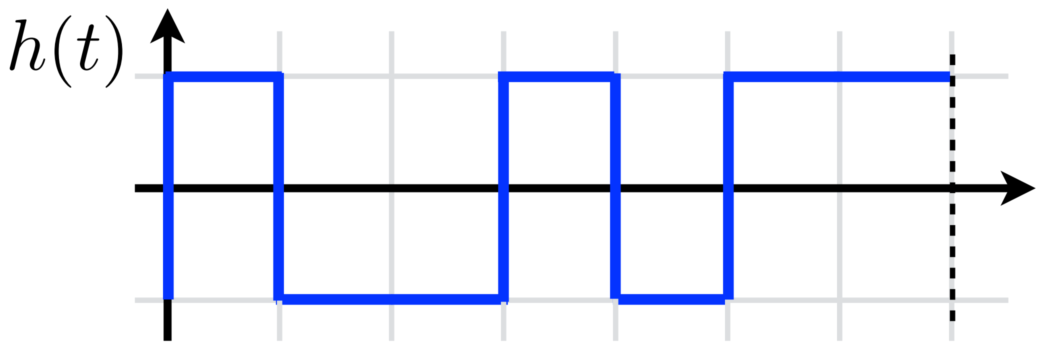

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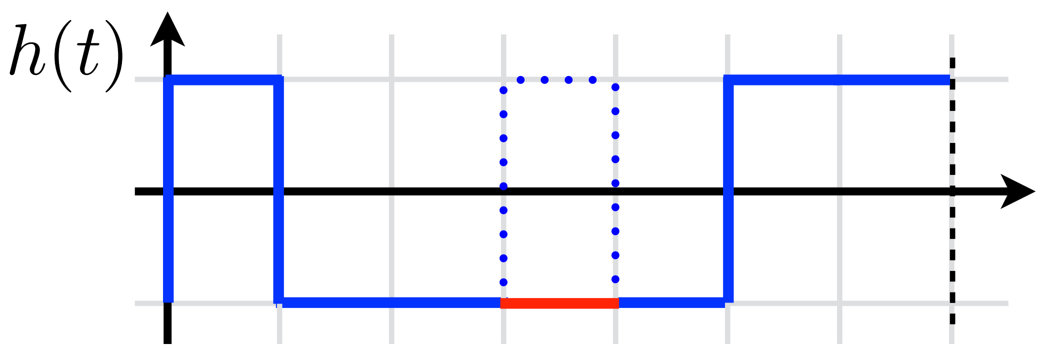
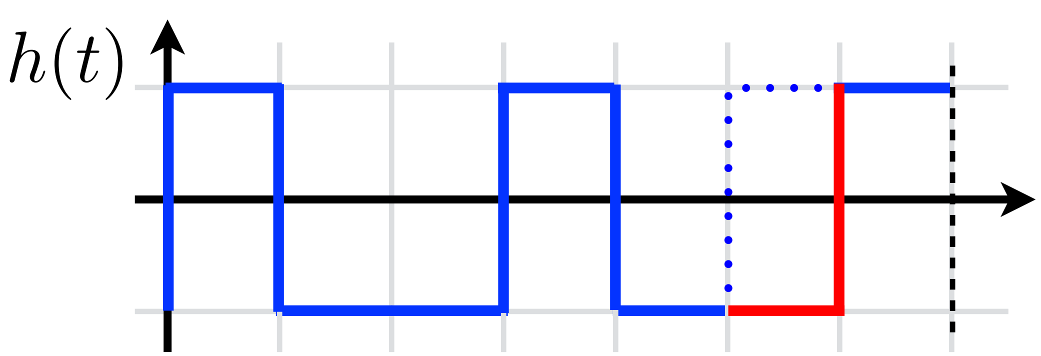


measurement: $F_h = 0.572$

control apparatus failed: it can't be!



measurement: $F_h = 0.657$

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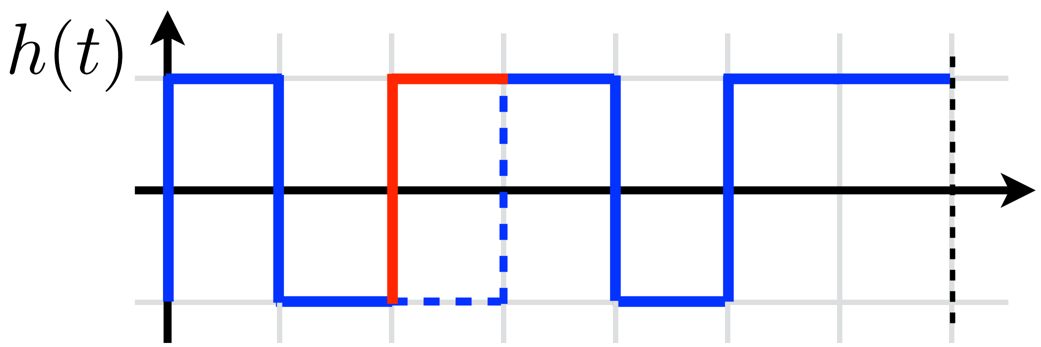
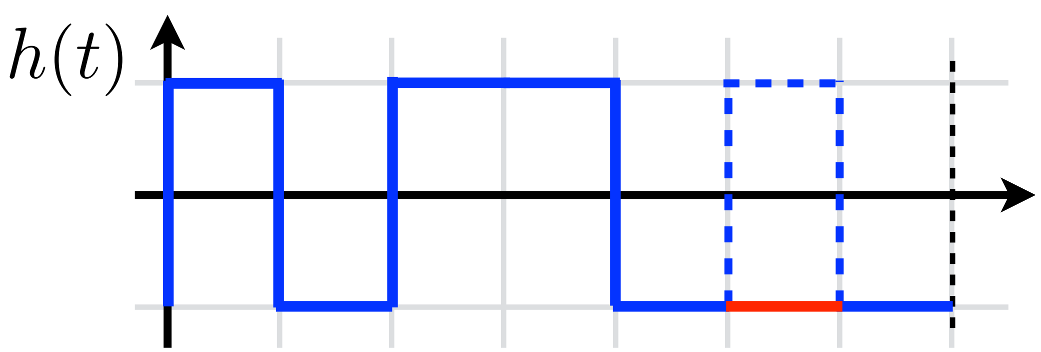
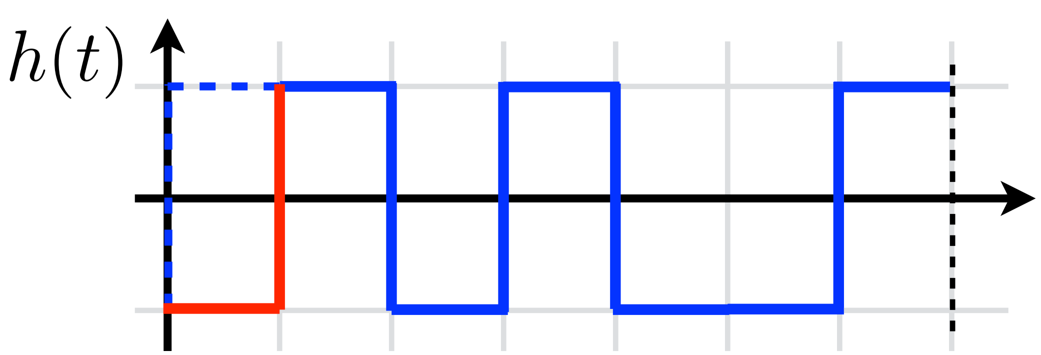
The Cruel Reality: all together (and probably much more!)



measurement: -1



measurement: $+1$



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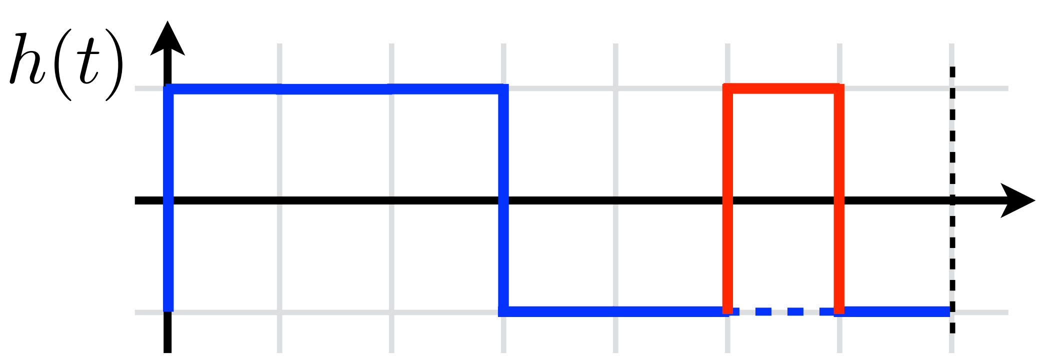

measurement: -1

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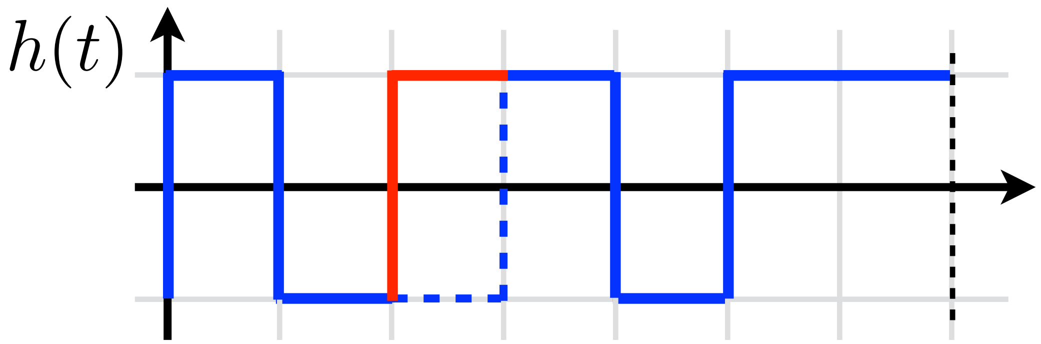
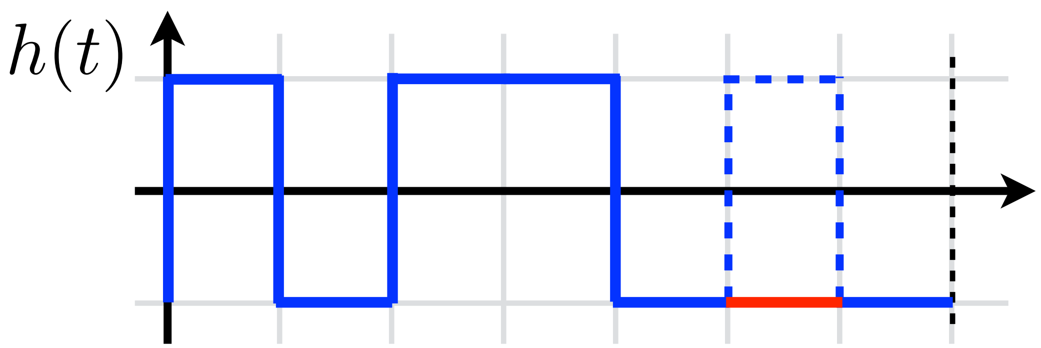
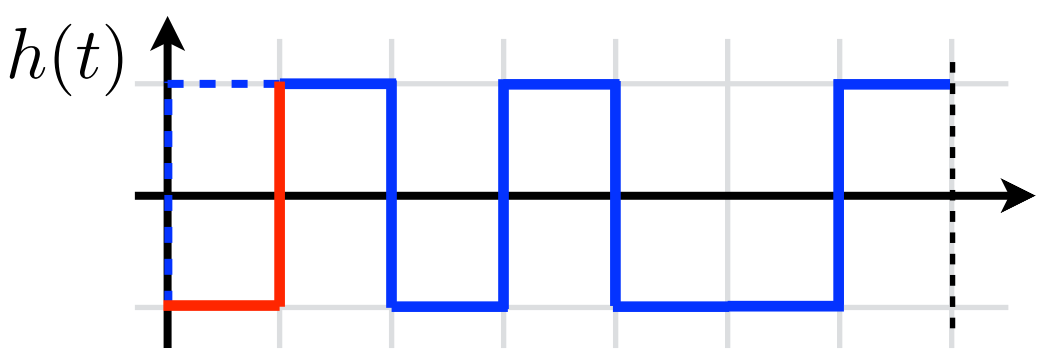


measurement: -1

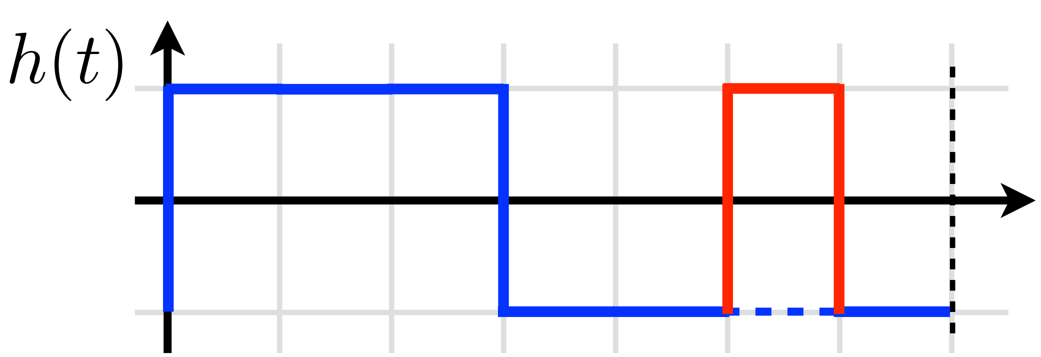


measurement: $+1$

extremely tedious task!



measurement: -1



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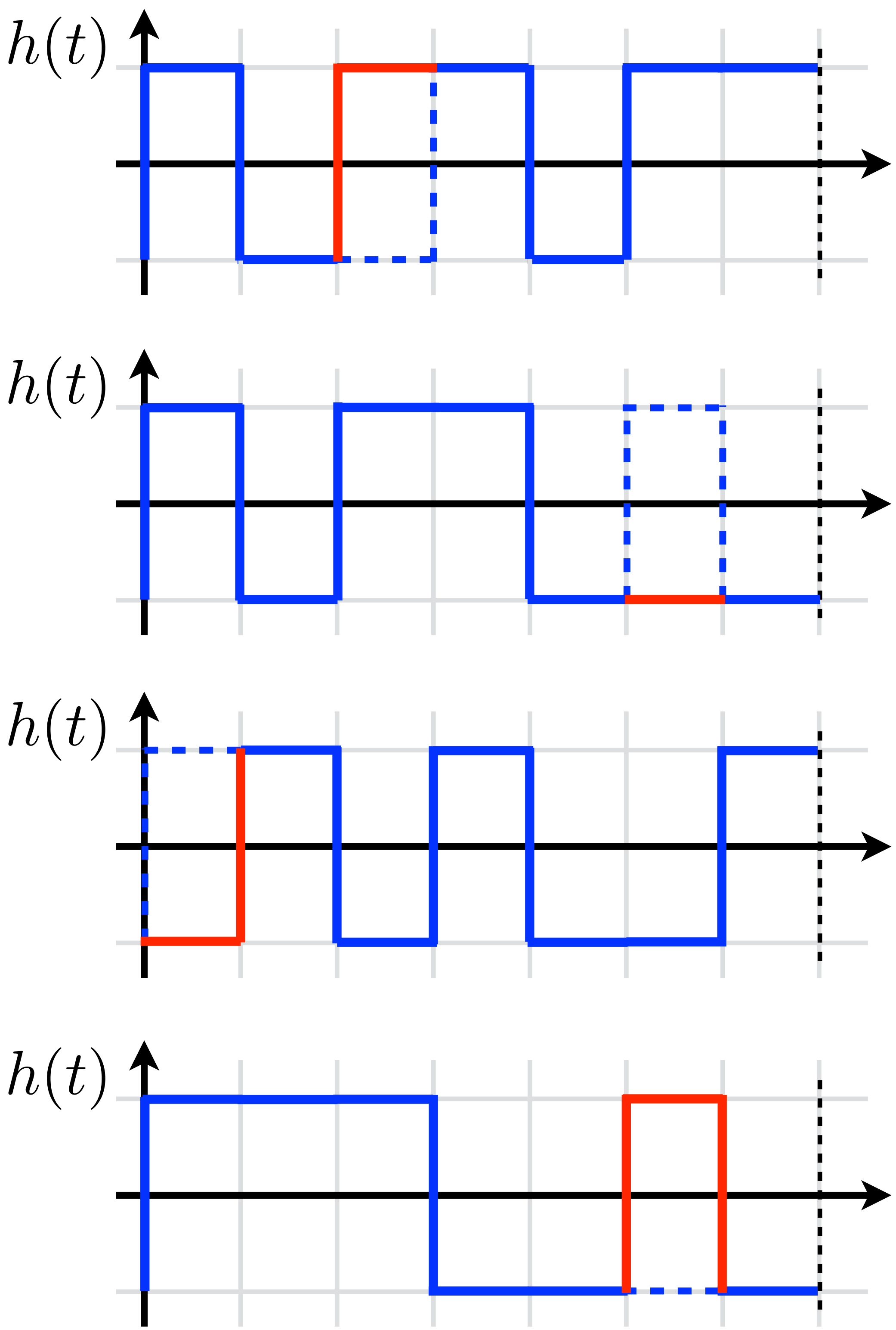

measurement: -1

measurement: $+1$

extremely tedious task!

measurement: -1

how do we solve it efficiently?

measurement: -1

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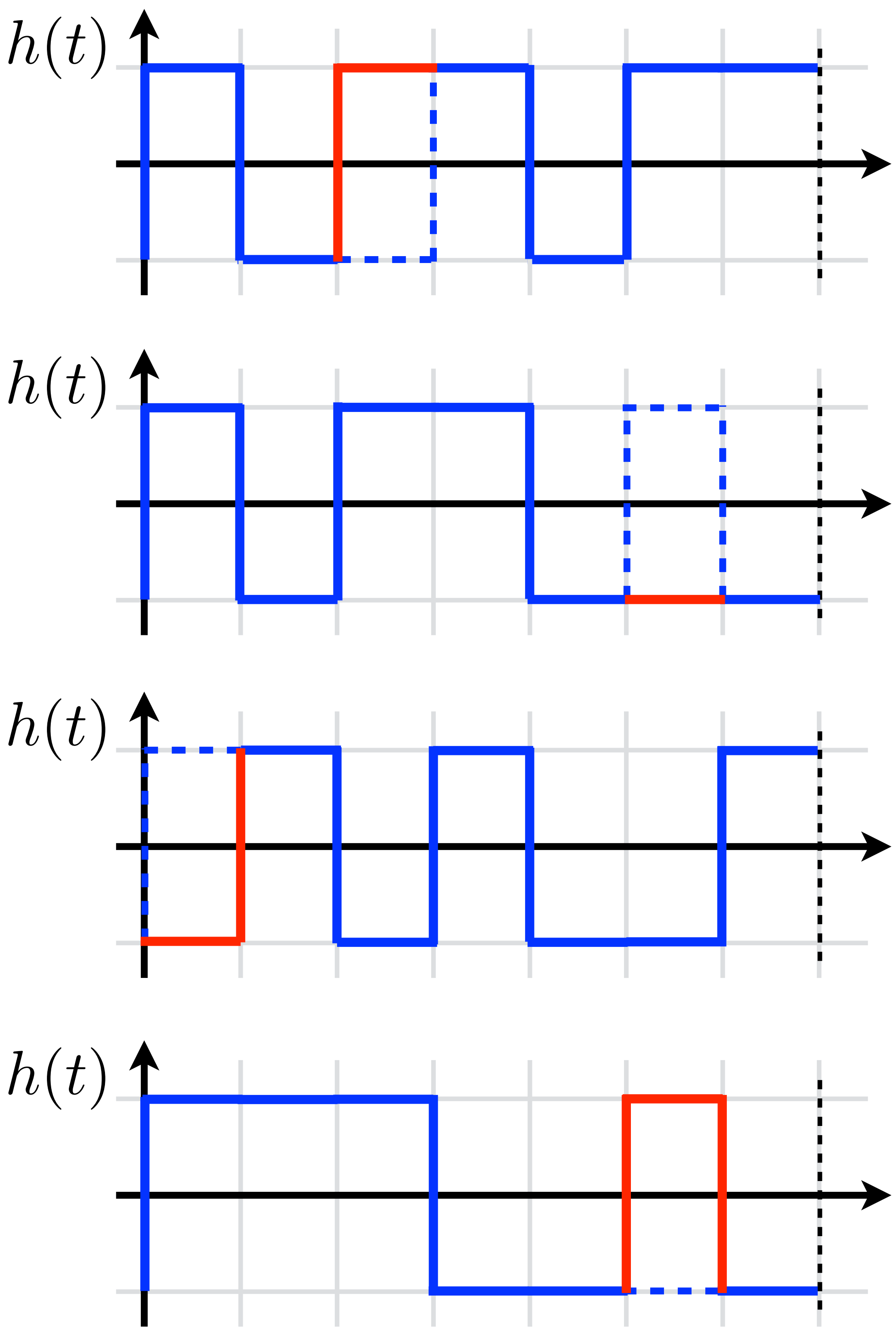
The Cruel Reality:
all together (and probably much more!)



measurement: -1

measurement: $+1$

extremely tedious task!

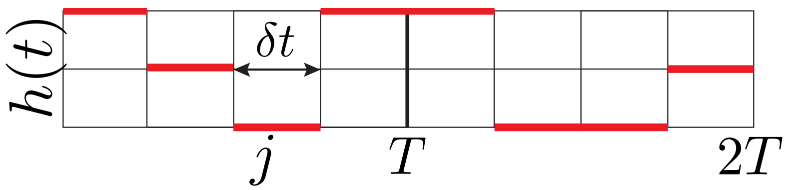
measurement: -1

how do we solve it efficiently?

measurement: -1

can we automate it?

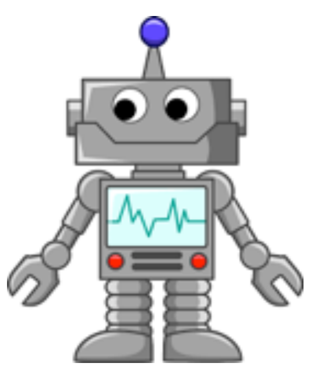
Reinforcement Learning to Prepare the Inverted Position Floquet State



4 driving cycles (periods), 32 steps (8 per period)

Kapitza pendulum

$t/T = 0.00,\ \theta(t) = 0.00\pi,\ p_\theta(t) = 0.00,\ r(t) = 0.00$



$h_{\max}/(m\omega_0) = 4.0$ $\Omega/(m\omega_0) = 10.0$ $A/(m\omega_0) = 2.0$

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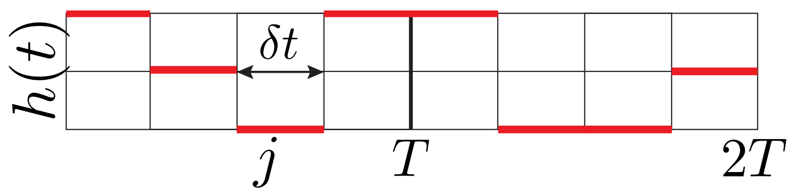
Reinforcement Learning to Prepare the Inverted Position Floquet State



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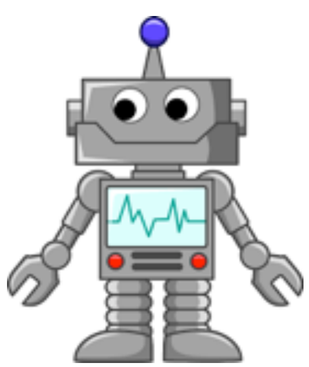

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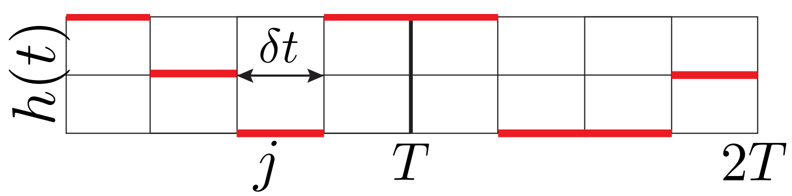
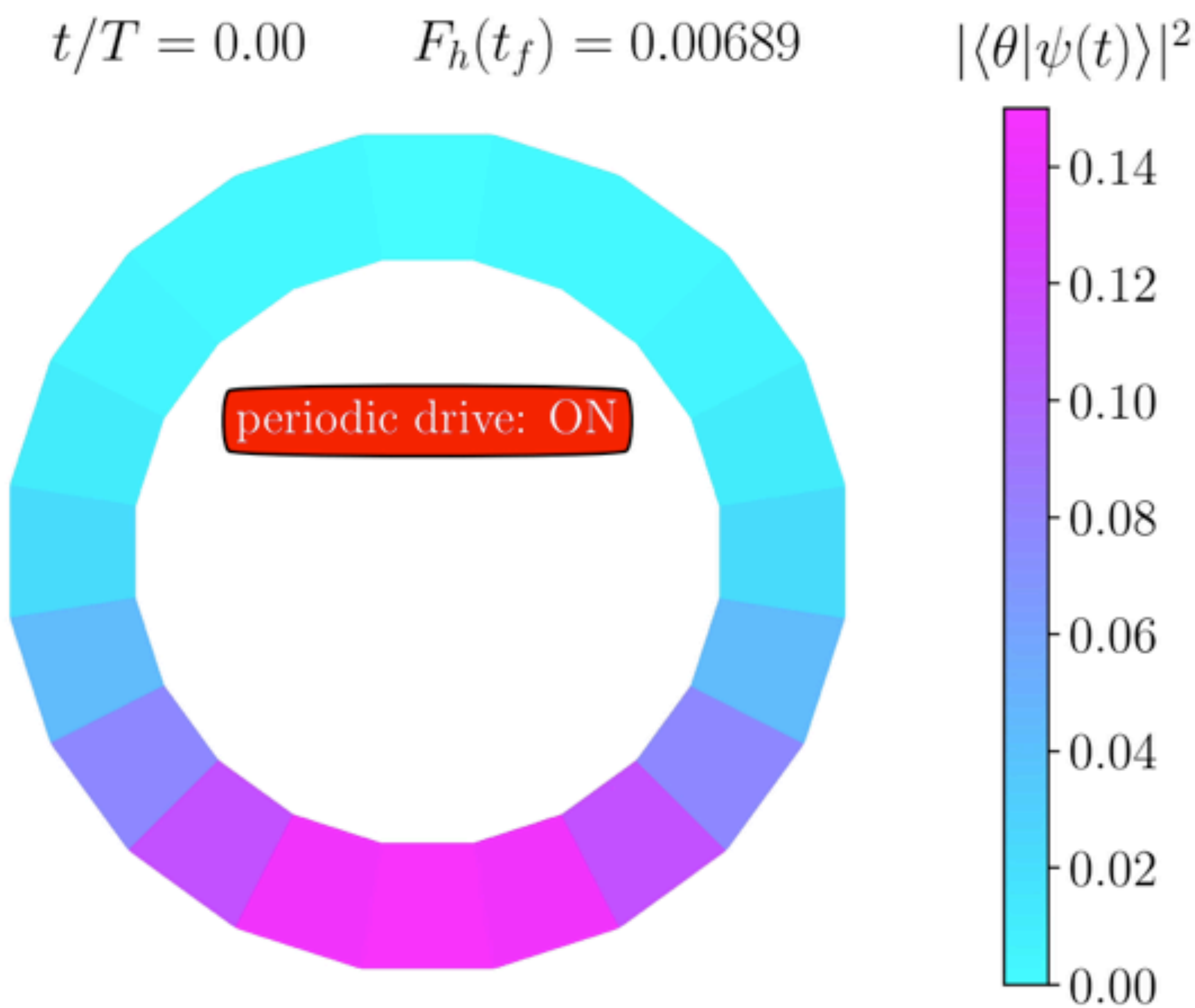
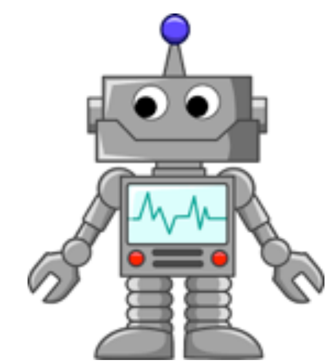
Reinforcement Learning to Prepare the Inverted Position Floquet State



15 driving cycles (periods), 120 steps (8 per period)

quantum Kapitza oscillator





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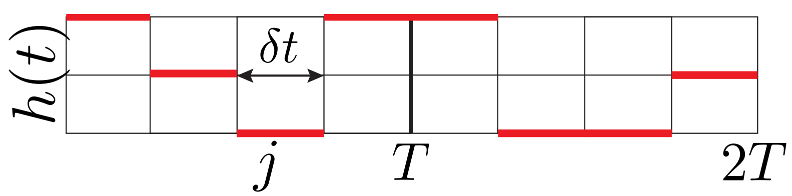

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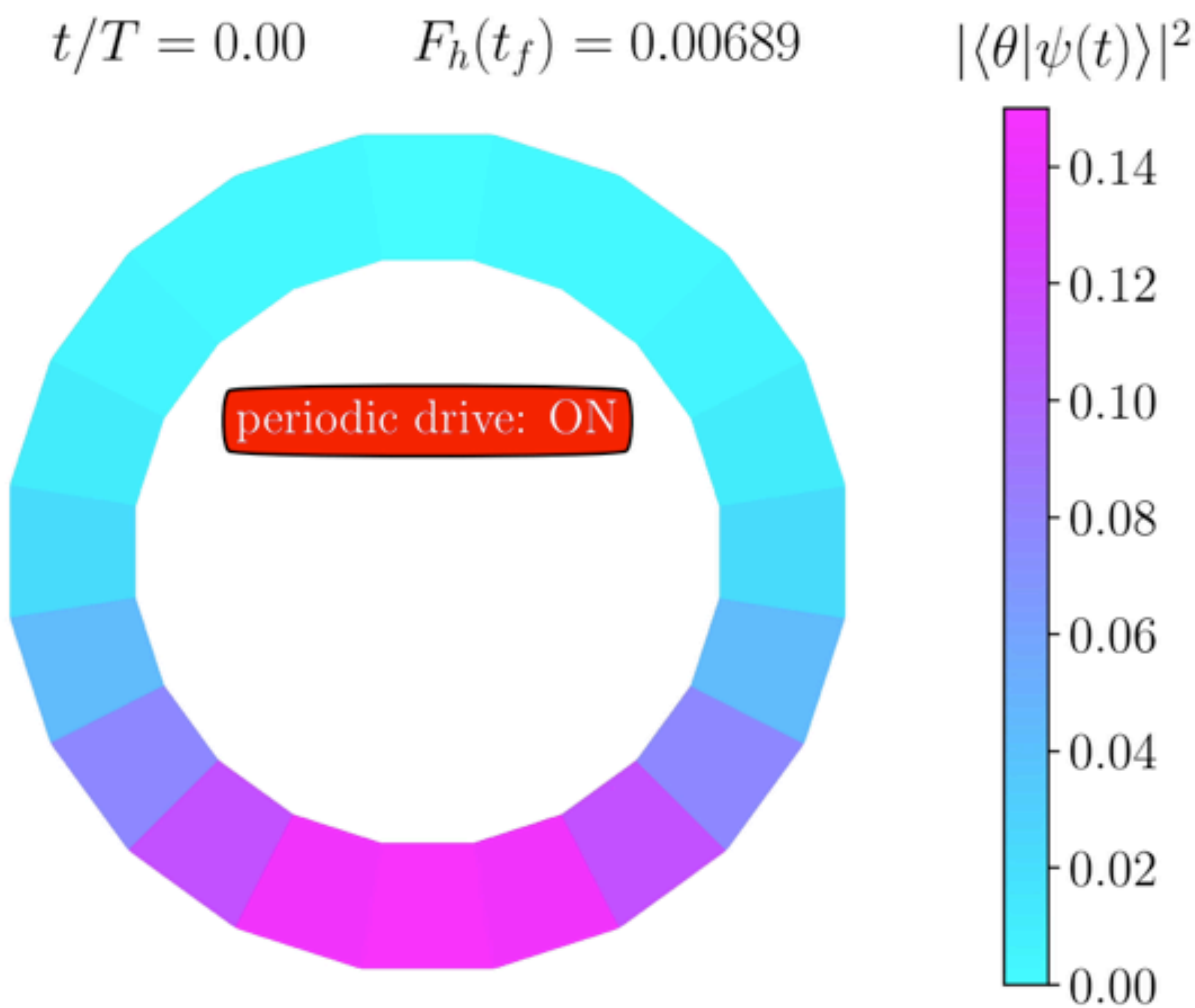

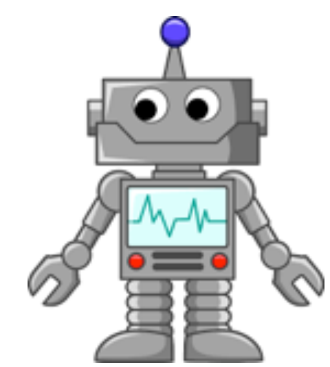

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Outlook

web: *mgbukov.github.io*

→ Which problems can we study with RL that we can't do otherwise?

→ Can RL lead to the discovery of new physics?

→ What's RL's most appropriate physics application as a toolbox?

funding: GORDON AND BETTY MOORE FOUNDATION

ML review with Jupyter notebooks: arXiv: *1803.08823*

RL in non equilibrium dynamics : *PRX 8 0311086 (2018)*, arXiv: *1808.08910*

control phase transitions: *PRA 97 052114 (2018)*, arXiv: *1803.10856*

QuSpin: *http://weinbe58.github.io/QuSpin*

python package for ED & many-body dynamics (with P. Weinberg, BU)

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