Near-term quantum simulation of nuclear dynamics

25th European Conference on Few-Body Problems in Physics

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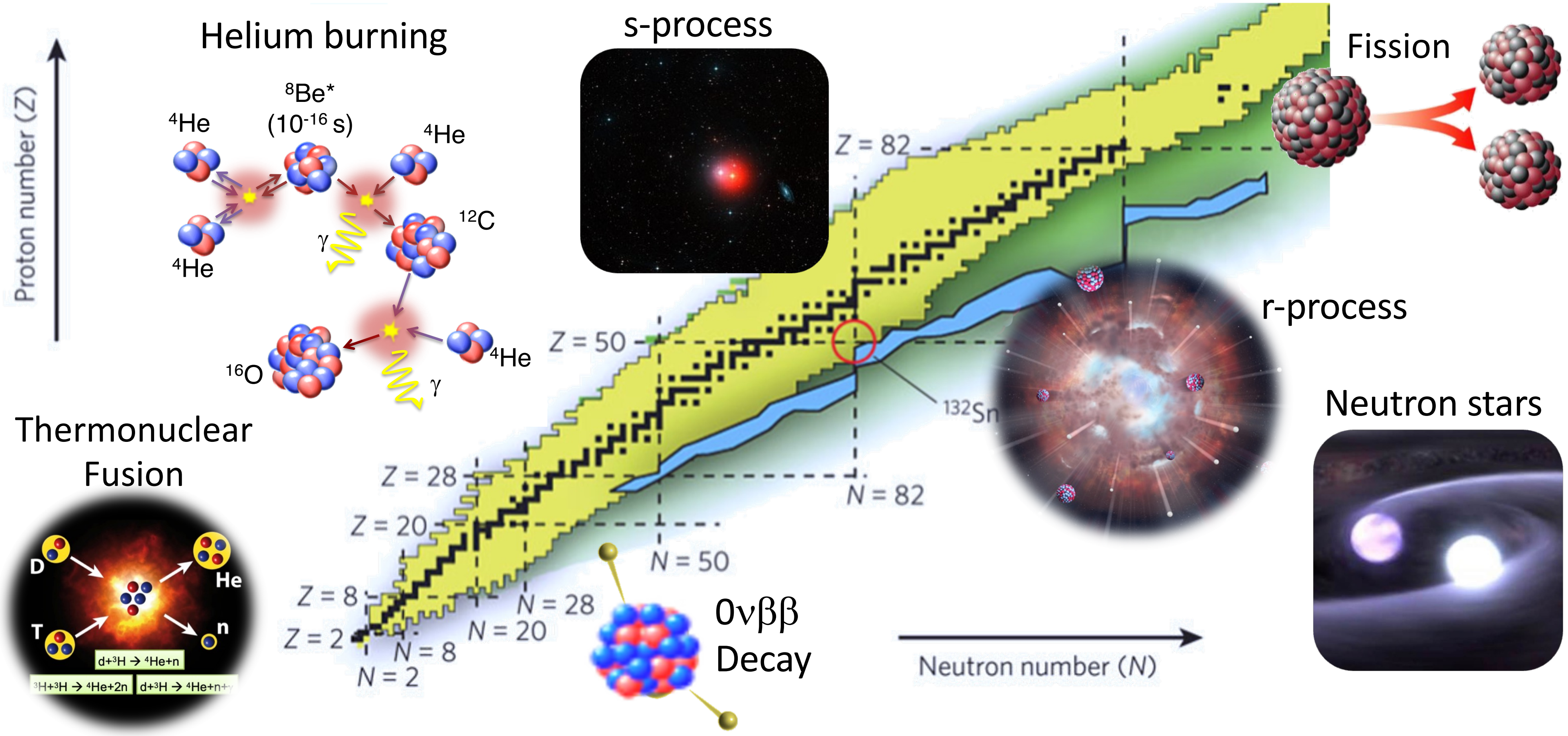
Nuclear & Chemical Sciences

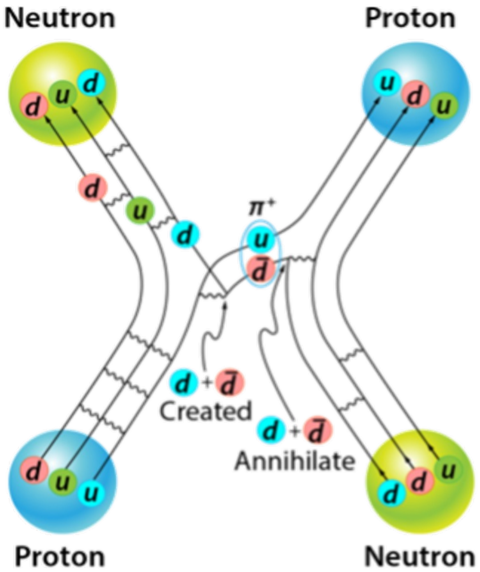
Lawrence Livermore National Laboratory

Goal:
Predictive understanding of nuclei and their interactions

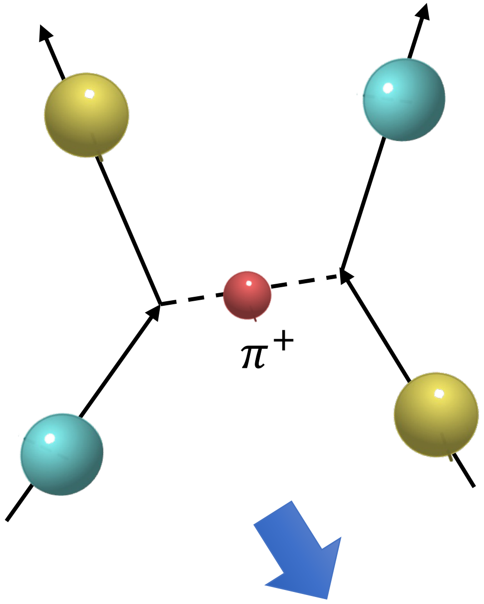


Currently best path to fundamental understanding combines effective field theory and ab initio methods

Quantum Chromodynamics

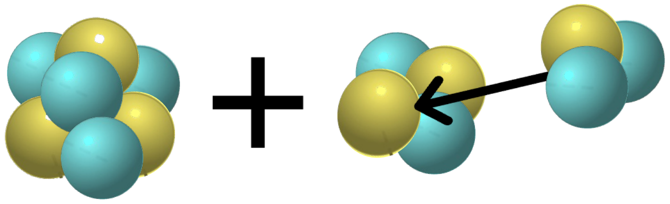


Chiral Effective Field Theory



Chiral NN+3N forces

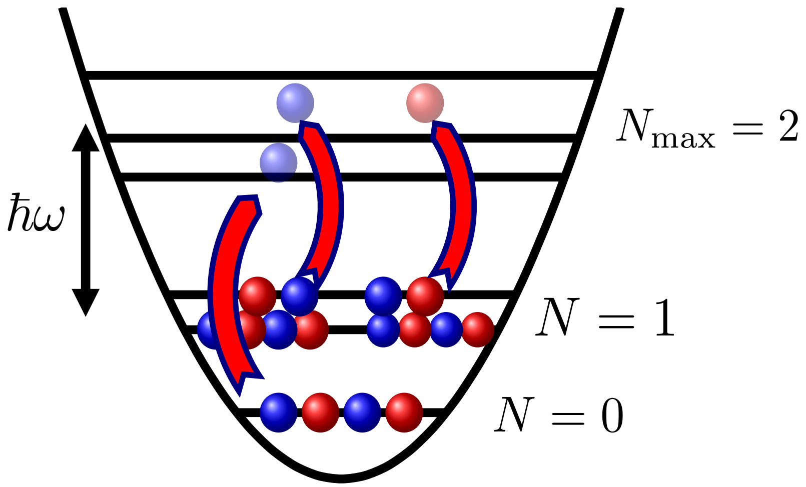
Unified ab initio many-body approach to structure and reactions

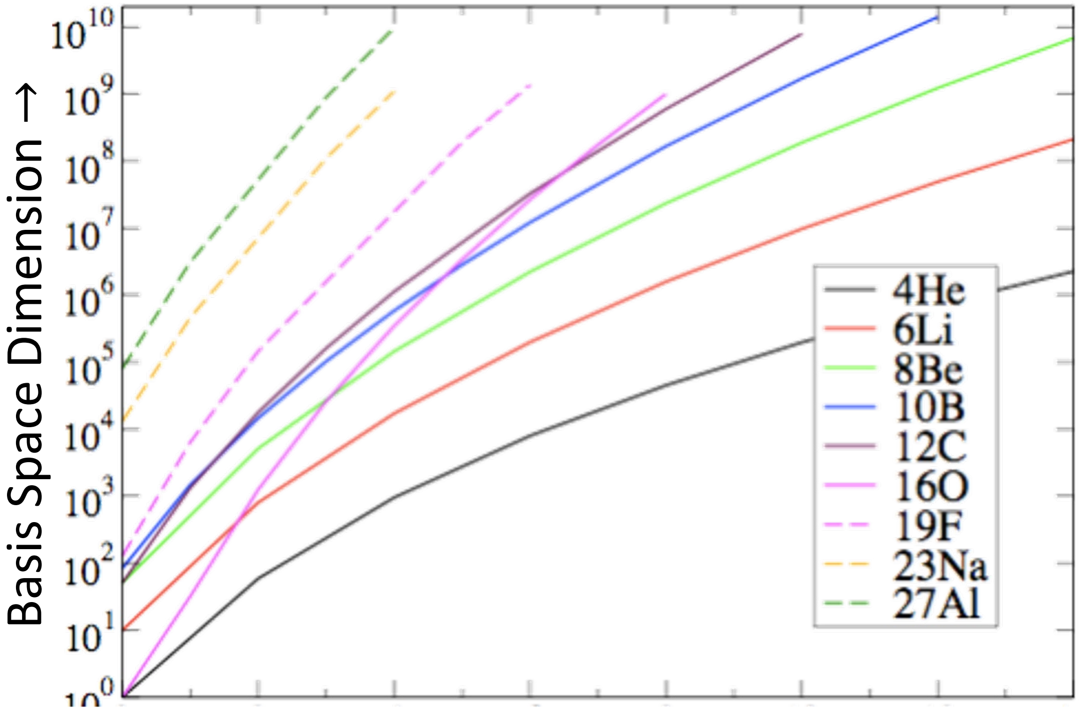


All active (pointlike) nucleons, non-relativistic quantum mechanics

Ab initio nuclear theory is among the most computationally intensive fields of science …

No-Core Shell Model:
bound states, static properties

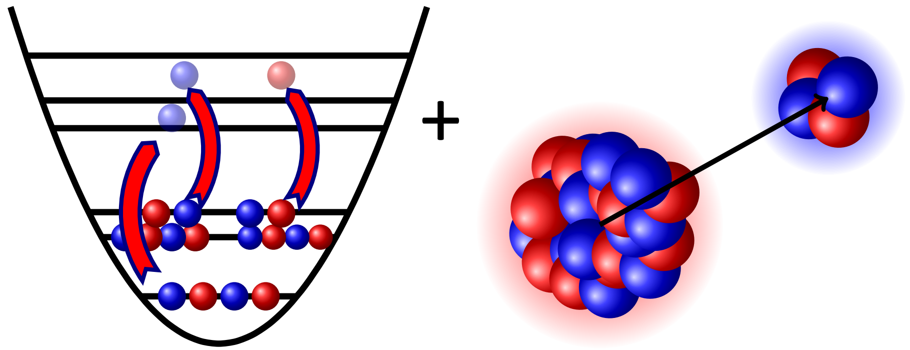


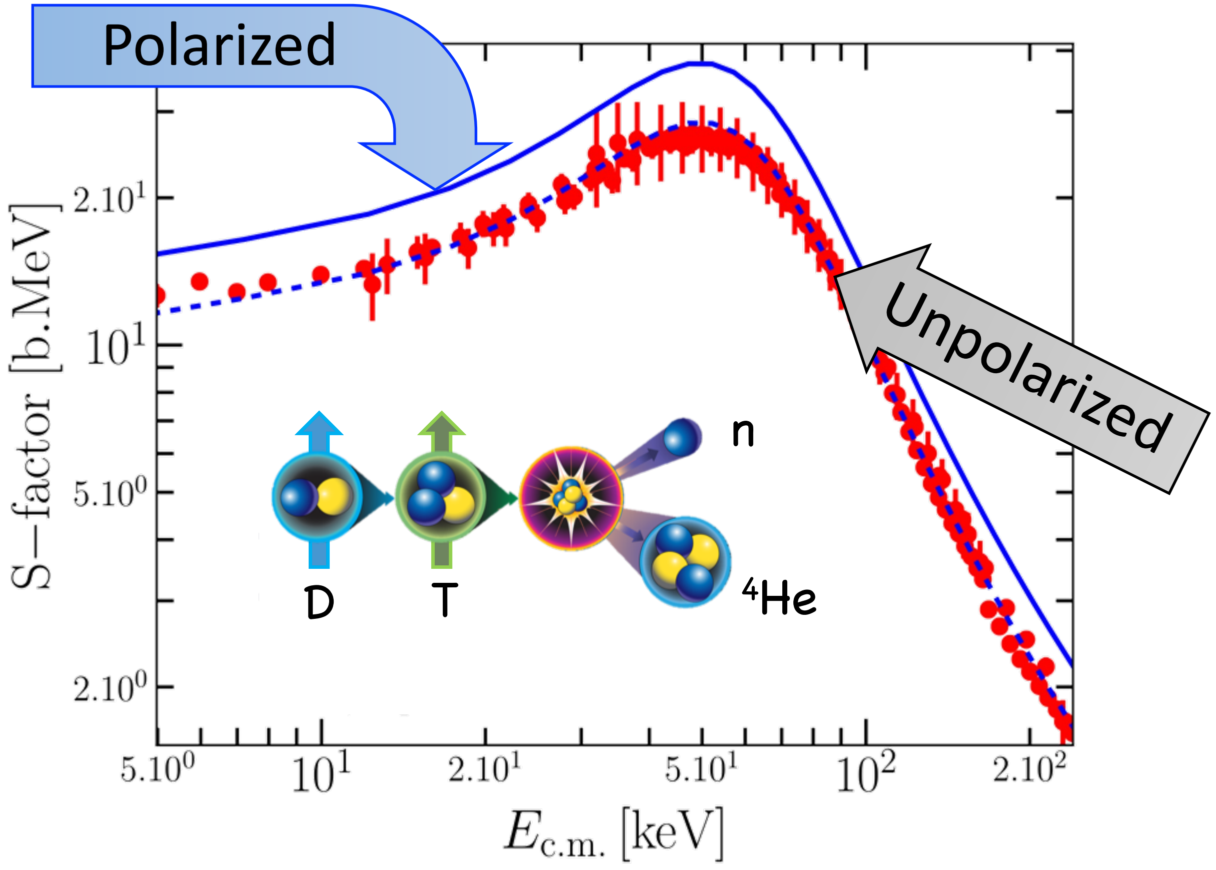


B. R. Barrett et al (2013), Prog. Part. Nucl. Phys. 69, 131

... and nuclear dynamical properties are among the most expensive to compute

No-Core Shell Model with Continuum:
resonances, scattering, reactions

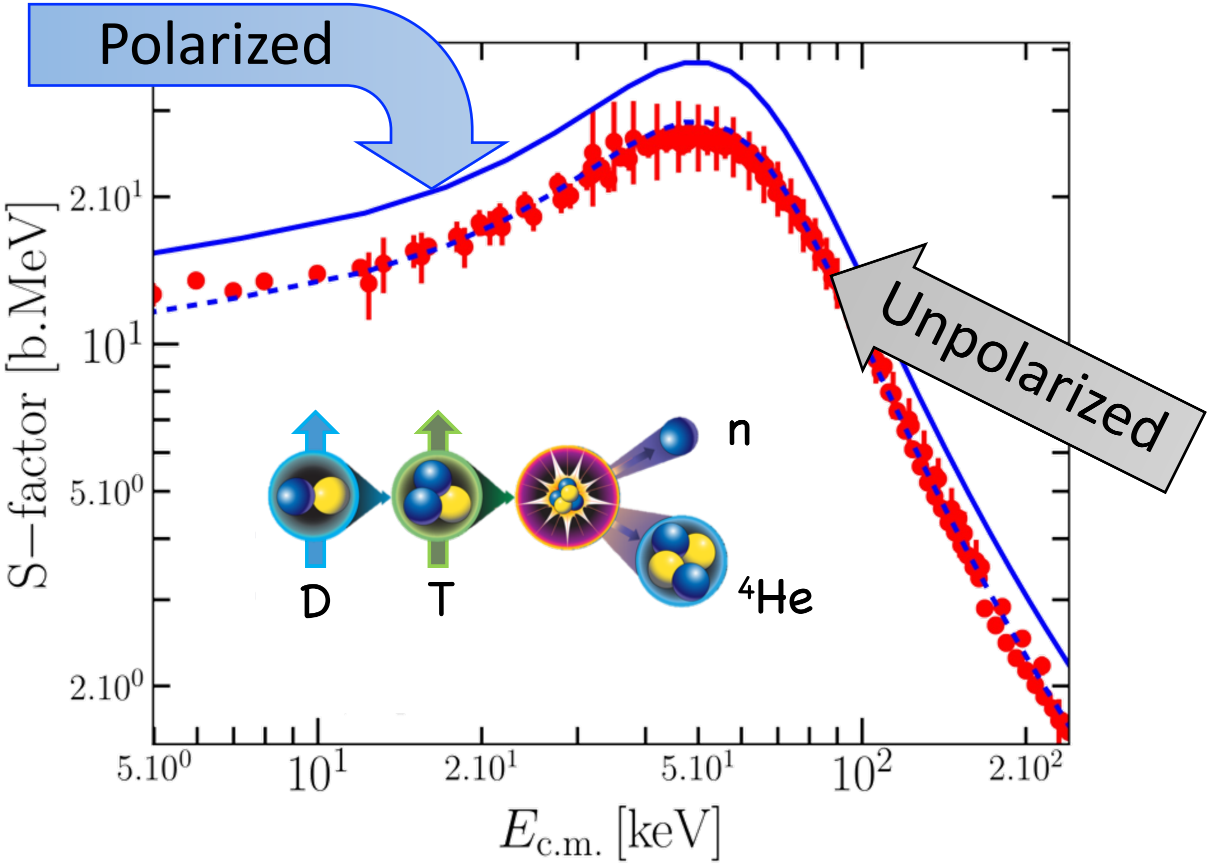




Navratil P et. al (2016), Physica Scripta 91, 053002

Hupin G et al. (2019), Nat. Comm. 10, 351

... and nuclear dynamical properties are among the most expensive to compute

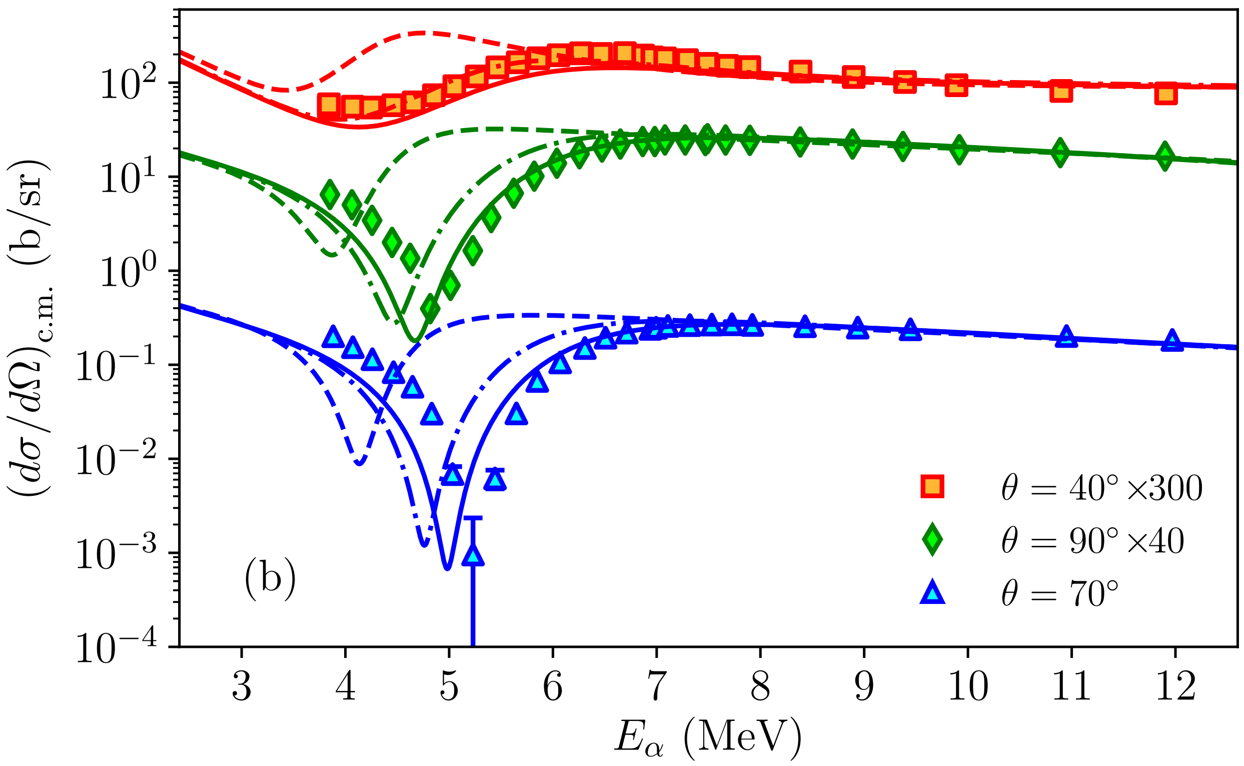


Hupin G et al. (2019), Nat. Comm. 10, 351

Advanced (CPU+GPU) architectures are enabling previously impossible ab initio reaction calculations

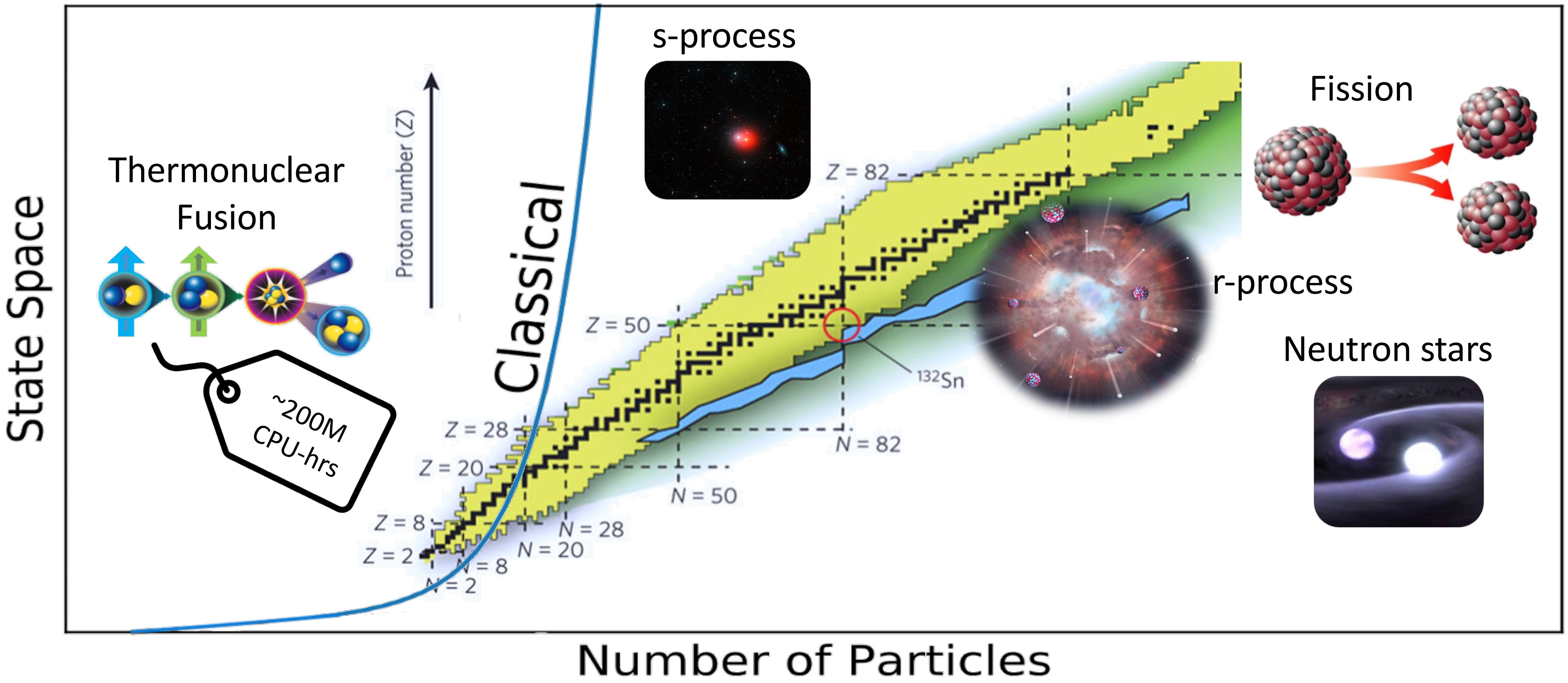
Memory of GPU cards present limiting factor

^{4}He + ^{4}He scattering

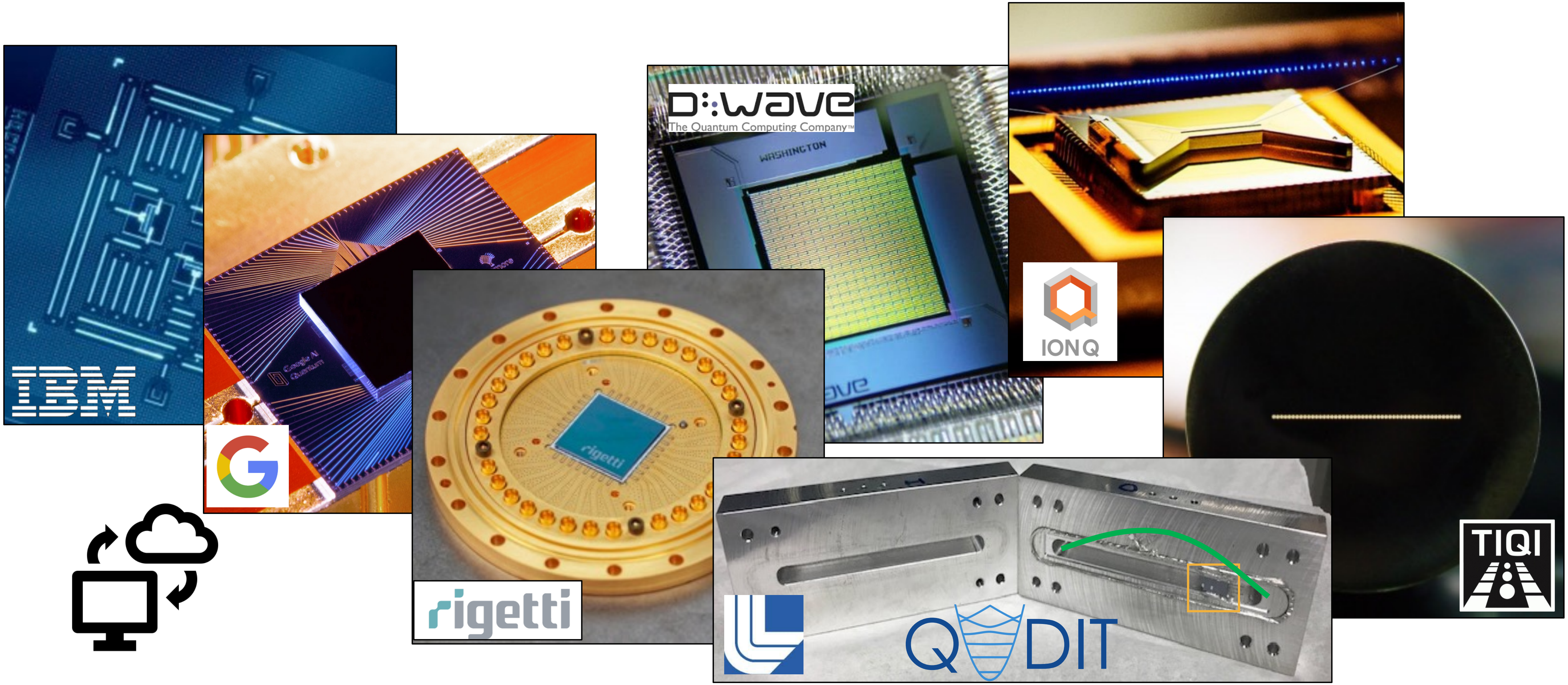


Kravvaris K et al., arXiv:2012.00228

Fundamental description of most nuclear dynamics remains a major challenge even with next-gen HPC



Several prototypes of quantum processors have emerged both in academia and industry



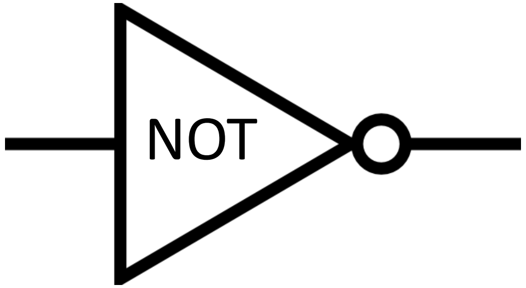
Quantum computers perform calculations by manipulating quantum states

$$|\psi_{targ}\rangle = U_{targ}\,|\psi_0\rangle$$

Desired state

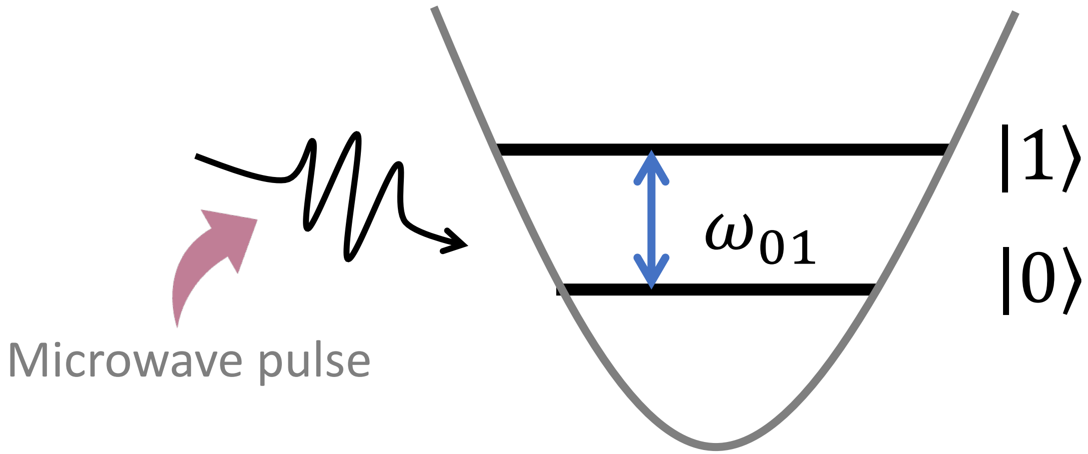
Initial state

Unitary operation (= gate)



Most quantum computers perform calculations by manipulating 2-level quantum systems or ‘qubits’

qubit



$$|\psi_{qubit}\rangle = \alpha|0\rangle + \beta|1\rangle$$

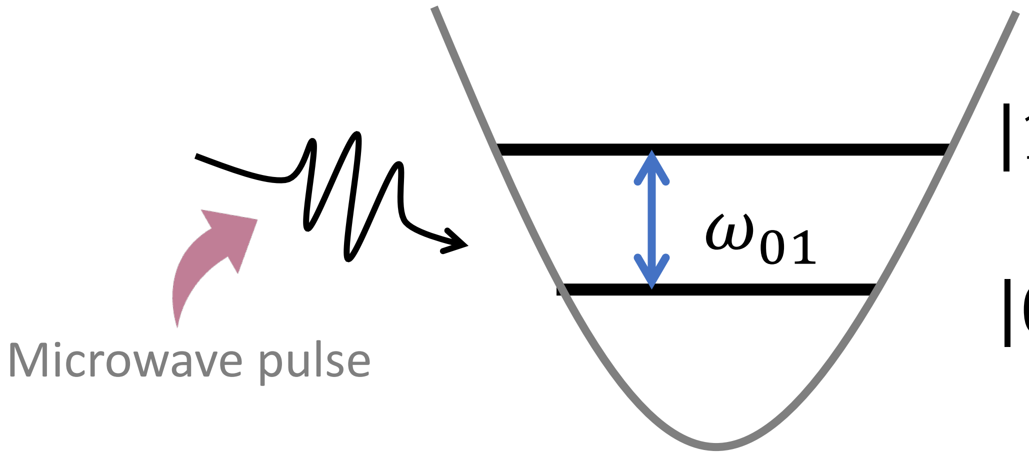
$$(|\alpha|^2 + |\beta|^2 = 1)$$

bit

Either 0 or 1

Most quantum computers perform calculations by manipulating 2-level quantum systems or ‘qubits’

qubit



$$|1\rangle = \begin{bmatrix} 0 \\ 1 \end{bmatrix}$$

$$|0\rangle = \begin{bmatrix} 1 \\ 0 \end{bmatrix}$$

$$|\psi_{qubit}\rangle = \alpha|0\rangle + \beta|1\rangle = \begin{bmatrix} \alpha \\ \beta \end{bmatrix}$$

$$(|\alpha|^2 + |\beta|^2 = 1)$$

bit

Either 0 or 1

A register of n qubits
has 2^n possible basis states (here $n = 2$) …

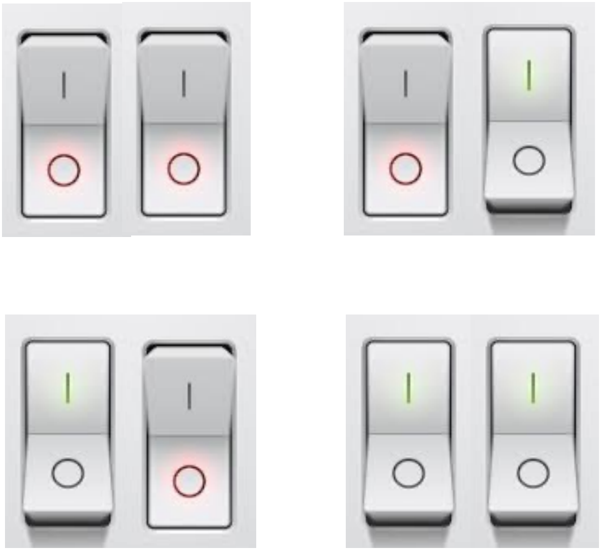
2-qubit register:

$$|00\rangle, |01\rangle, |10\rangle, |11\rangle$$

qubit 1 qubit 2

2^n basis states

2-bit register:



2^n possible configurations

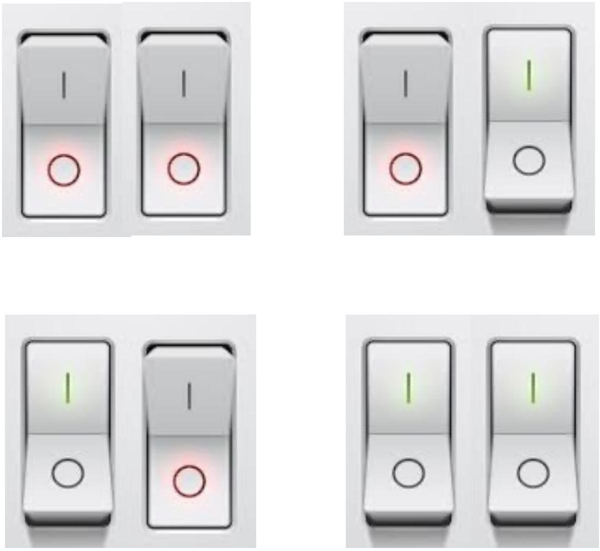
... can store, process 2^n basis states simultaneously.
Well suited for many-particle entangled quantum states!

2-qubit register:

$$|\psi_{2-qubit}\rangle = \alpha_{00}|00\rangle + \alpha_{01}|01\rangle + \alpha_{10}|10\rangle + \alpha_{11}|11\rangle$$

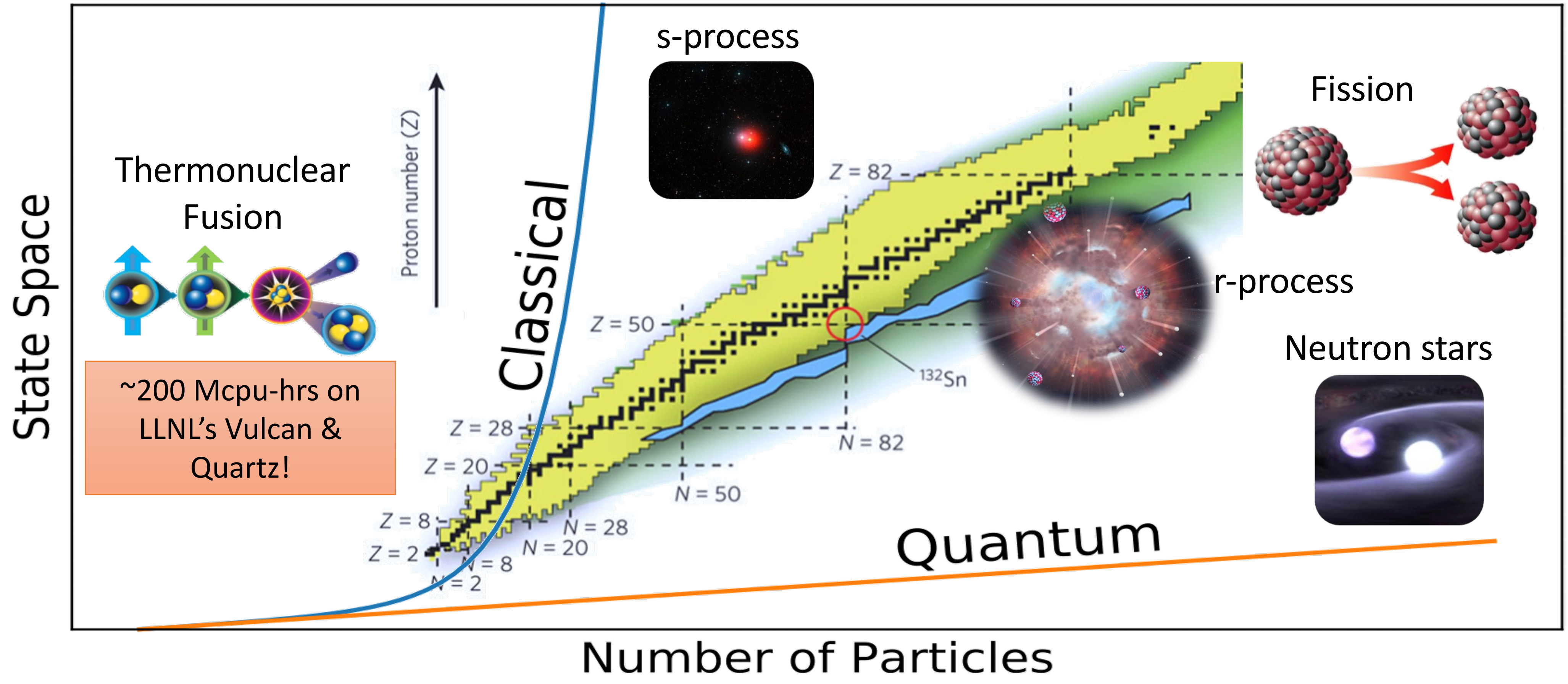
Can store superpositions of
2^n basis states simultaneously

2-bit register:



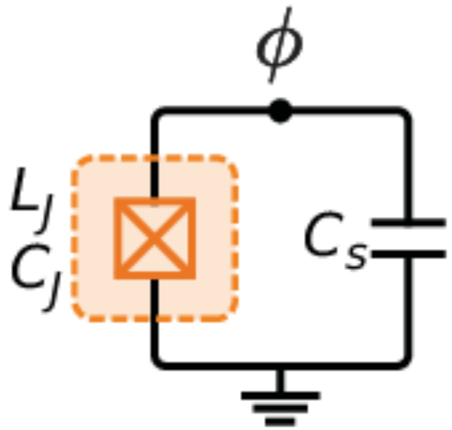
can only store one configuration

Quantum computing holds the promise of exact simulations of nuclear matter and dynamics

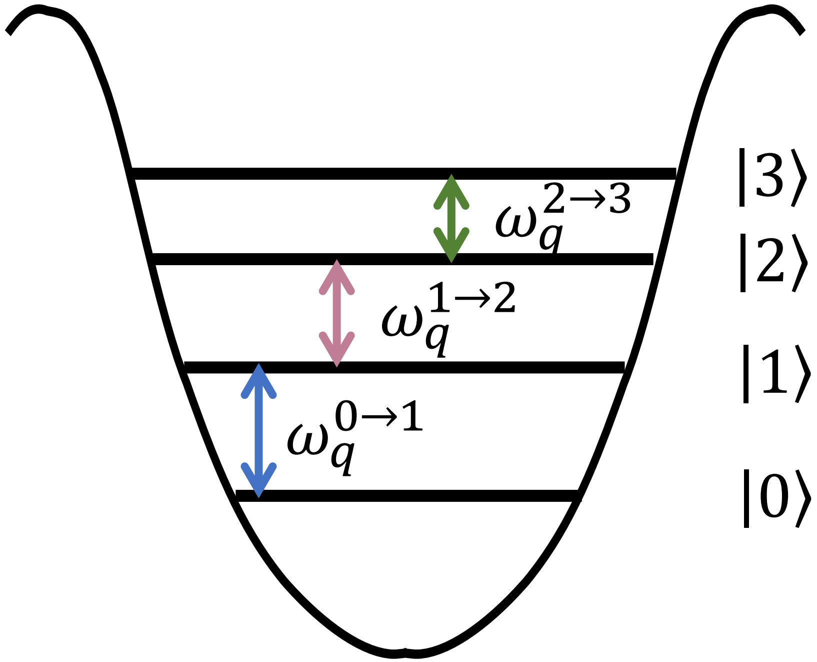


A physical realization of a qubit is a transmon

Quantized transmon:



$$H = \hbar\omega_q \, a^+ a + \frac{\alpha}{2} a^+ a^+ a a$$



Krantz P et al. (2019), Applied Physics Reviews 6, 021318

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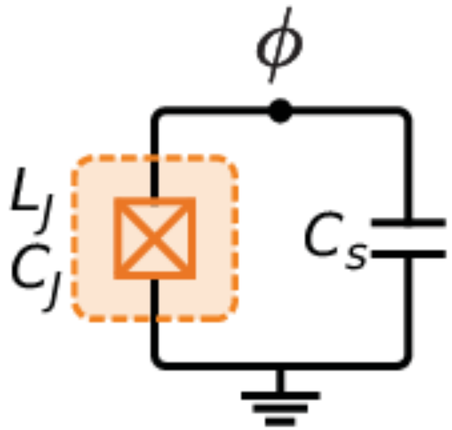
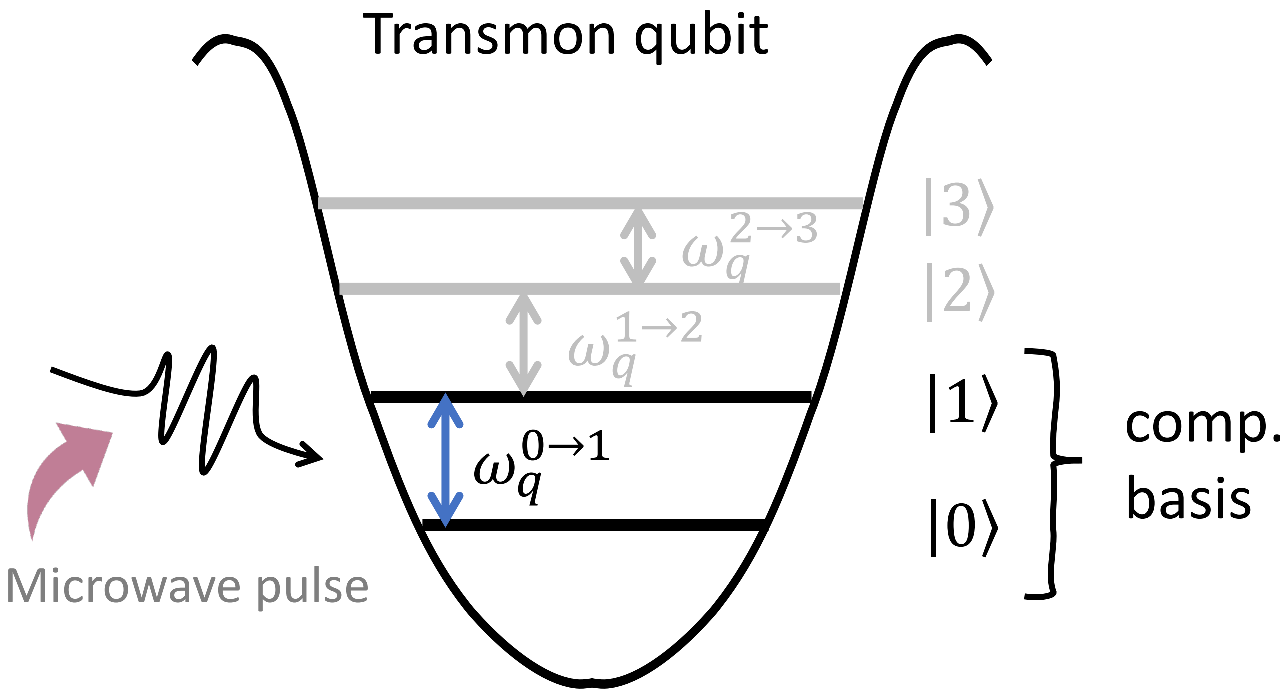
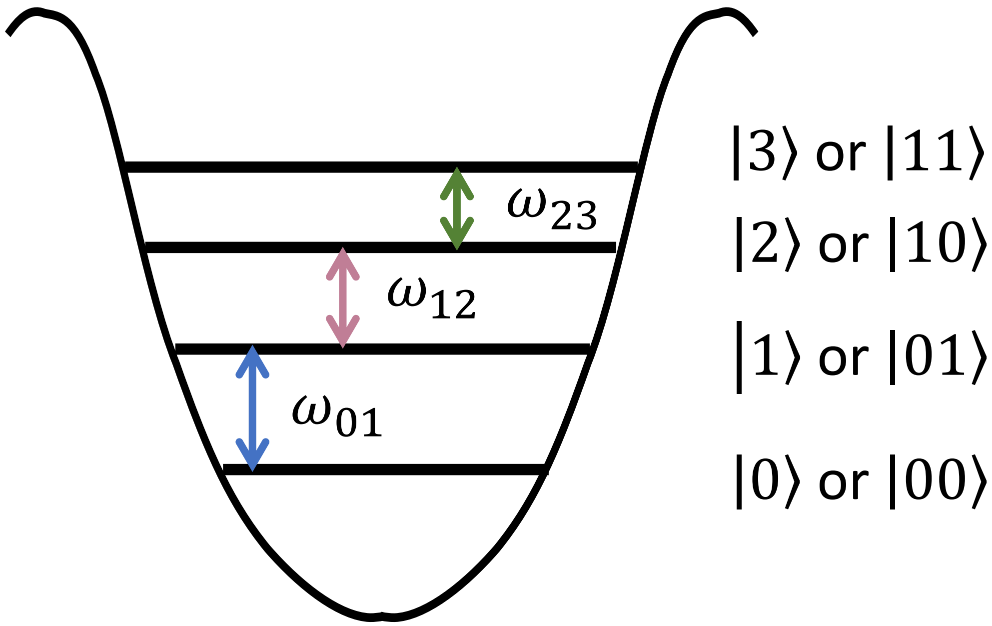


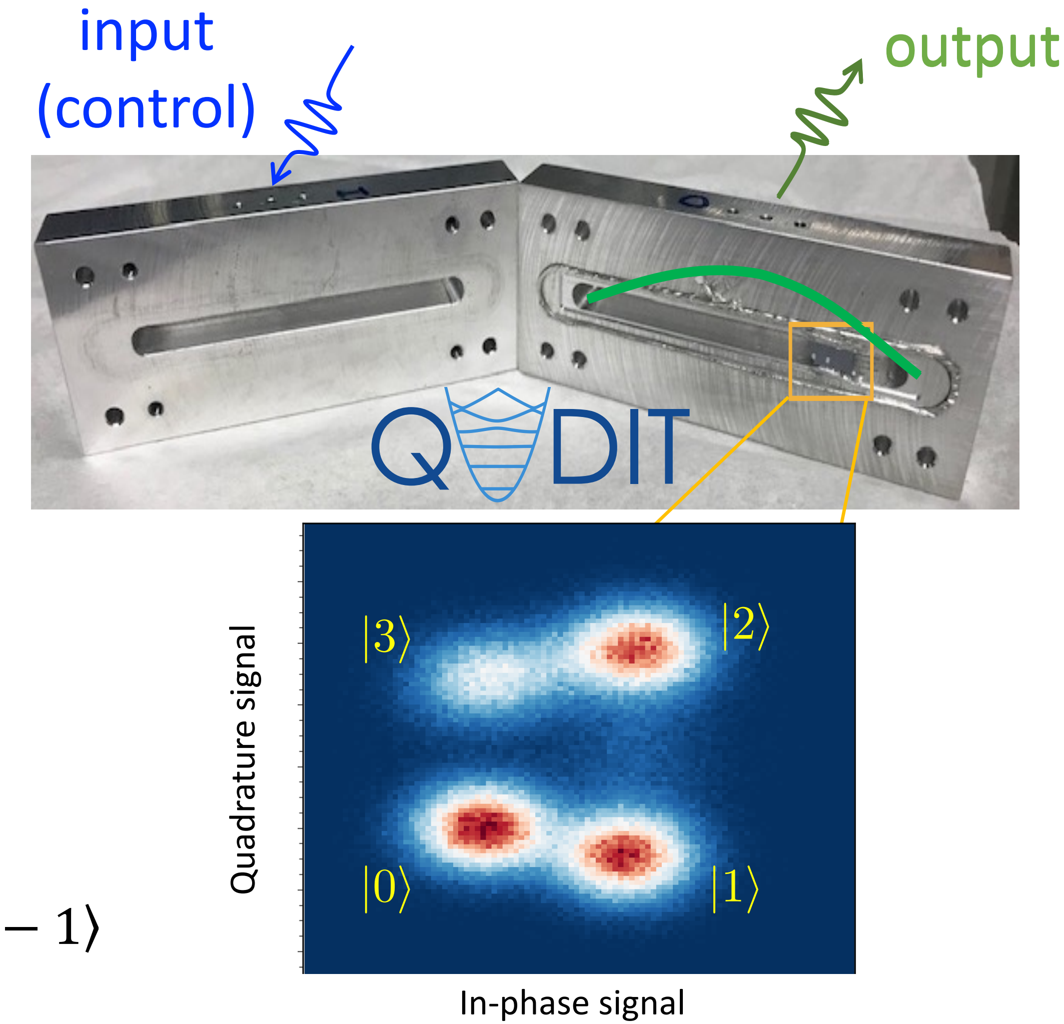


$$H = \hbar\omega_q\, a^+a + \frac{\alpha}{2} a^+a^+aa$$

Krantz P et al. (2019), Applied Physics Reviews 6, 021318

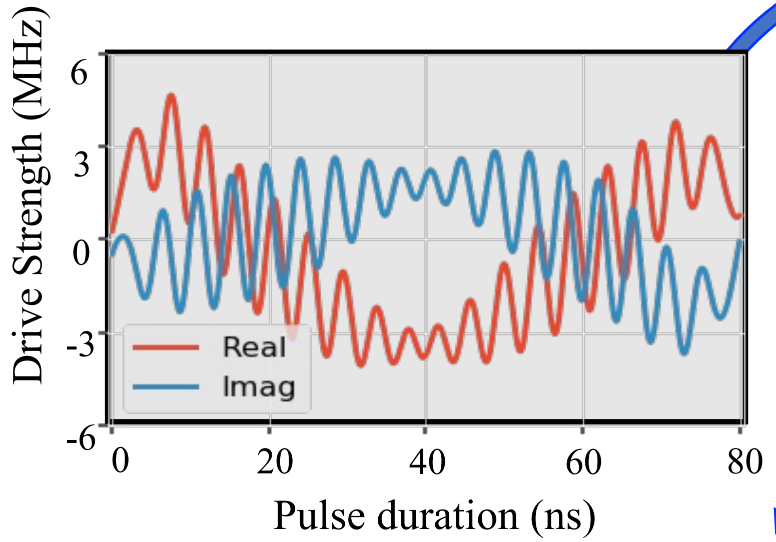
One can also work with registers of d-level quantum systems or ‘qudits’

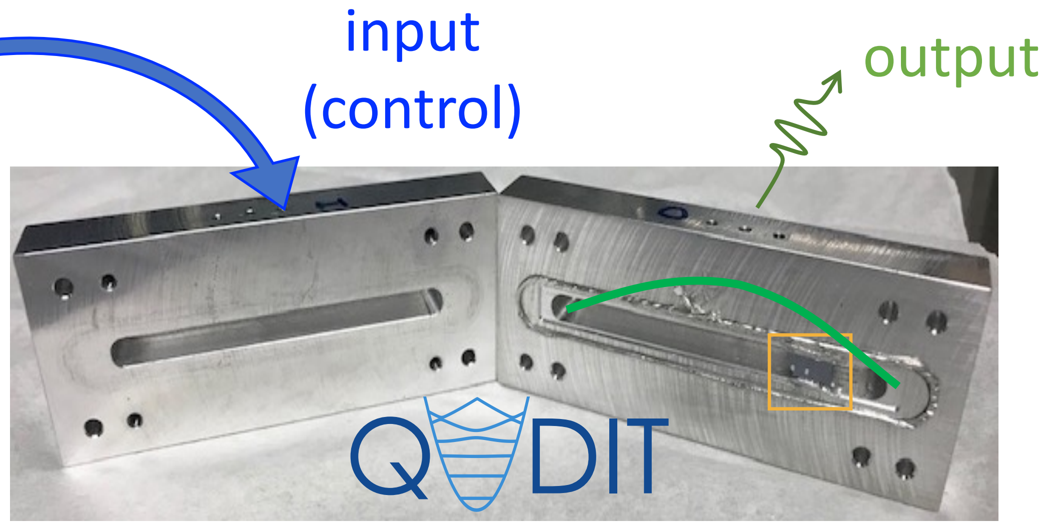




$$|\psi_{qudit}\rangle = \alpha_0|0\rangle + \alpha_1|1\rangle + \alpha_2|2\rangle + \alpha_3|3\rangle + \cdots \alpha_{d-1}|d-1\rangle$$

Physically, quantum gates are realized by controlling the device with microwave pulses engineered with optimization techniques





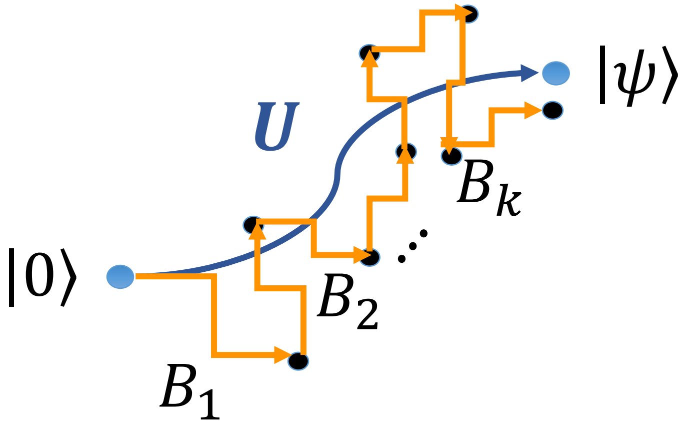
$$U_{targ} \approx U_{opt} = \mathcal{T}exp\left[-\frac{i}{\hbar}\int_0^{T_g}\left(H_0+\sum_{k=1}^{2n} u_k(t)H_k\right)dt\right]$$

Solve time evolution for quantum device

Quantum programs (sequence of unitaries) can be compiled through digital or analog gates, or a combination of both

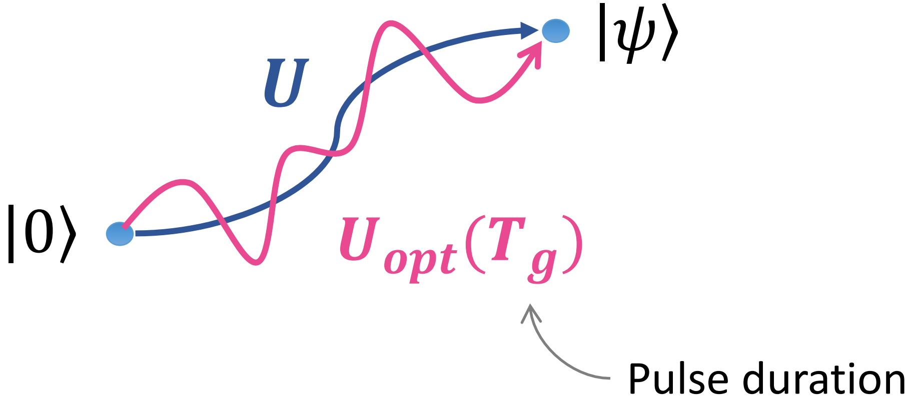
$$U \approx B_k \cdots B_2 B_1$$

Universal set of gates,
Digital simulation



$$U \approx U_{opt}(T_g)$$

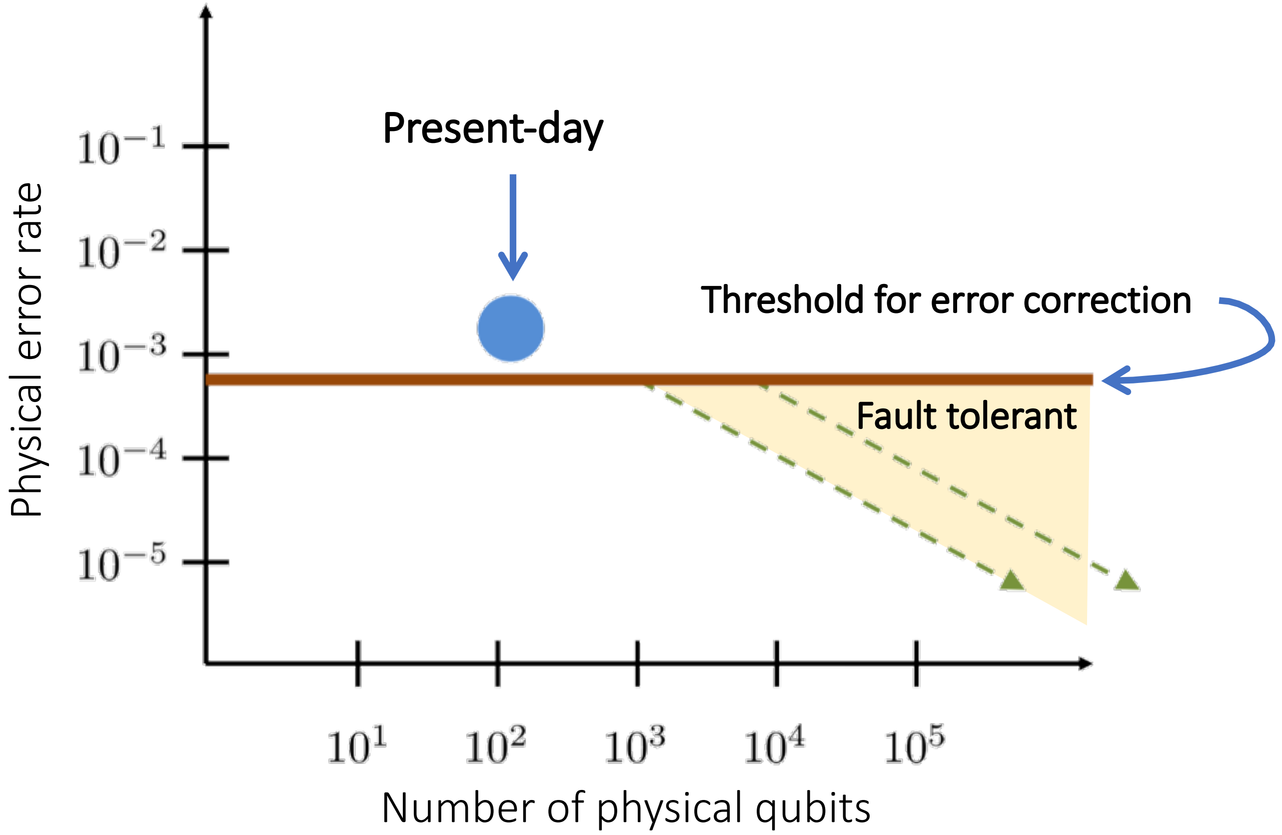
Custom gate,
Analog simulation



A challenge is to formulate quantum algorithms, measurement schemes to simulate nuclear physics

Controlled quantum systems	Must use distinguishable qubits to simulate indistinguishable fermions	Which encodings will be most effective?
		Can we efficiently adapt our 'classical' methods to quantum computing?
$\vert\psi_f\rangle = U\,\vert\psi_i\rangle$	Simulations must be framed in terms of qubits' unitary operations	Can we exploit the nature of quantum devices to develop new methods?
$P(10011\cdots) = \vert\langle 10011\cdots\vert\psi_f\rangle\vert^2$	Desired quantities must be extracted from positive semi-definite distributions	Can we design analog and digital-analog quantum simulations tailored to hadrons?

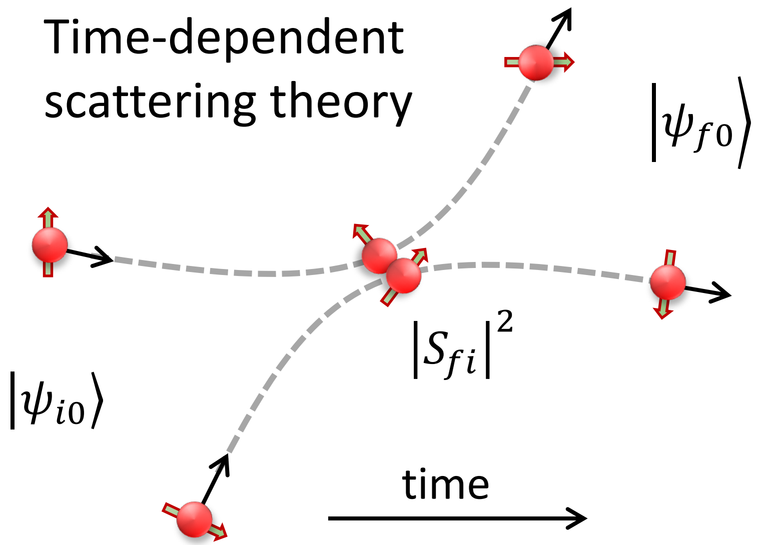
Another challenge is to realize useful quantum simulations in the noisy and intermediate scale (NISQ) quantum era



What are noise-resilient protocols that will enable useful quantum simulations of hadron dynamics in the near term?

Quantum computing offers a natural framework for simulating nuclear dynamics, classically very hard!

Time-dependent scattering theory



$$P = |S_{fi}|^2 = |\langle\psi_f(0)|\psi_i(0)\rangle|^2$$

$$\approx |\langle\psi_{f0}(0)|\Omega_+^\dagger\Omega_-|\psi_{i0}(0)\rangle|^2$$

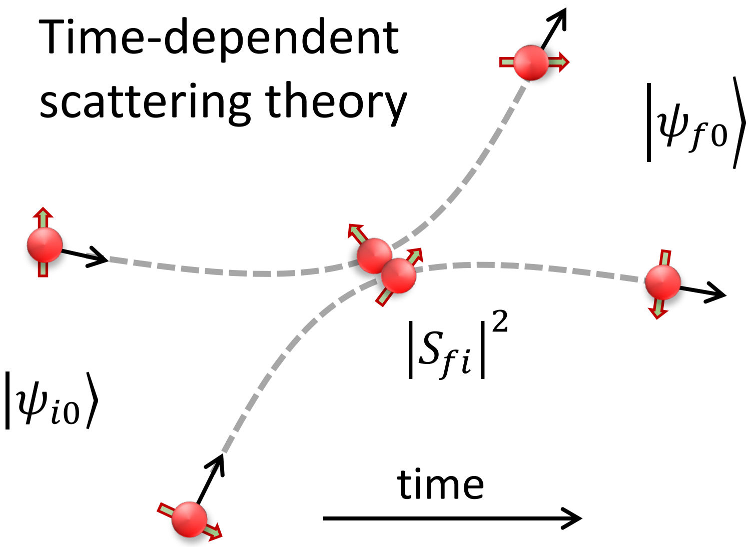
↑

$$e^{-iHt}e^{iH_0t}$$

Application of unitary transformations (= gates)

Quantum computing offers a natural framework for simulating nuclear dynamics, classically very hard!

Time-dependent scattering theory



$$P = |S_{fi}|^2 = |\langle\psi_f(0)|\psi_i(0)\rangle|^2$$

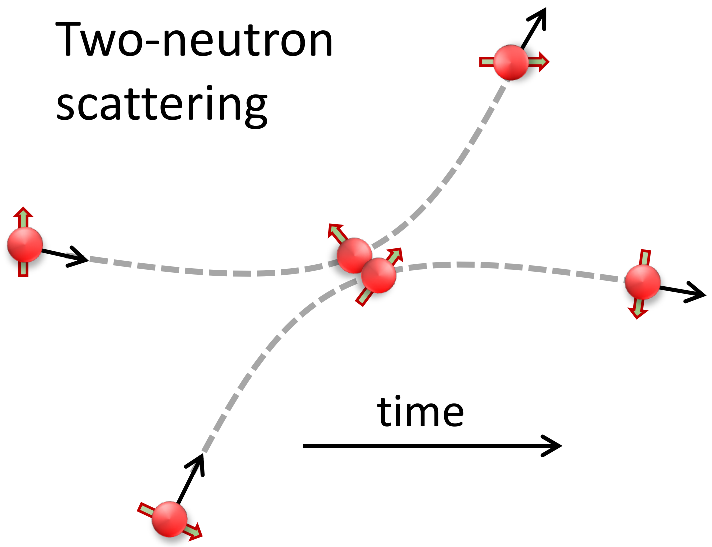
$$\approx |\langle\psi_{f0}(t)|e^{-2iHt}|\psi_{i0}(-t)\rangle|^2$$

$U(2t)$

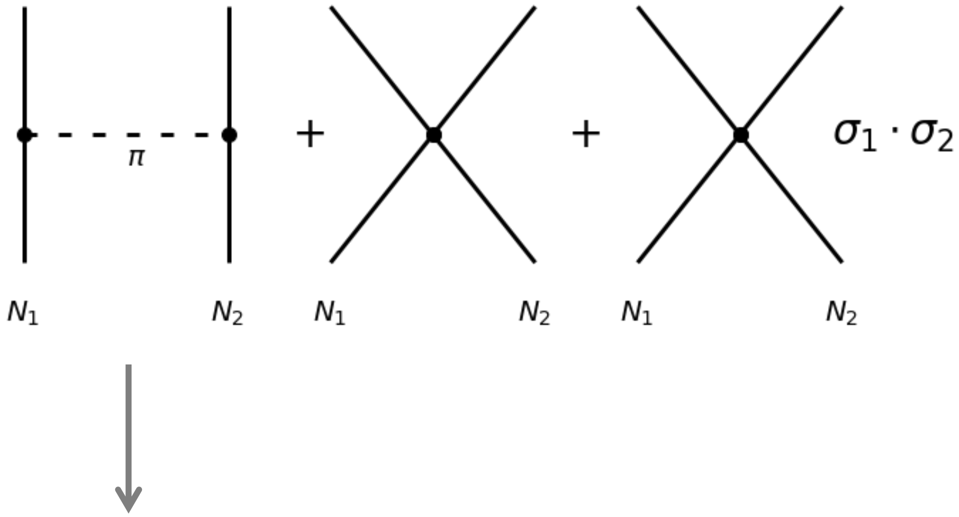
State preparation

Real-time evolution

Target problem: prototypical two-neutron scattering

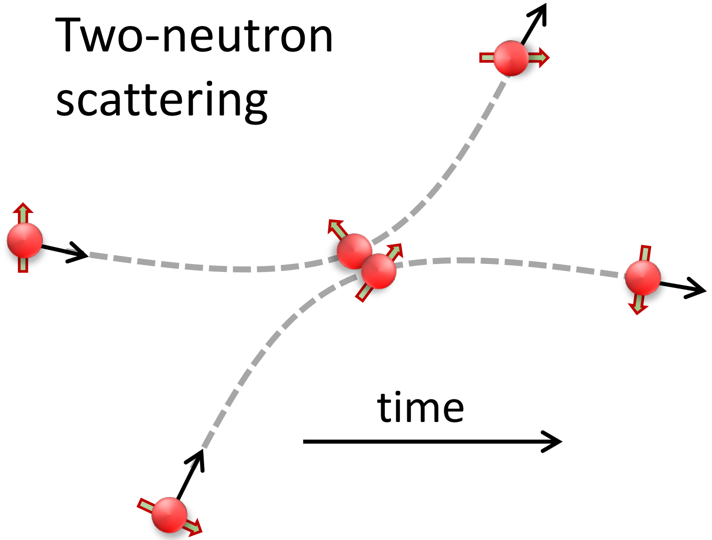


NN force @LO of chiral EFT

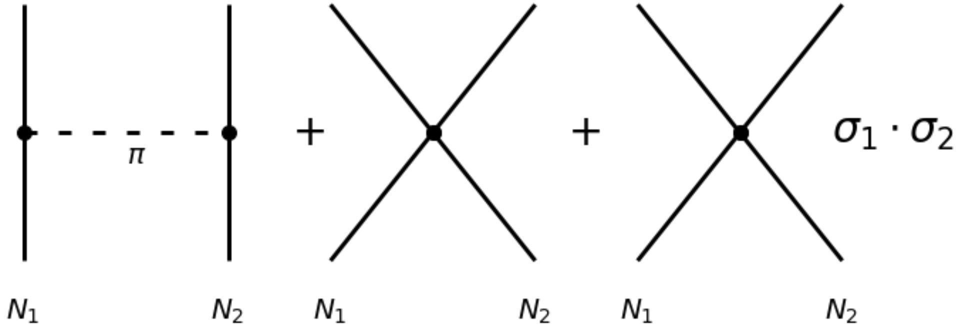


$$S_{12} = 3\left(\vec{\sigma}^1 \cdot \hat{r}\right)\left(\vec{\sigma}^2 \cdot \hat{r}\right) - \vec{\sigma}^1 \cdot \vec{\sigma}^2$$

Target problem: prototypical two-neutron scattering



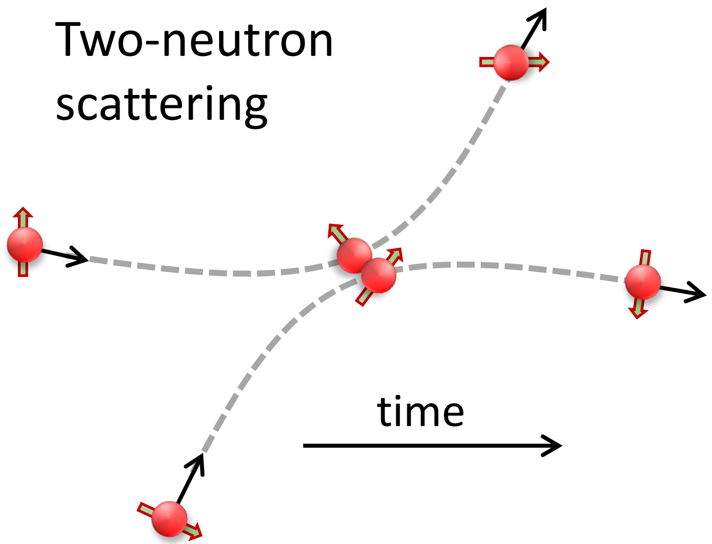
NN force @LO of chiral EFT

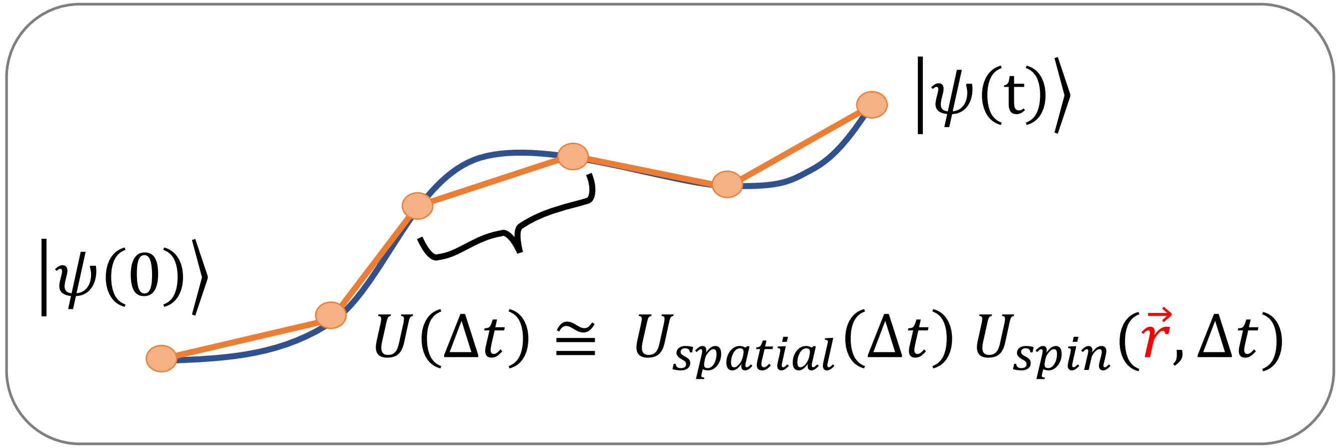


$$H_{LO}(\vec{r},\vec{\sigma}_1,\vec{\sigma}_2) = \underbrace{T(\vec{r}) + V_{SI}(\vec{r})} + V_{SD}\,(\vec{r},\vec{\sigma}_1,\vec{\sigma}_2)$$

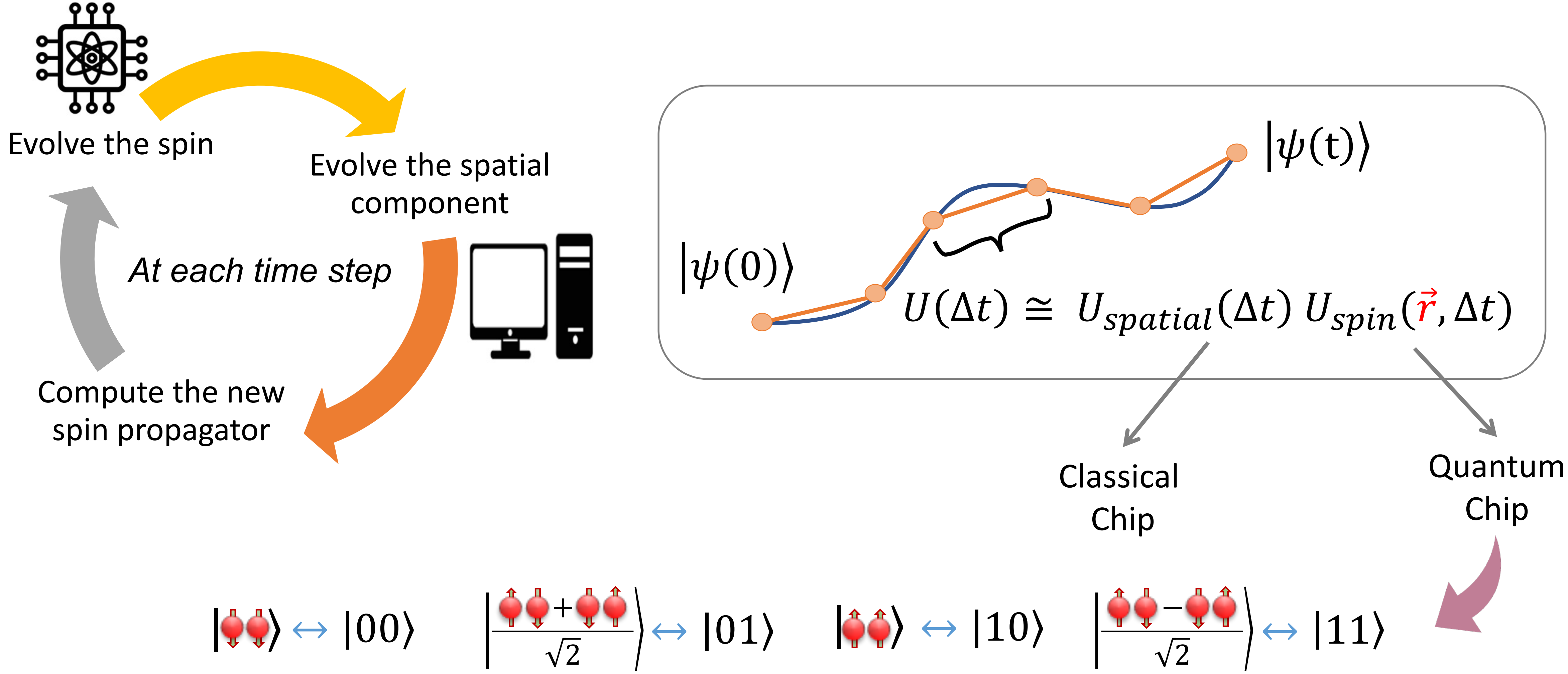
$$U(\Delta t) \cong U_{spatial}(\Delta t)\; U_{spin}(\vec{r},\Delta t)$$

Target problem: prototypical two-neutron scattering

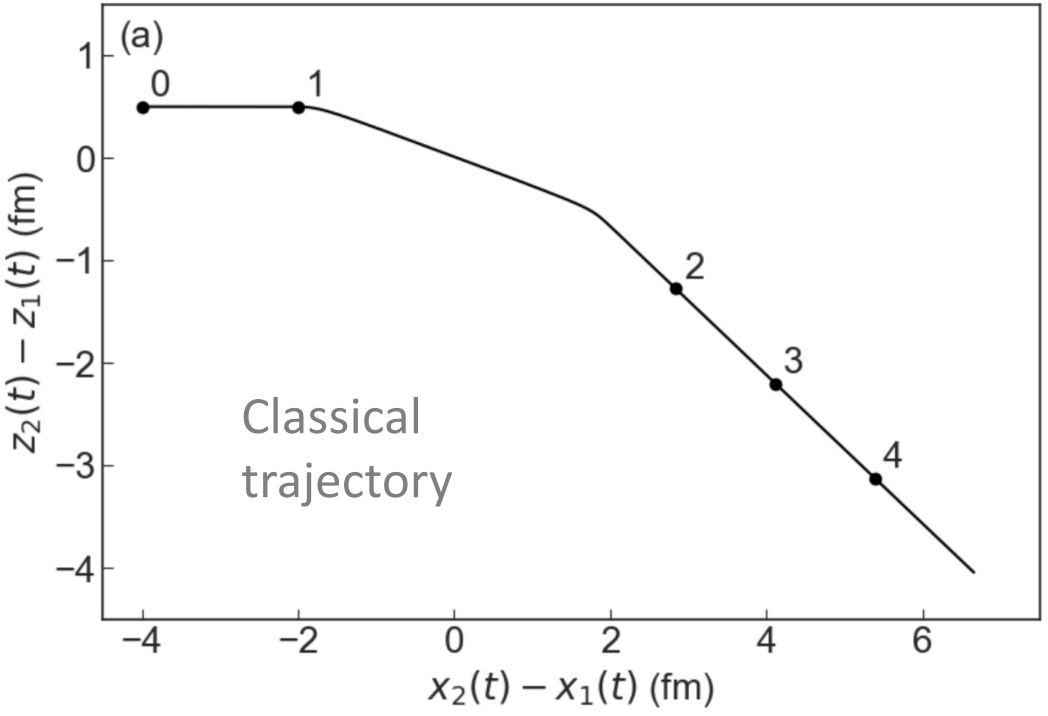


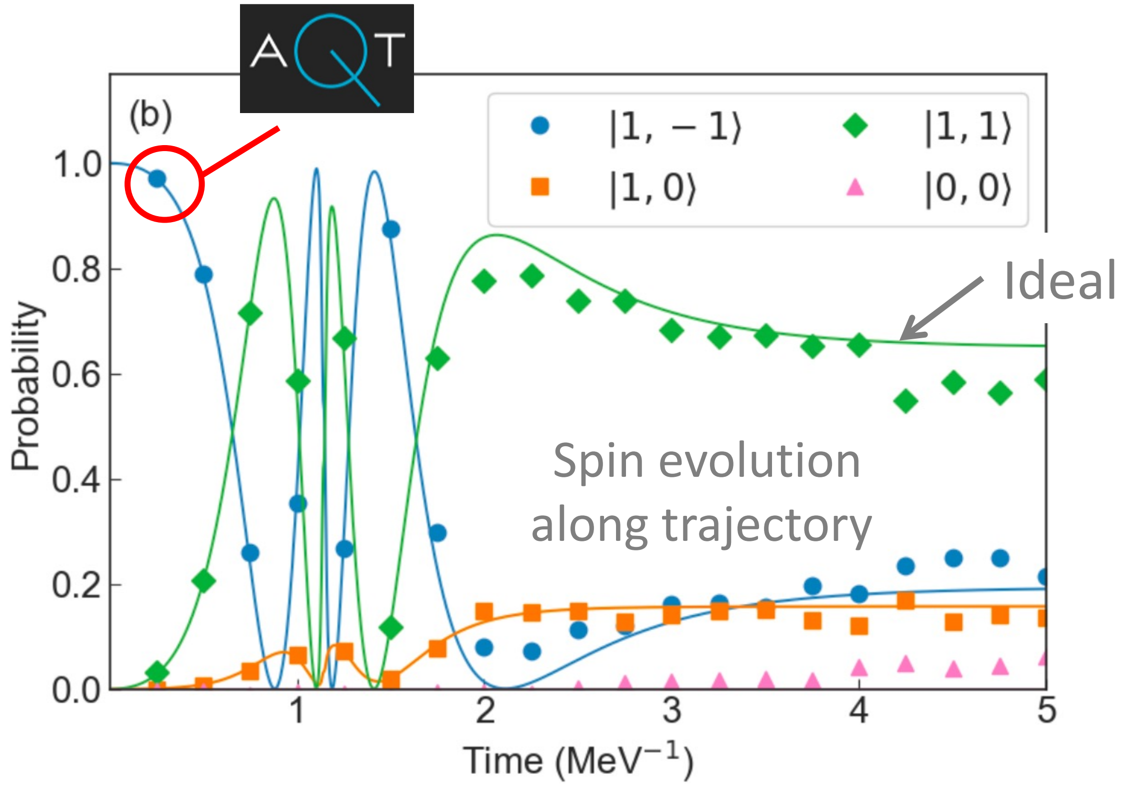


Target problem: prototypical two-neutron scattering



Quantum-classical coprocessing scheme works on present hardware, could enable path-integral simulations of scattering

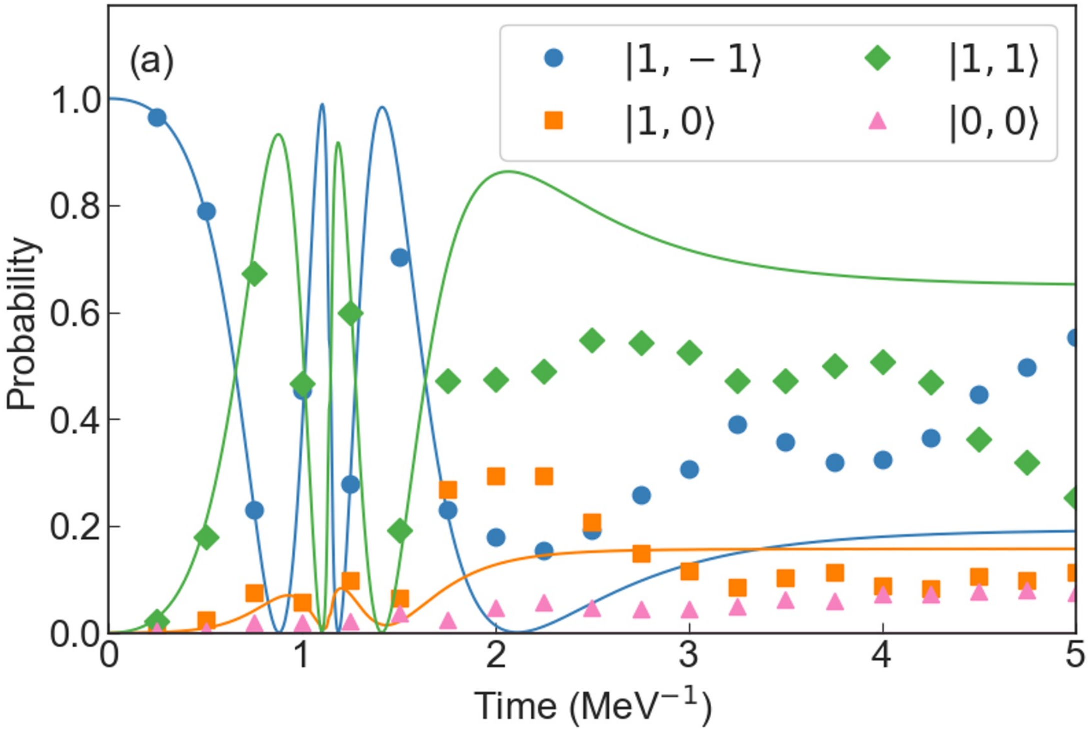




Turro F, Chistolini T. et al. (2023), Phys. Rev. A (submitted), arXiv:2302.06734

However, it first required (scalable) error mitigation: randomized compiling, state purification

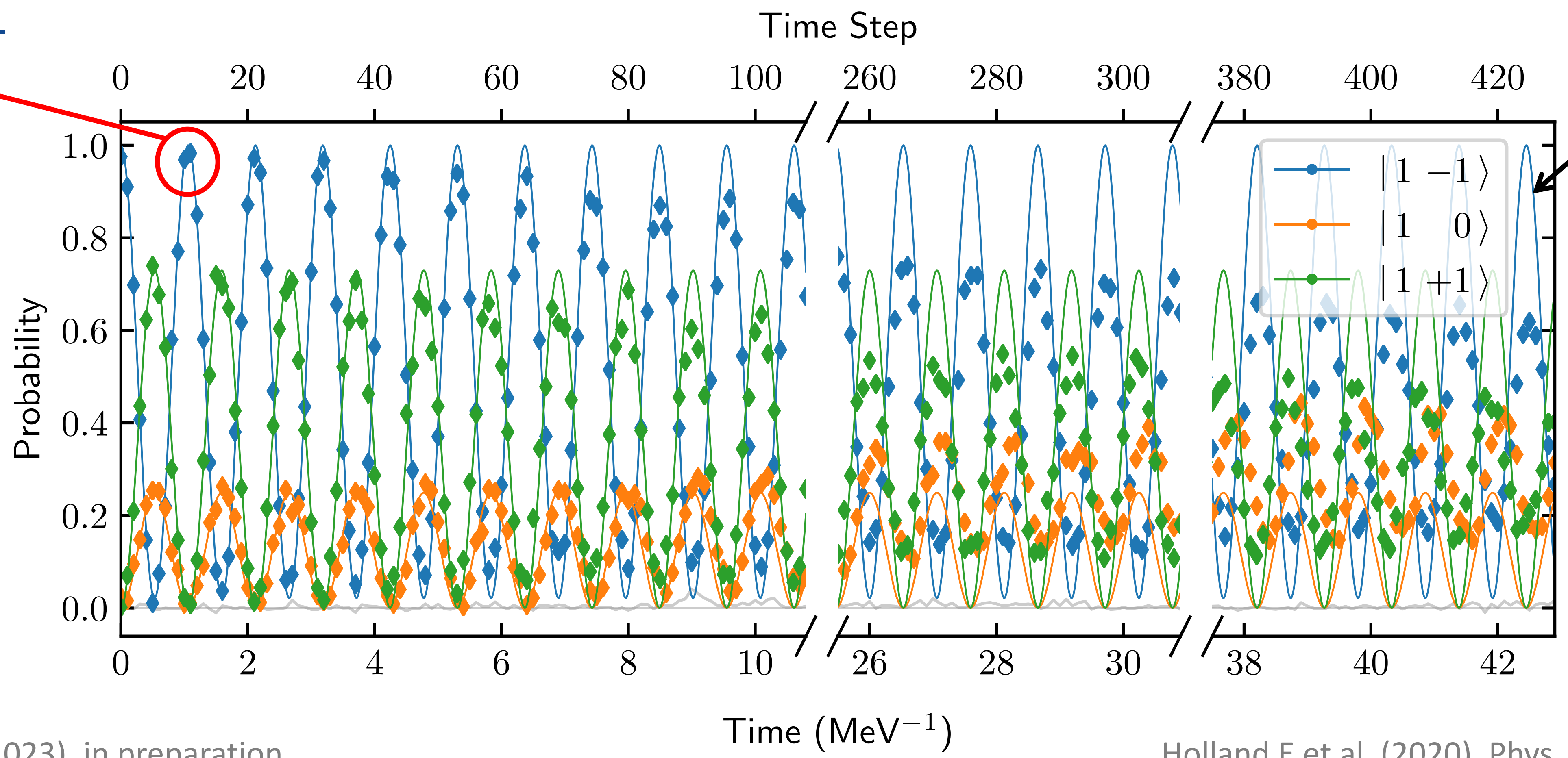
Before error mitigation



Time step	# 2-qubit gates	# Total gates
1	3	27
4	12	135
8	24	243
12	36	351
16	48	459
20	60	540

Turro F, Chistolini T. et al. (2023), Phys. Rev. A (submitted), arXiv:2302.06734

Digital-analog simulation with custom two-spin short-time propagator gates provides enhanced resilience to noise

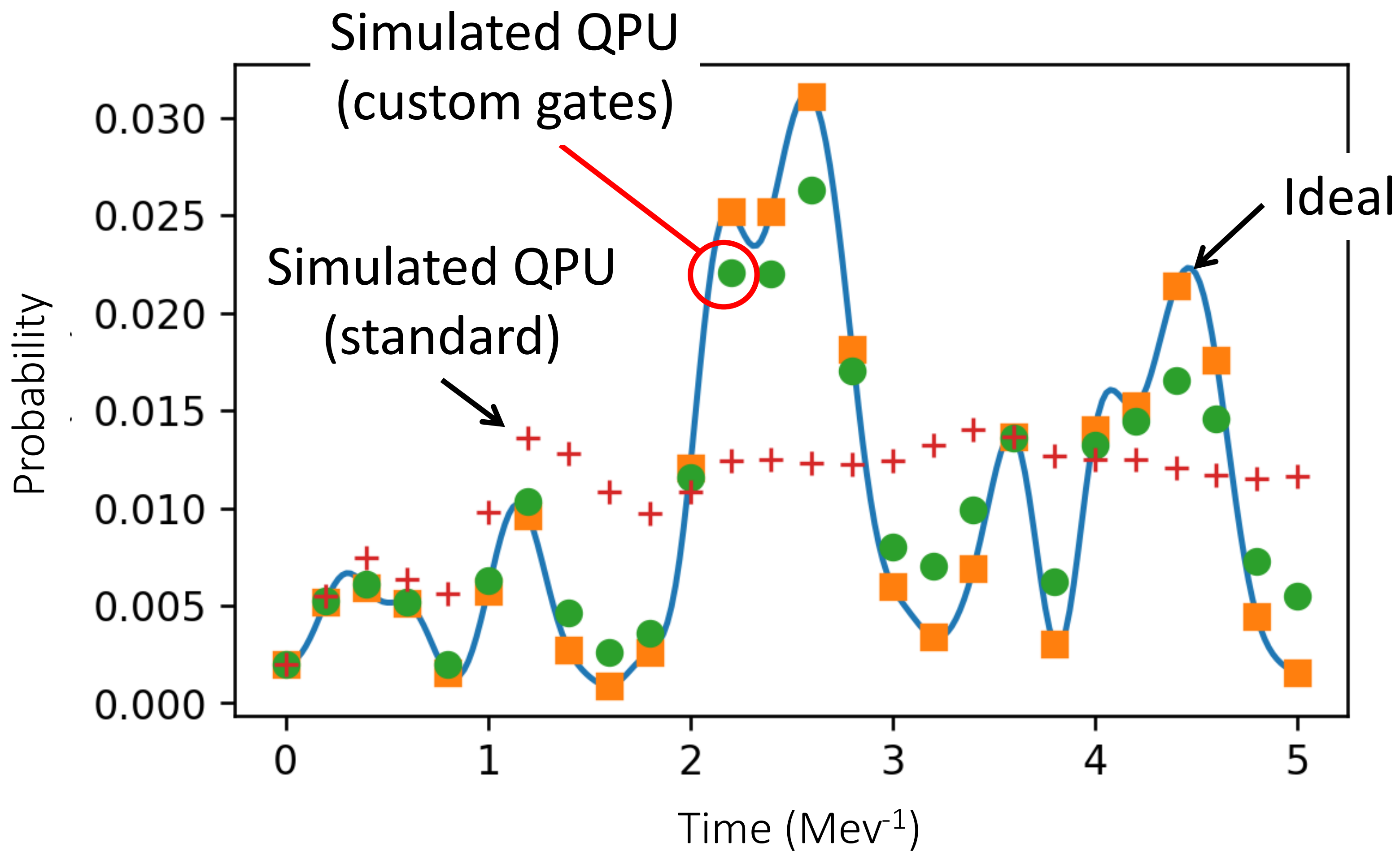


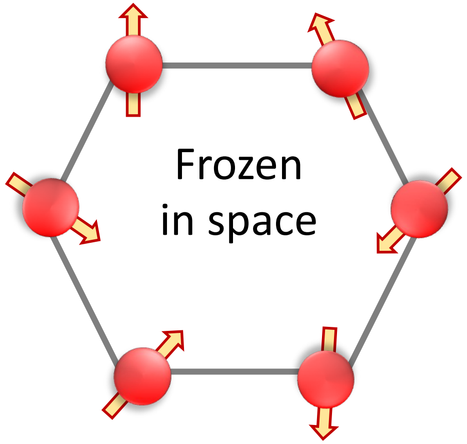
Ideal solution

Wu X et al. (2023), in preparation

Holland E et al. (2020), Phys. Rev. A 101, 062307

With custom gates, designed noise-resilient algorithm for quantum simulation of multi-nucleon spin dynamics





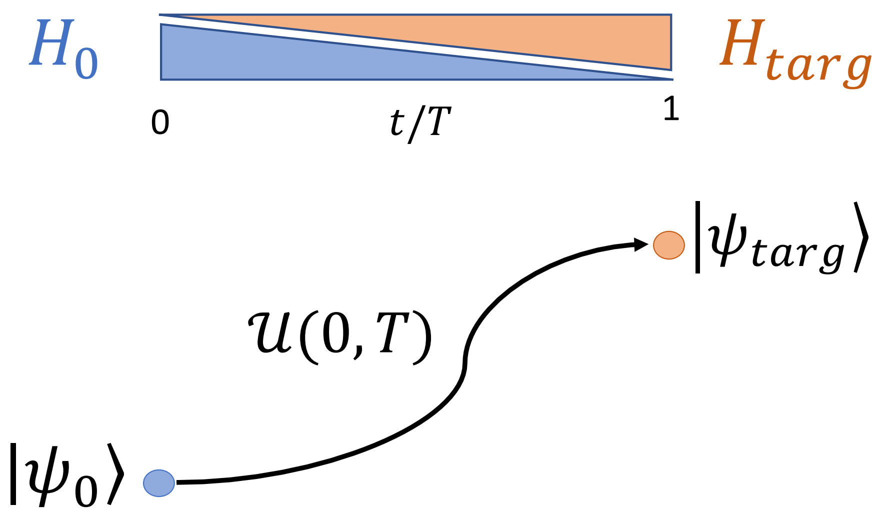
≡ 6 qubits

Polynomial scaling
with number of particles

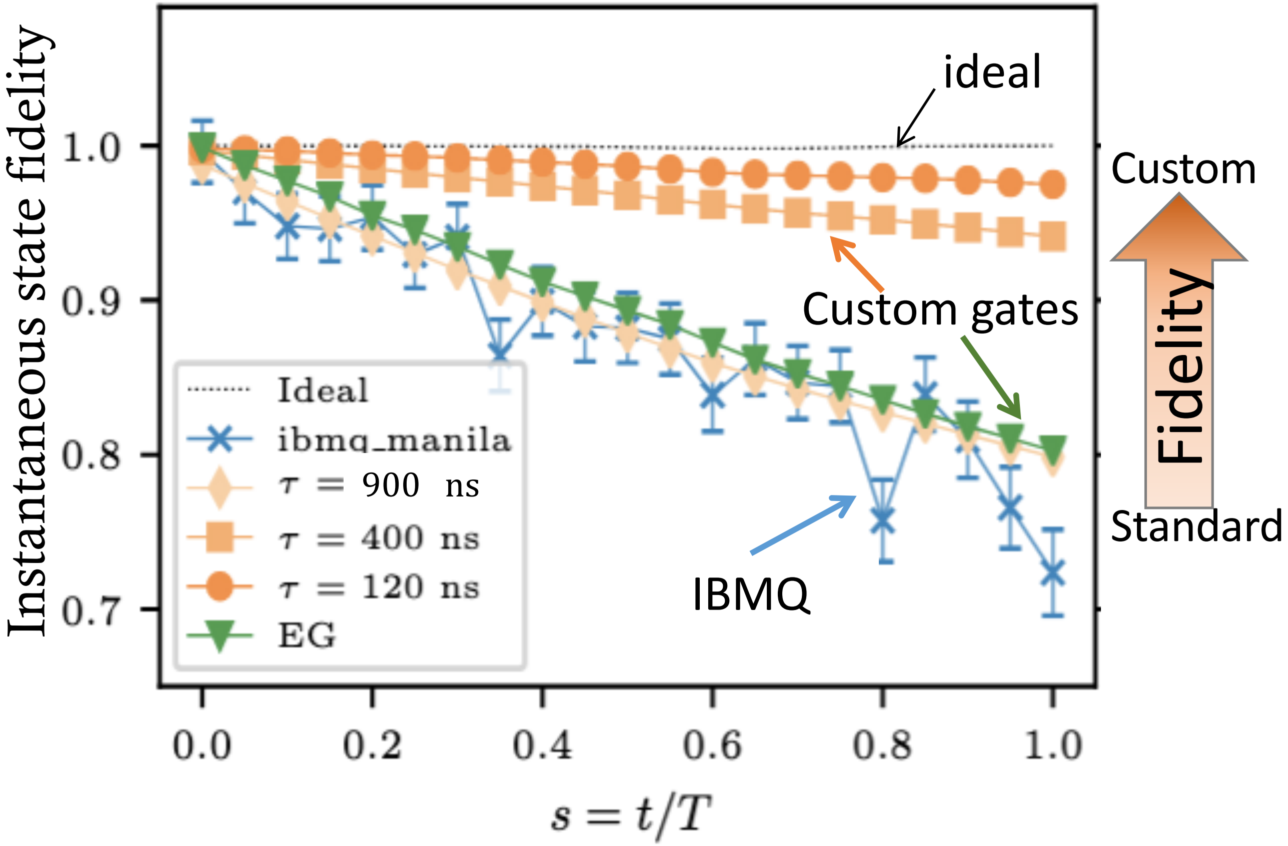
Wendt KA et al, in progress

Digital-analog simulations with custom gates enable major performance improvements for state preparation

Adiabatic evolution



E.g.: 2-spin system



Coello-Perz, EA et al. (2022), Phys. Rev. A 105, 032403

The LLNL/Trento QC team and collaborators

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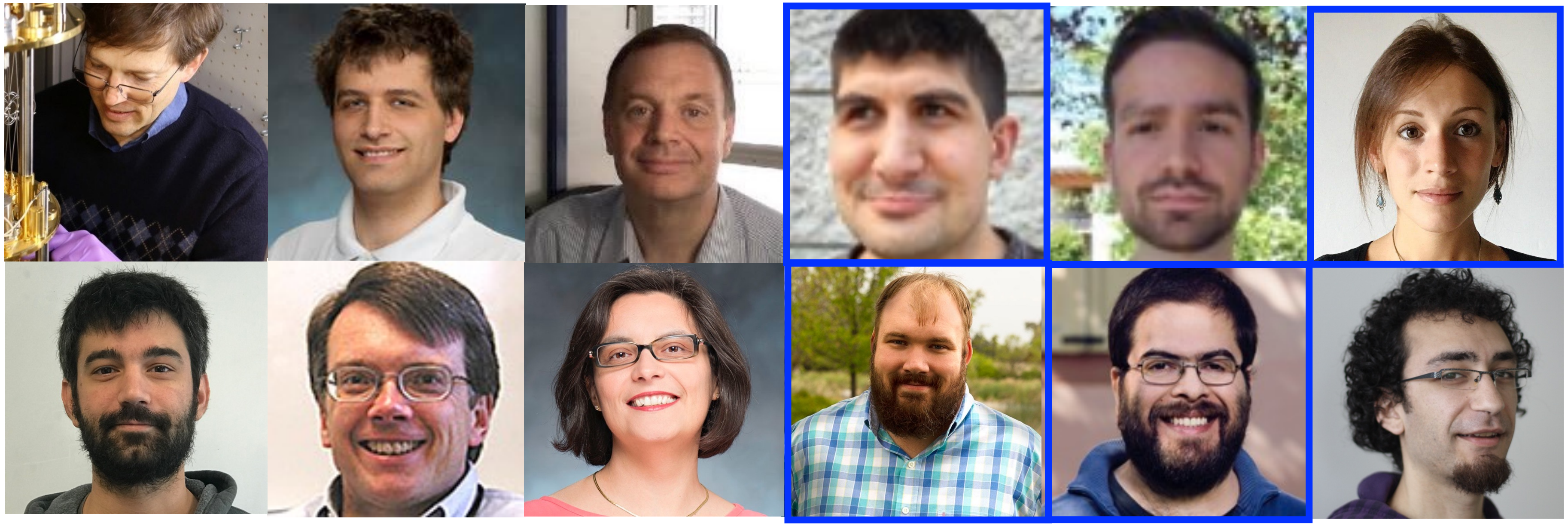

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Joey Bonitati (MSU)
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Collaborator

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Chistolini
& AQT Team

This is an exciting time for paving the way to exact quantum simulations of few- & many-body dynamics

In the near term, noise-resilient quantum simulations will require hybrid algorithms and customized gates

Understanding, exploiting the underlying characteristics of near-term quantum devices will be key

Lots of (few-body) work ahead to develop
noise-resilient quantum simulations
that scale with particle number

PROGRAM Upcoming @INT

OCTOBER 7 - NOVEMBER 8, 2024

Quantum Few- and Many-Body Systems in Universal Regimes (INT)

A. Bergschneider, S. Gandolfi,
M. Gattobigio, S. Quaglioni
Embedded Workshop: October 21 - 25

FEW-BODY TOPICAL GROUP

The APS Topical Group On Few-Body Systems and Multiparticle Dynamics

Graduate/Postdoctoral Travel Grants

International, European, Asian-Pacific Conferences on Few-body Problems in Physics

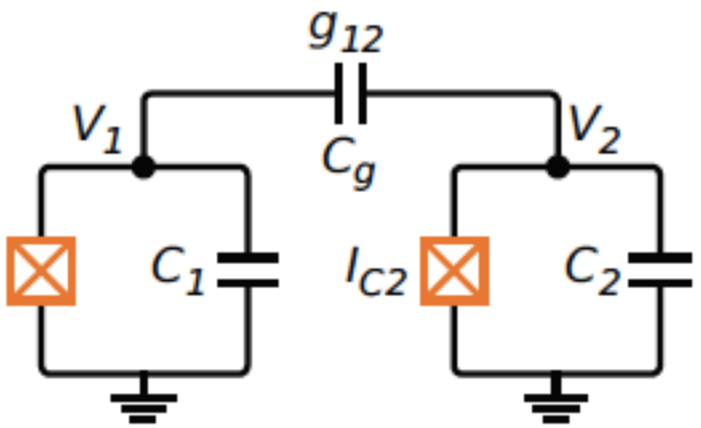
APS Fellowship, Faddeev Medal

https://engage.aps.org/gfb/home

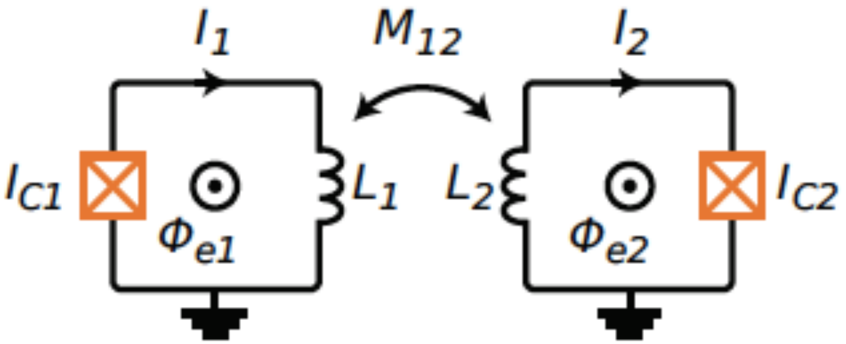
Thank You

To generate entanglement (build registers n of qubits), superconducting qubits must be coupled (here $n = 2$)

Ex: Direct capacitative coupling



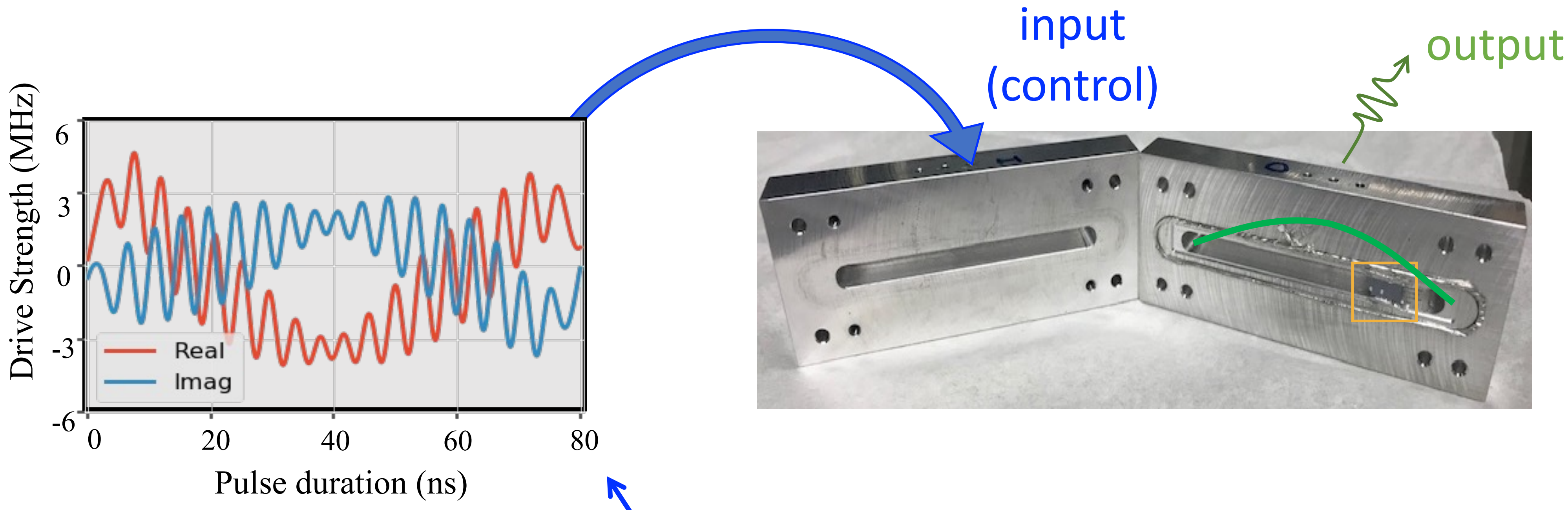
Ex: Direct inductive coupling



$$H = H_0 + H_{int} = \sum_{i \in 1,2} \left[\hbar\omega_i \, a_i^{+} a_i + \frac{\alpha_i}{2} a_i^{+} a_i^{+} a_i a_i \right] - g(a_1 - a_1^{+})(a_2 - a_2^{+})$$

Krantz P et al. (2019), Applied Physics Reviews 6, 021318

‘Basic’ quantum gates are realized with optimization techniques, hinging on a realistic model of the physical quantum device



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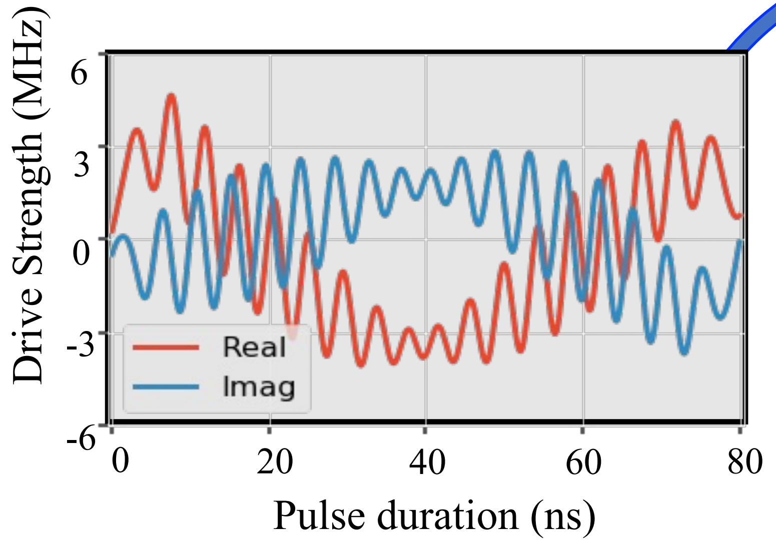
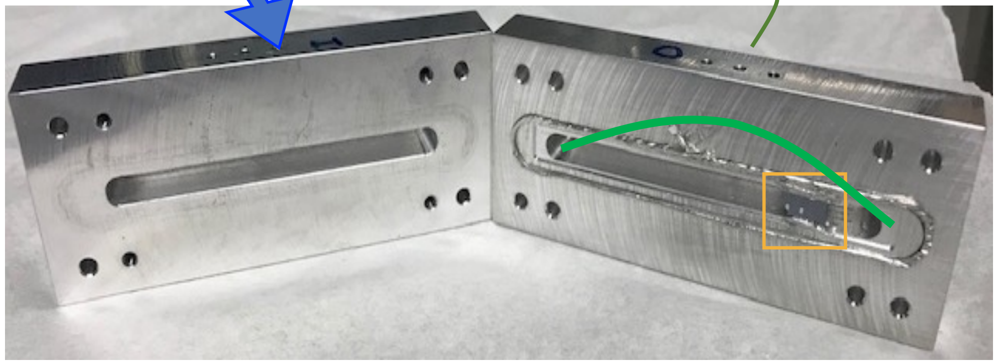
Solve time evolution for quantum device

‘Basic’ quantum gates are realized with optimization techniques, hinging on a realistic model of the physical quantum device



input
(control)

output



$$U_{targ} \approx U_{opt} = \mathcal{T}exp\left[-\frac{i}{\hbar}\int_{0}^{T_g}[H_0 + u_R(t)(a+a^+) + iu_I(t)(a-a^+)]dt\right]$$

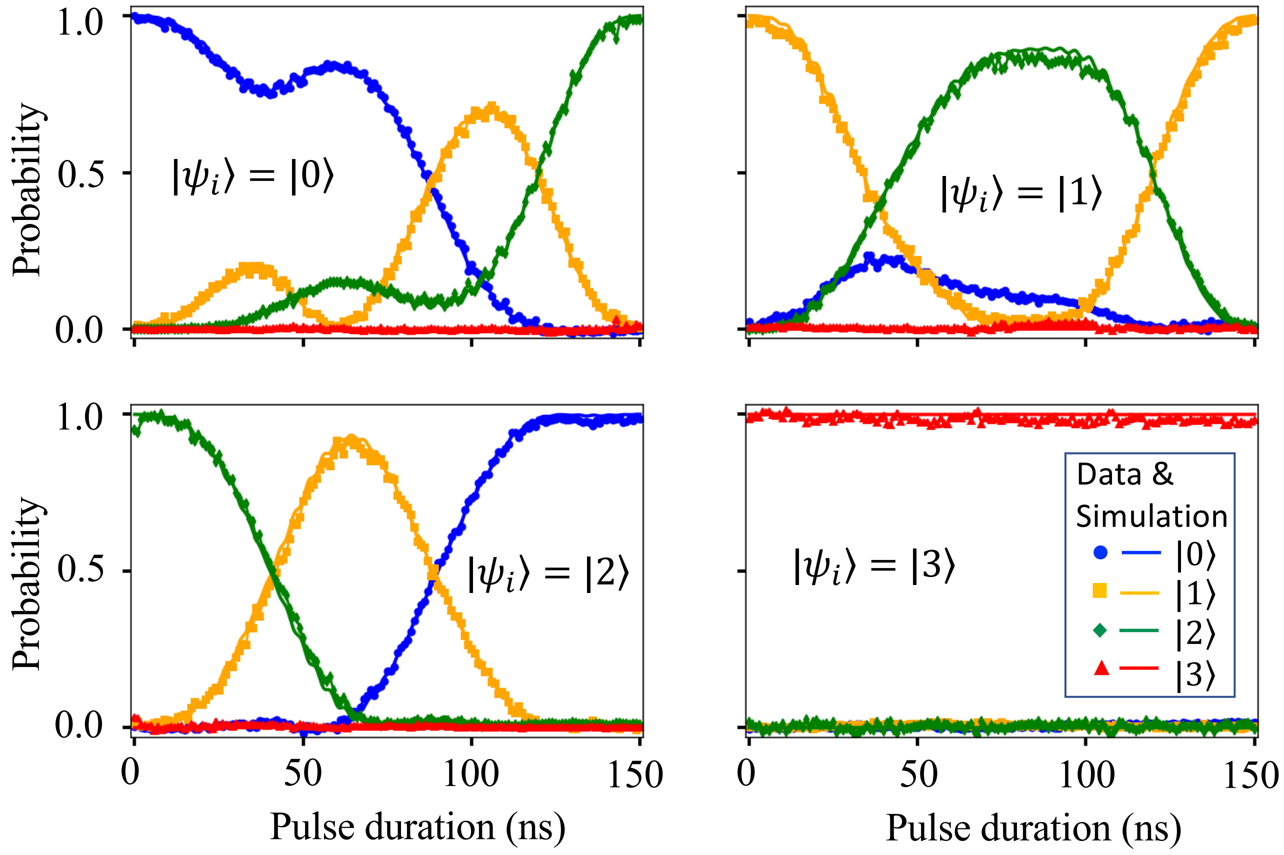
The $0 \leftrightarrow 2$ swap gate was realized with high fidelity on the LLNL qudit

$|0\rangle \rightarrow |2\rangle$

$|1\rangle \rightarrow |1\rangle$

$|2\rangle \rightarrow |0\rangle$

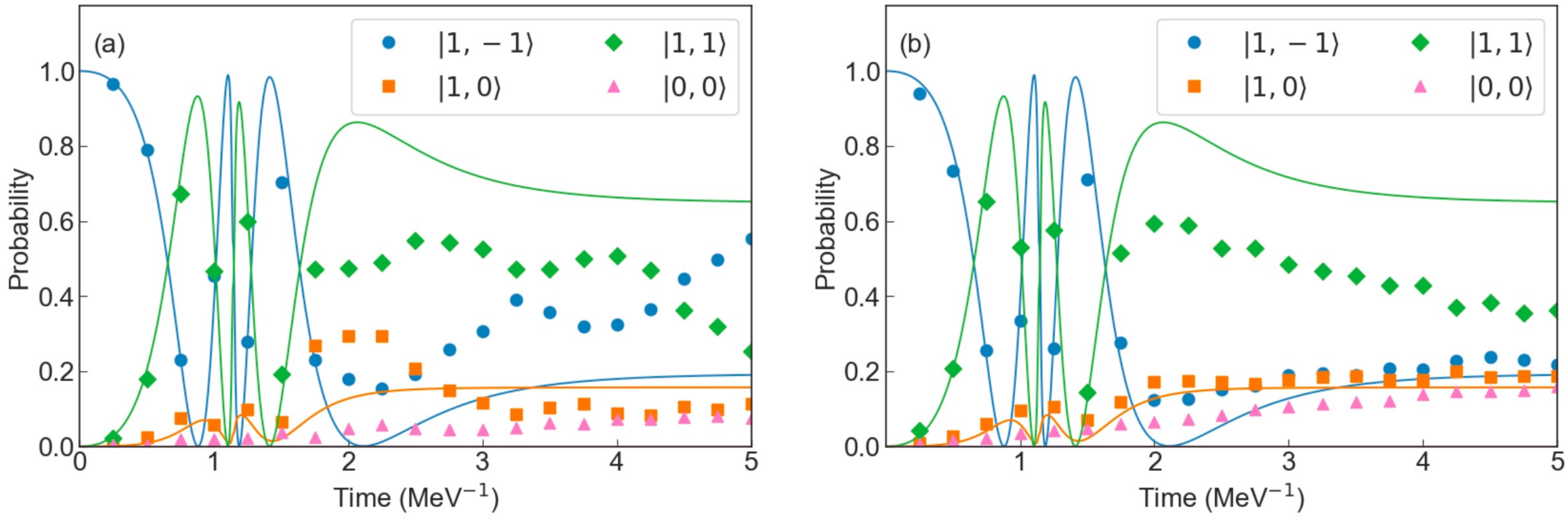
$|3\rangle \rightarrow |3\rangle$



X Wu et. al. PRL 125,170502 (2020)

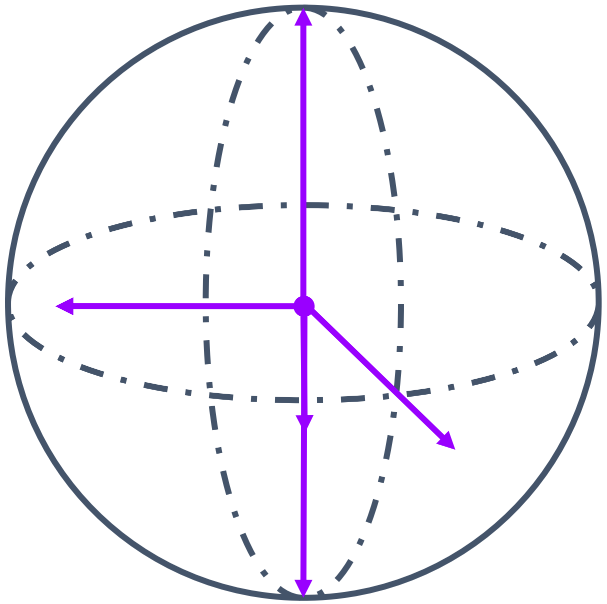
Randomized compiling

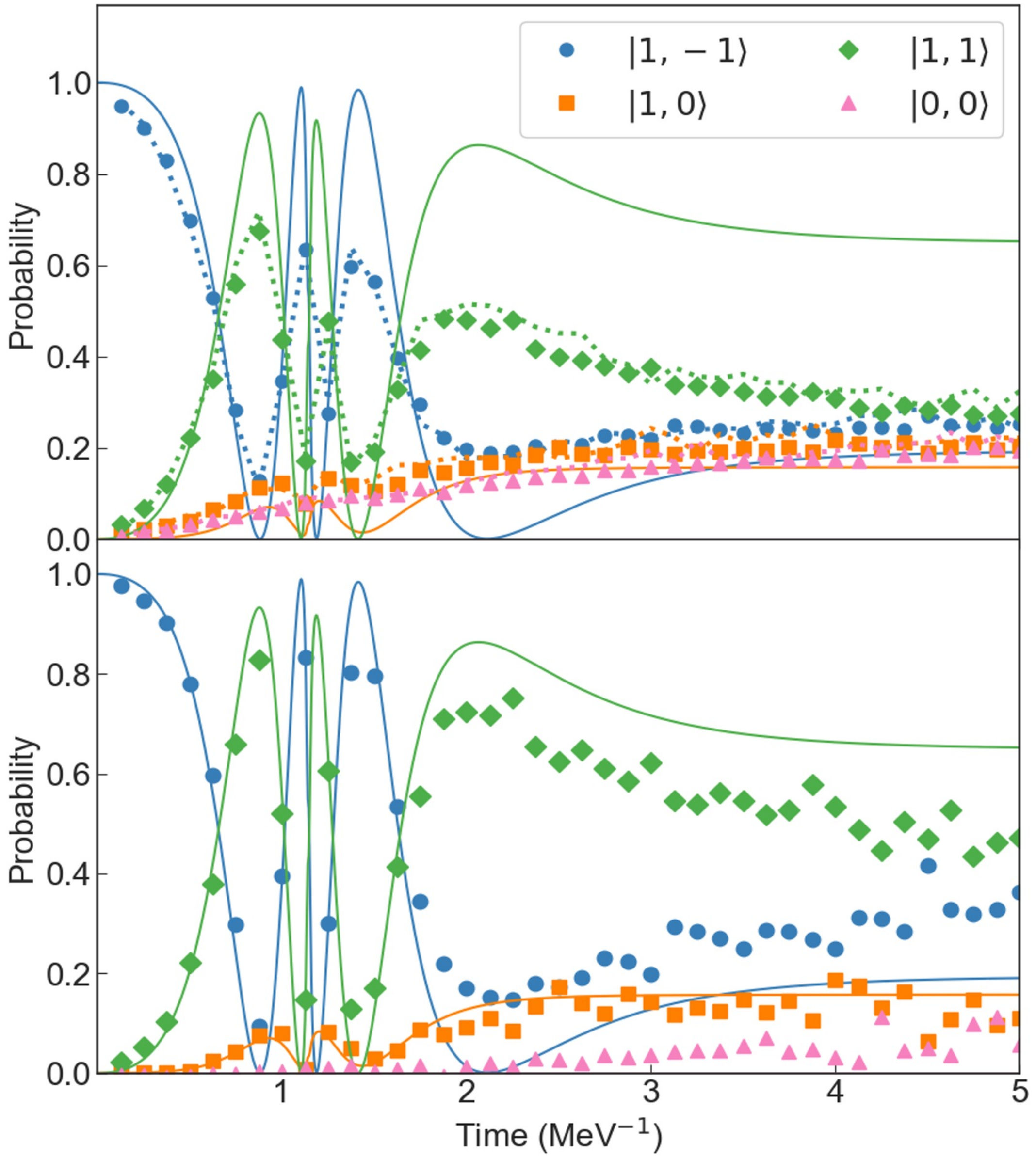
- New circuit by inserting random virtual twirling gates, corresponding inverting gates
- Translate coherent error to stochastic error using multiple random, logically equivalent circuits



State purification

1. Estimate extent that Bloch vector shrinks upon each gate application
2. Renormalize length to unity in post-processing

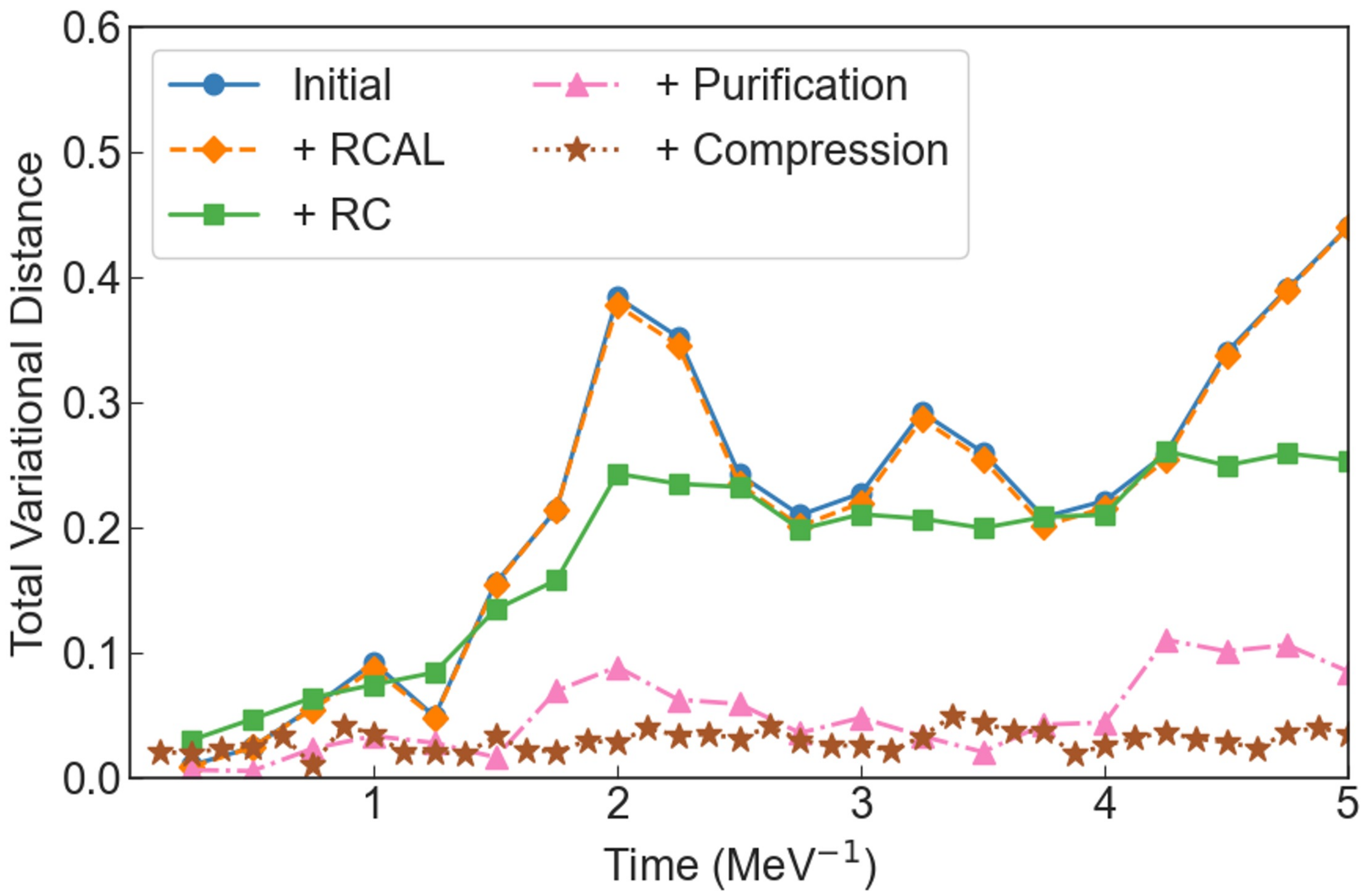




Summary of results: Total variational distance

Total variational distance

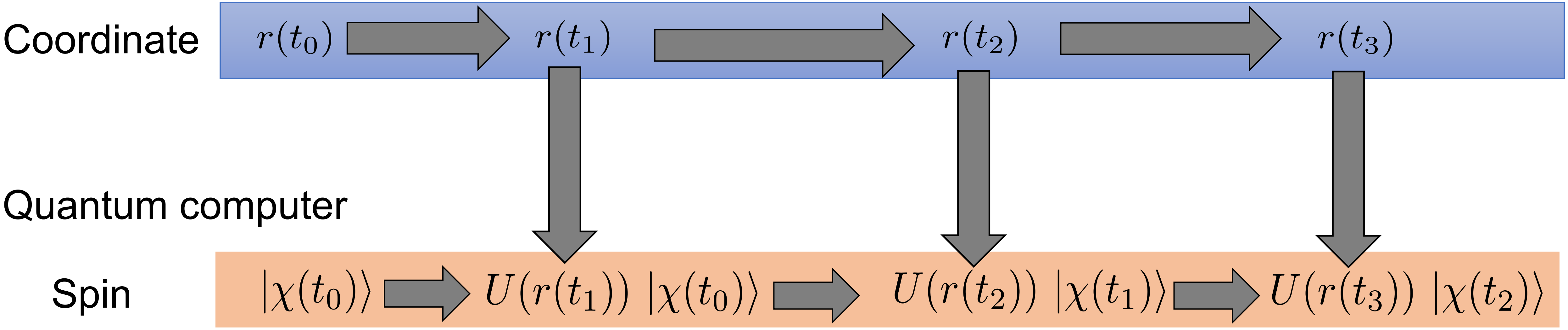
- Metric of absolute difference between two probability distributions
- Here: experimental versus ideal, to evaluate accuracy



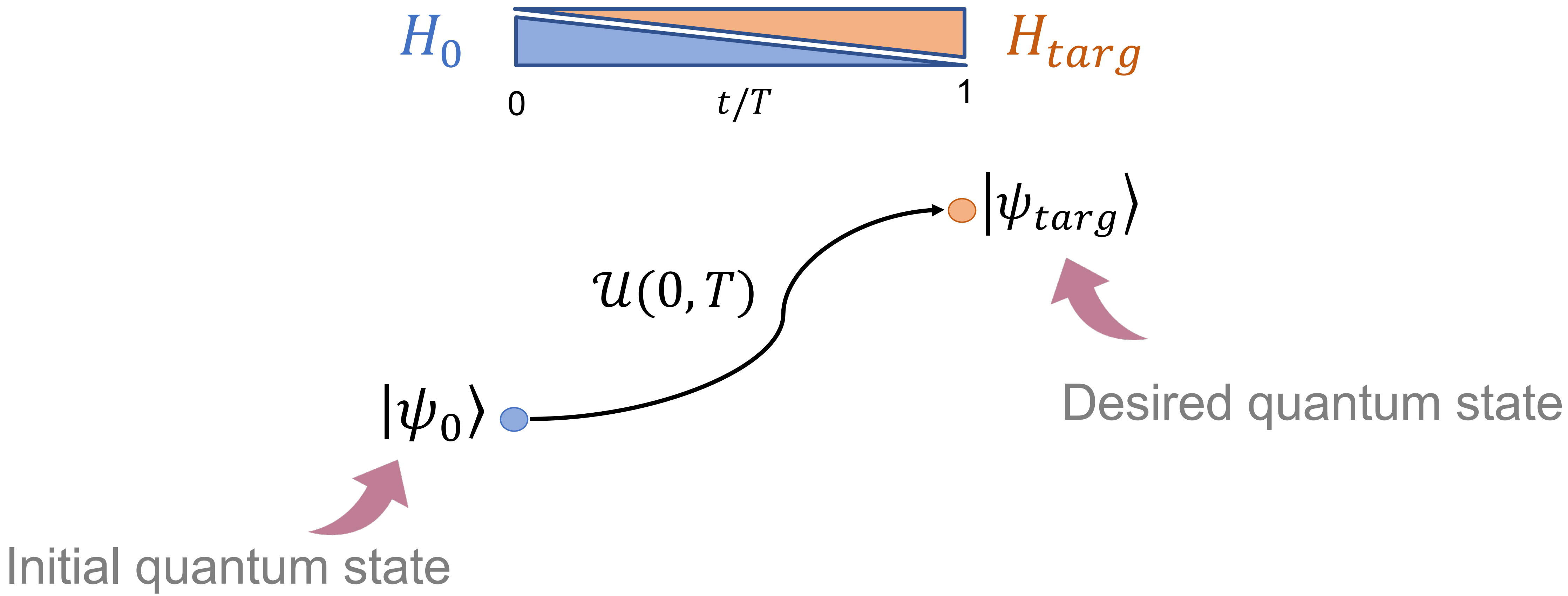
Further approximation: Semiclassical approximation

<u>Approximation:</u> the spatial evolutions are computed on a classical device by solving the Newton equation (**saddle point approximation**)

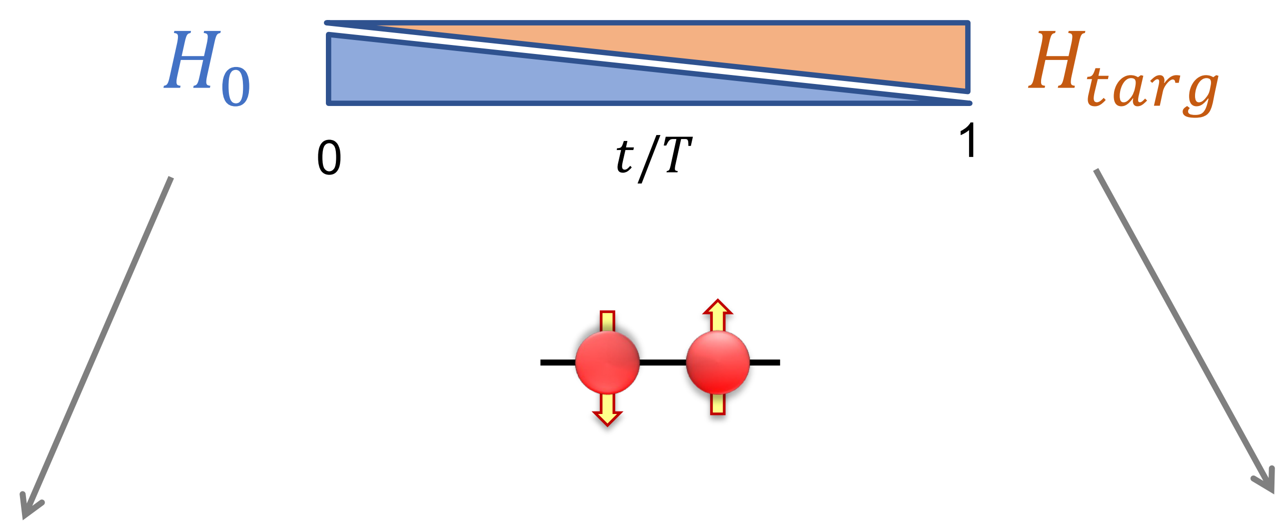
Classical device: Solving the Newton equation



To simulate scattering also need state preparation approach, e.g., adiabatic evolution



As an initial target problem, we consider
the adiabatic evolution of a simple two-spin system



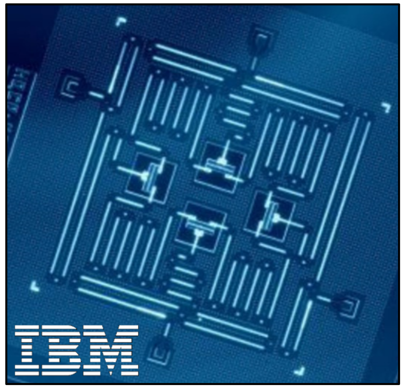
$$\sum_i \sigma_x^i$$

$$\sum_{ij} \left(\sigma_x^i \sigma_x^j + \sigma_y^i \sigma_y^j + \frac{1}{2} \sigma_z^i \sigma_z^j \right) - \sum_i \sigma_z^i$$

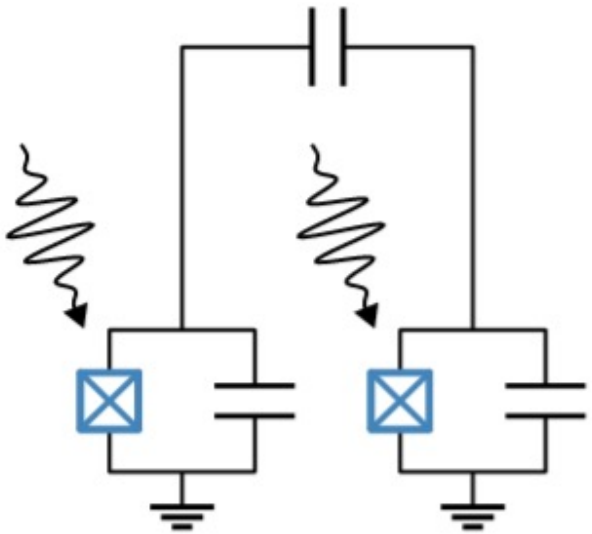
As before, we consider two strategies:
1) gate-based approach; and 2) customized gates approach

$$\mathcal{U}(0,T) \approx \prod_{k=1}^{n} U(t_k) = \prod_{k=1}^{n} e^{-iH(t_k)\Delta t}$$

1) Experimental quantum simulations



2) Classical device-level simulations



Customized gates significantly improve state fidelity, allow for accurate extraction of state properties