‘Classical’ and quantum simulations of nuclear dynamics

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LLNL-PRES-835850
This work was performed under the auspices of the U.S. Department of Energy by Lawrence Livermore National Laboratory under contract DE-AC52-07NA27344. Lawrence Livermore National Security, LLC

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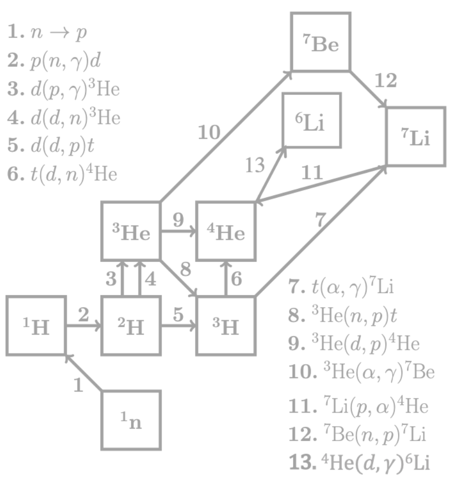
UNIVERSITY OF TRENTO - Italy

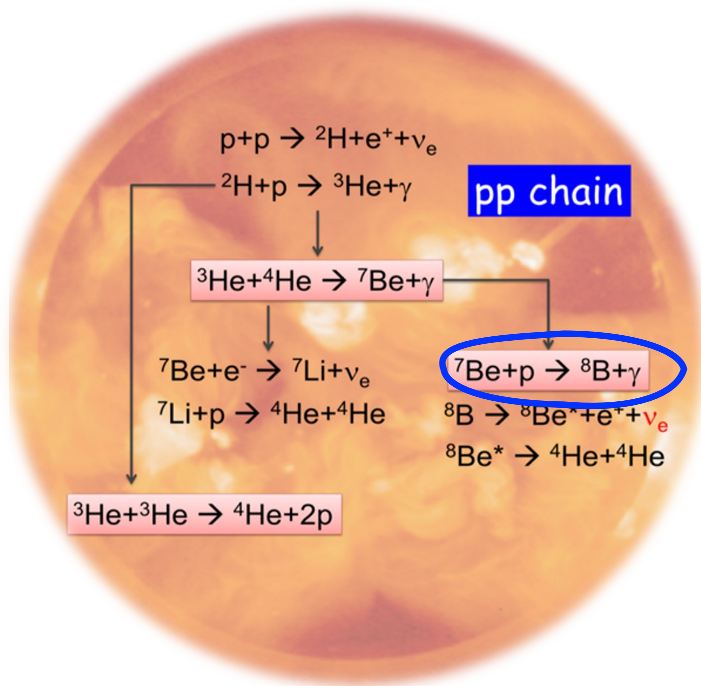
INFN

Reactions ‘R’ Us

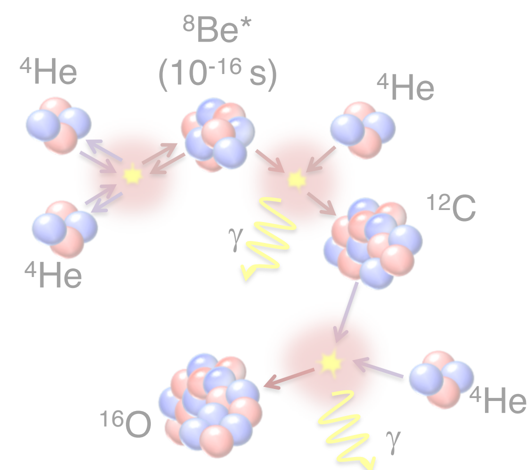
Solar Fusion

Big Bang





Helium Burning



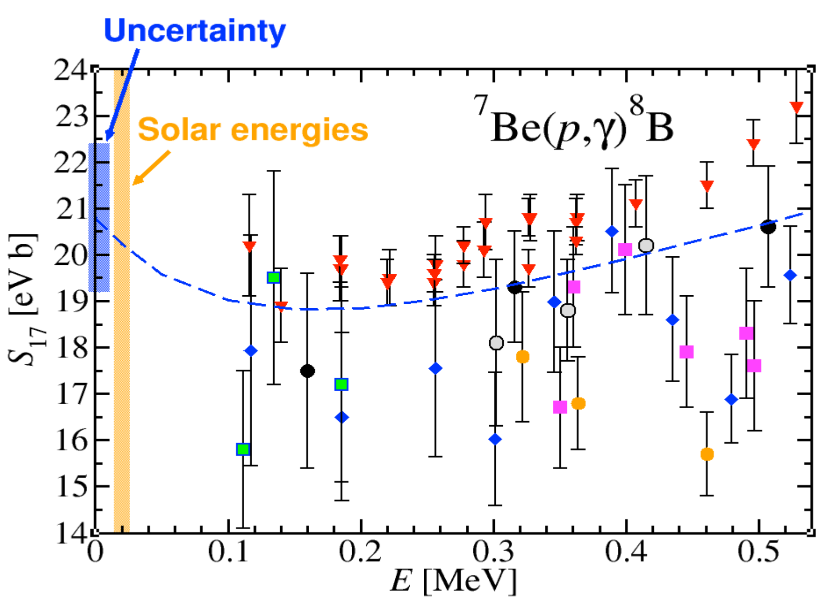
We need reliable theory to accurately evaluate S-factors at stellar energies

$$S_{17}(0) = 20.8 \pm (0.7)_{\text{exp}} \pm (1.4)_{\text{th}} \text{ eV·b}$$

Astrophysical S-factor: nuclear contribution

$$\sigma(E) = \frac{S(E)}{E} \exp\left(-\frac{2\pi Z_1 Z_2 e^2}{\hbar\sqrt{2E/m}}\right)$$

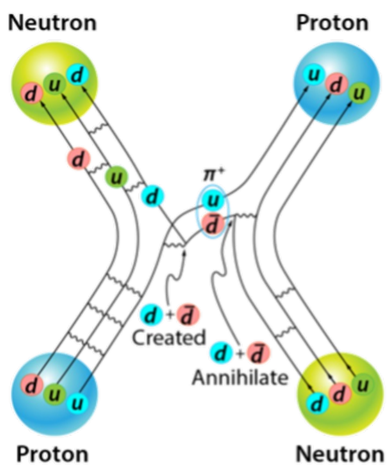
'Coulomb' contribution (tunneling)



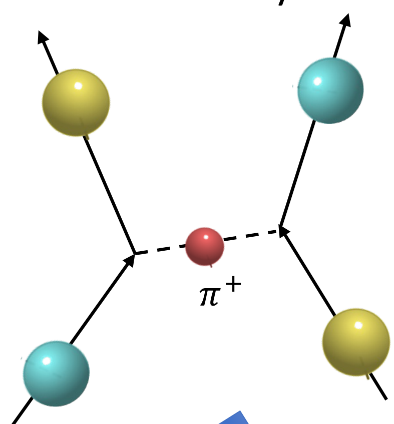
Adelberger EG et al. (2011), Rev. Mod. Phys. 83, 195

We combine nuclear forces derived within chiral effective field theory and ab initio methods

Quantum
Chromodynamics

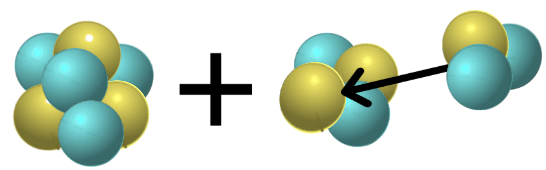


Chiral Effective
Field Theory



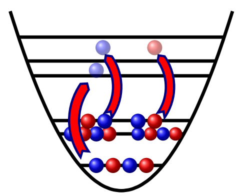
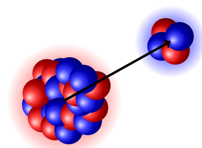
Chiral NN+3N forces

Unified ab initio many-body approach
to structure and reactions



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

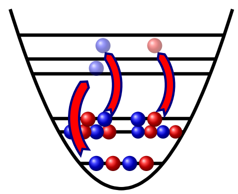
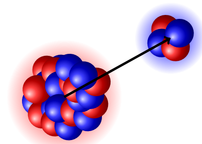
Structure, scattering and reactions obtained with unified treatment of bound and unbound states

$$\Psi = \sum_{\lambda} c_{\lambda} \Big|$$

$$\Big\rangle + \sum_{\nu} \int dr\, u_{\nu}(r) \Big|$$

$$\Big\rangle$$

No Core Shell Model with continuum
(NCSMC)

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

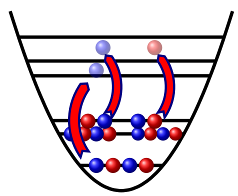
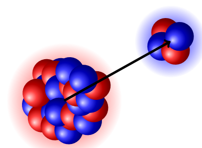
Structure, scattering and reactions obtained with unified treatment of bound and unbound states

$\Psi = \sum_{\lambda} c_{\lambda} \,|$  $\rangle + \sum_{\nu} \int dr\, u_{\nu}(r) \,|$  $\rangle$

Static solutions for aggregate system, describe all nucleons close together

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

Structure, scattering and reactions obtained with unified treatment of bound and unbound states

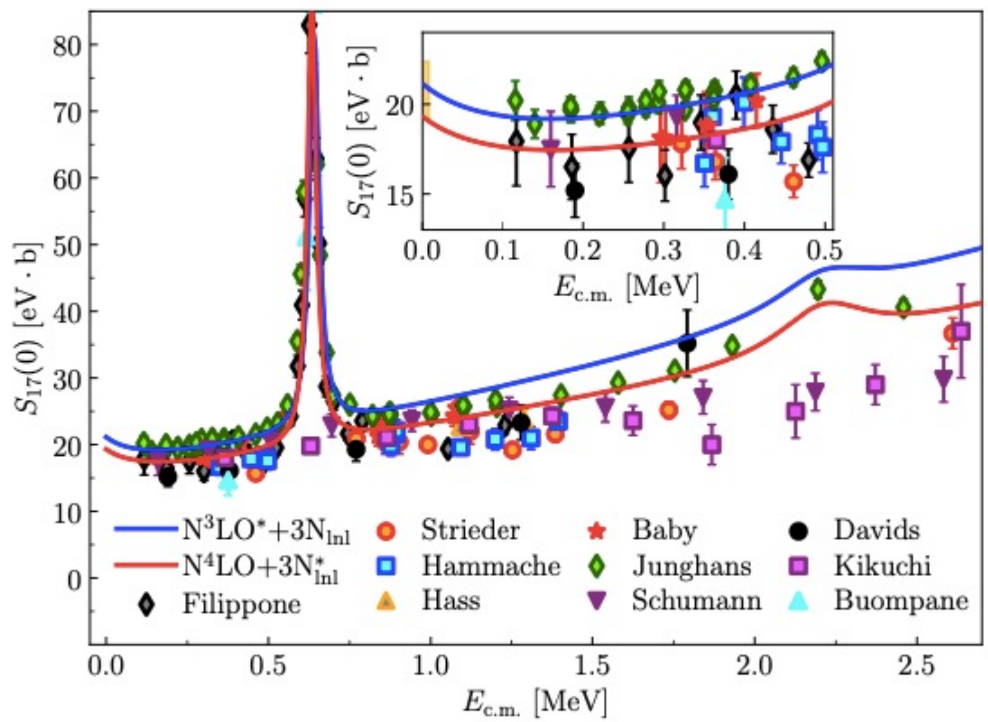
$\Psi = \sum_{\lambda} c_{\lambda} |$  $\rangle + \sum_{\nu} \int dr\, u_{\nu}(r) |$  $\rangle$

Continuous microscopic cluster states, describe separated projectiles & targets

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

We can apply the NCSMC framework to compute the ^{7}Be(p,γ)^{8}B capture rate ...

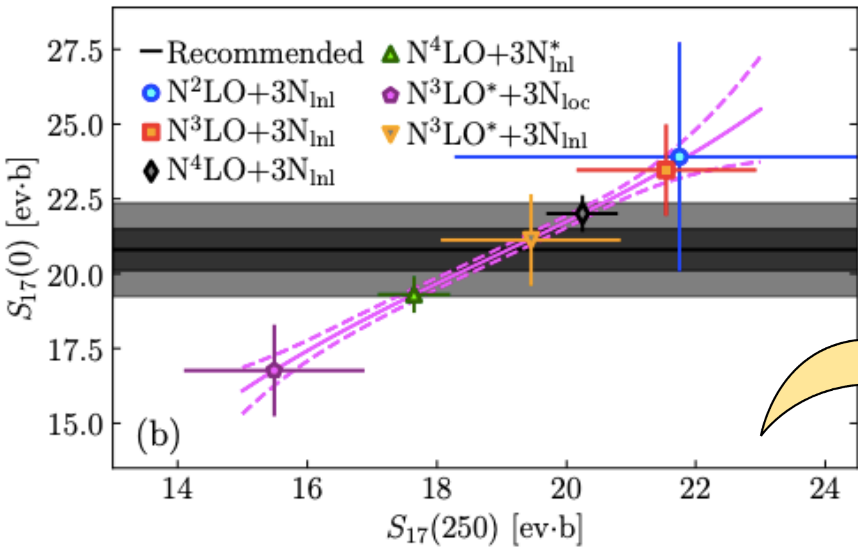
	C_1	C_2	a_1	a_2	$S_{17}(0)$
N^2LO+3N_{lnl}	0.384	0.691	4.4(1)	-0.5(1)	23.9(38)
N^3LO+3N_{lnl}	0.390	0.678	1.3(1)	-4.7(1)	23.5(15)
N^4LO+3N_{lnl}	0.354	0.669	1.6(1)	-4.4(1)	22.0(6)
$N^4LO+3N^*_{lnl}$	0.343	0.621	1.3(1)	-5.0(1)	19.3(6)
$N^3LO^*+3N_{lnl}$	0.334	0.663	0.1(1)	-7.7(1)	21.1(15)
$N^3LO^*+3N_{loc}$	0.308	0.584	2.5(1)	-3.6(2)	16.8(15)
Ref. [42]	0.315(9)	0.66(2)	$17.34^{+1.11}_{-1.33}$	$-3.18^{+0.55}_{-0.50}$	

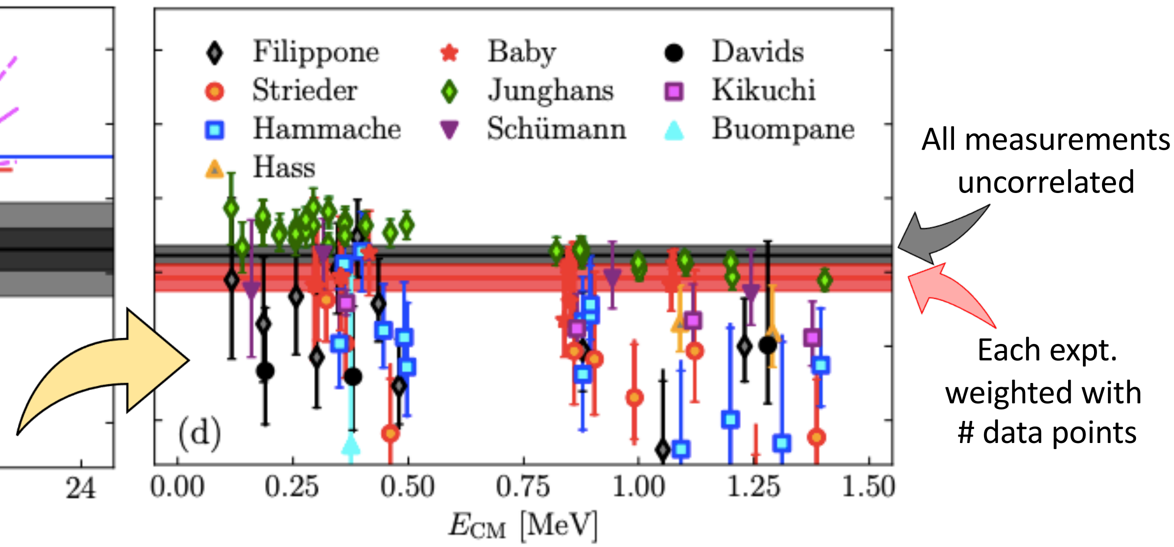


Kravvaris K et al. (2022), arXiv:2202.11759

… combine it with experimental data to arrive at an improved evaluation of $S_{17}(0)$

$S_{17}(0) = 19.8 \pm 0.3$ eV·b

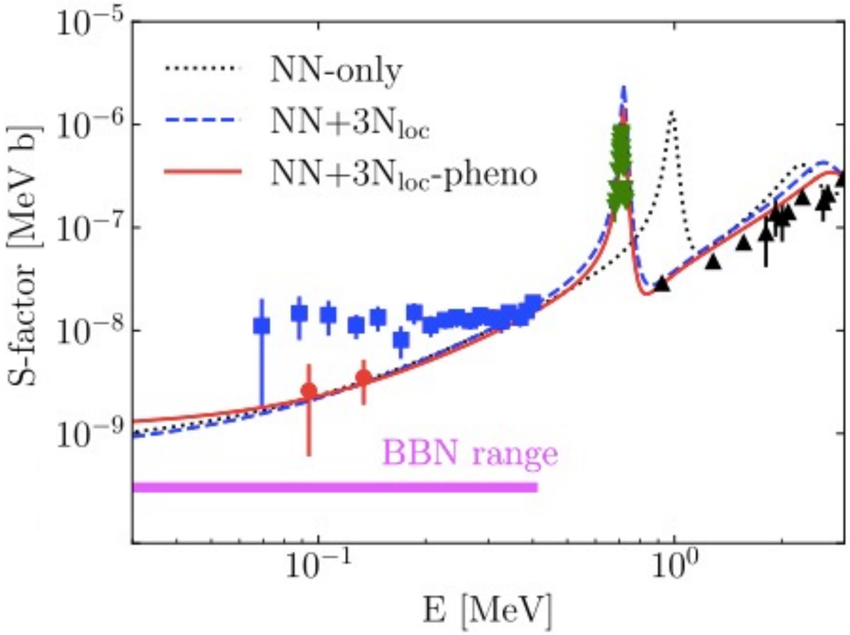




Kravvaris K et al. (2022), arXiv:2202.11759

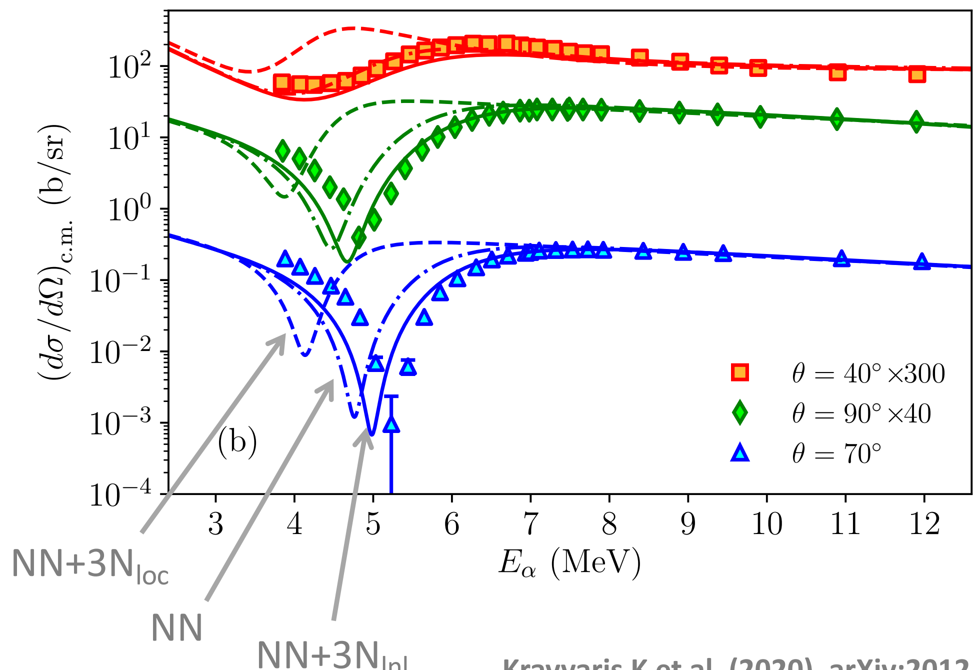
The NCSMC also successfully applied to Big-Bang and helium burning reactions …

^{4}He(d,γ)^{6}He S-factor (Big Bang)



Hebborn C et al. (2022), arXiv:2203.15914

^{4}He-^{4}He Scattering (helium burning)



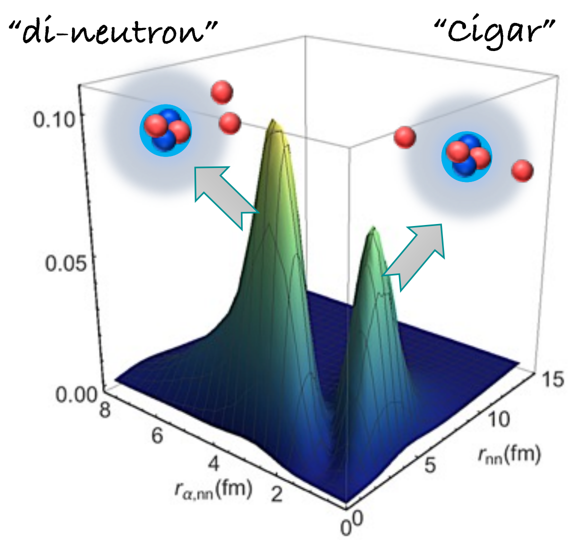
Kravvaris K et al. (2020), arXiv:2012.00228

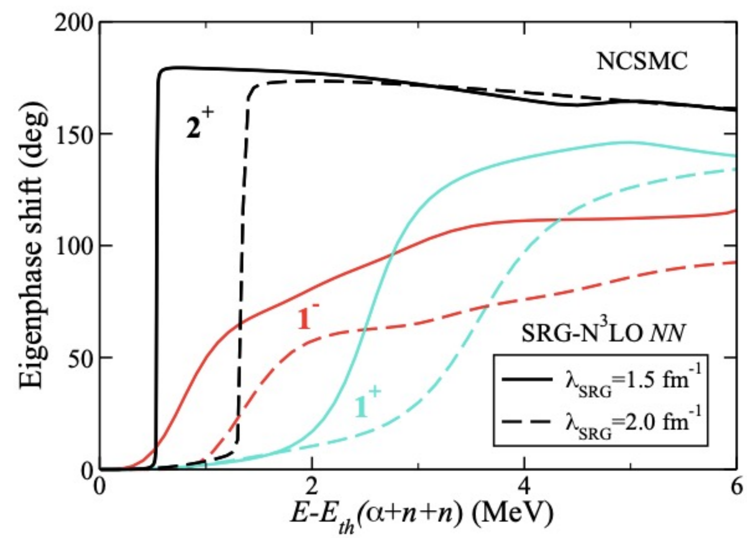
… and can also be applied to describe clustering phenomena, halo nuclei, ternary dynamics

$$\Psi^{(A)} = \sum_\lambda c_\lambda \left| ^{(A)}, \lambda \right\rangle + \sum_\nu \int\int d\vec{x}\, d\vec{y}\, \hat{A}_\nu \left| \vec{y}\ \vec{x}\ , \nu \right\rangle$$

e.g., Hyperspherical Harmonics

e.g:
^{4}He+n+n bound
& scattering states





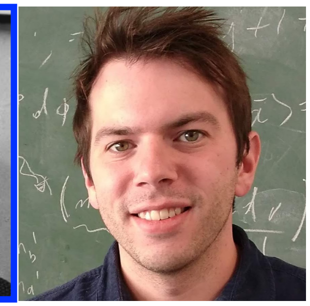
The ab initio structure and reactions team

Sofia Quaglioni

Kostas Kravvaris

Linda Hlophe

Chloë Hebborn



Mack Atkinsons

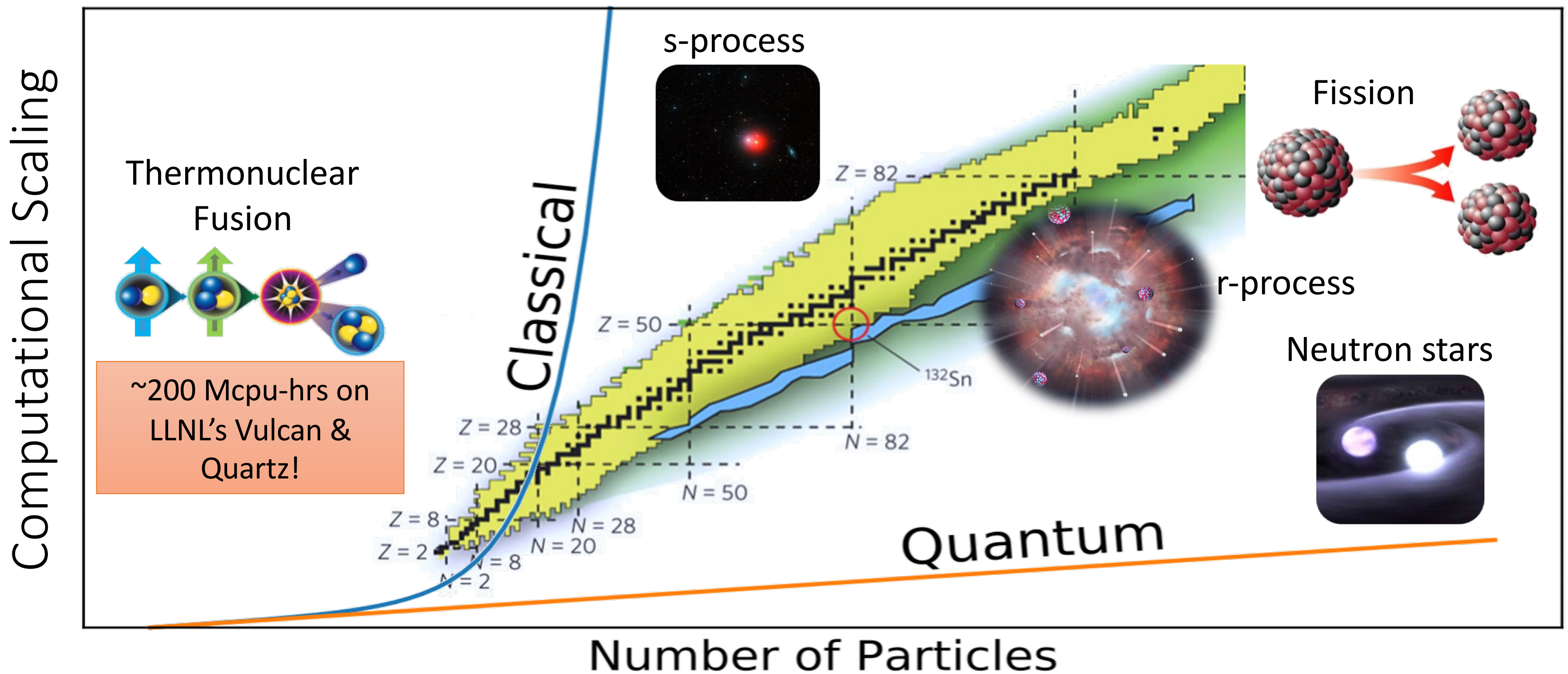
Guillaume Hupin

IN2P3

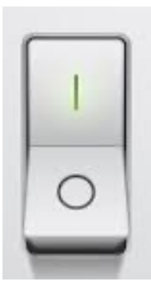
Petr Navratil

TRIUMF

Quantum computing holds the promise of exact simulations of quantum mechanical systems, e.g., nuclear matter and dynamics



Quantum computers perform calculations by manipulating quantum states

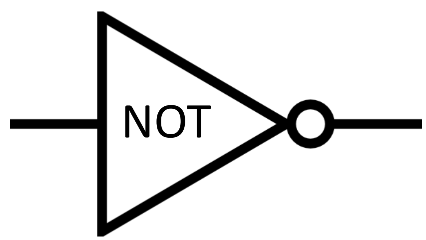


$$|\psi_{targ}\rangle = U_{targ}\,|\psi_0\rangle$$

Desired state

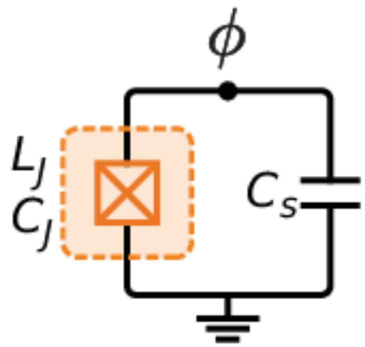
Initial state

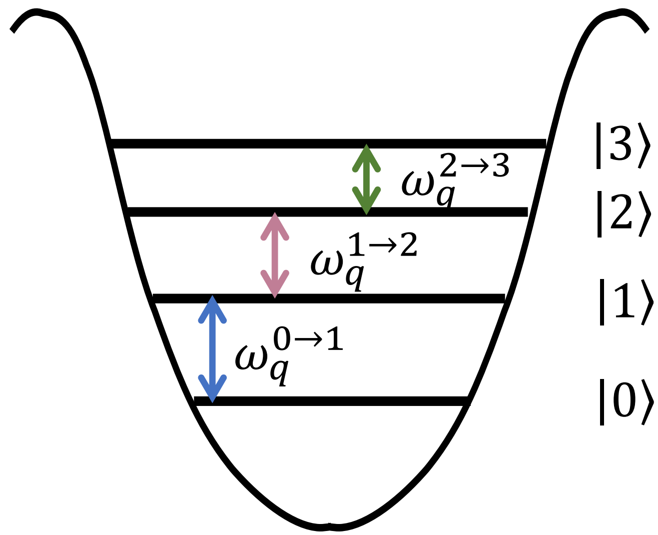
Unitary operation (= gate)



A physical realization of a qubit is a transmon

Quantized transmon:



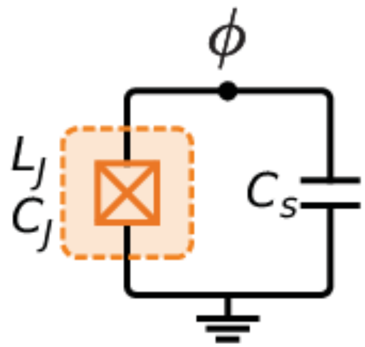


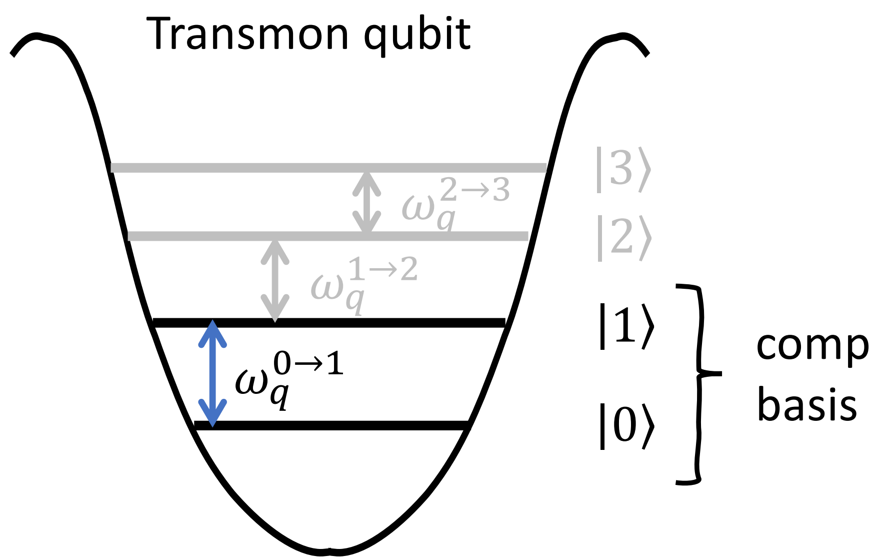
$$H = \hbar\omega_q\, a^+a + \frac{\alpha}{2}a^+a^+aa$$

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

A physical realization of a qubit is a transmon

Quantized transmon:



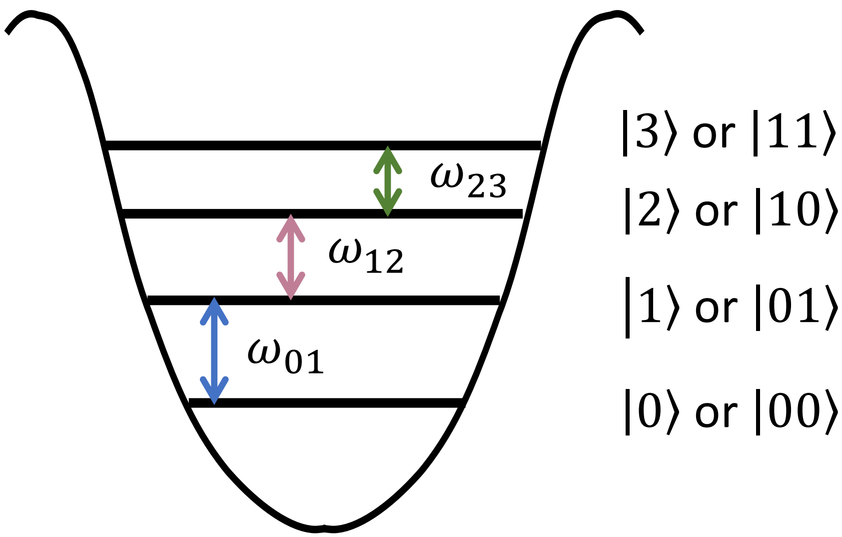


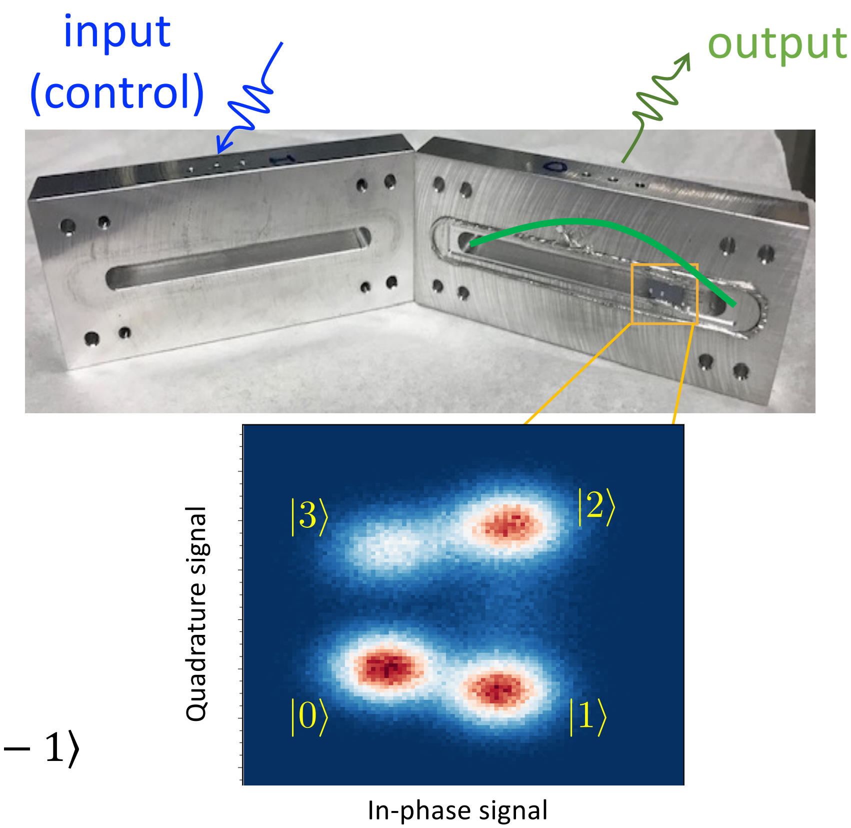
$$H = \hbar\omega_q\, a^+ a + \frac{\alpha}{2} a^+ a^+ a a$$

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

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

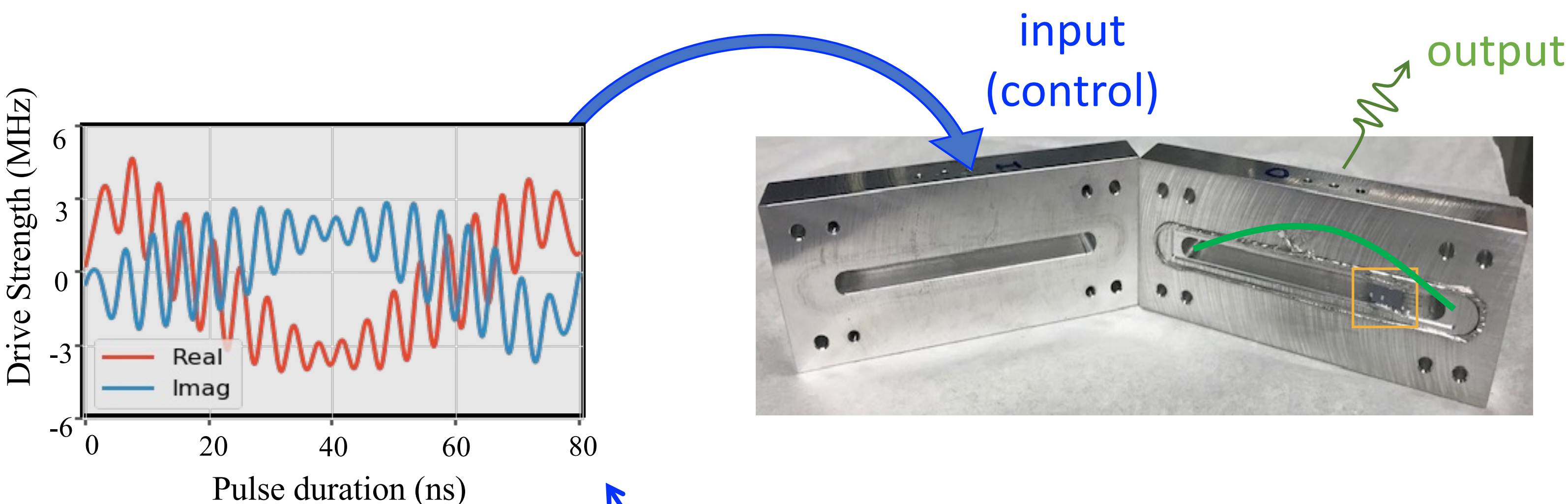
One can also work with registers of d-level quantum systems or ‘qudits’





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

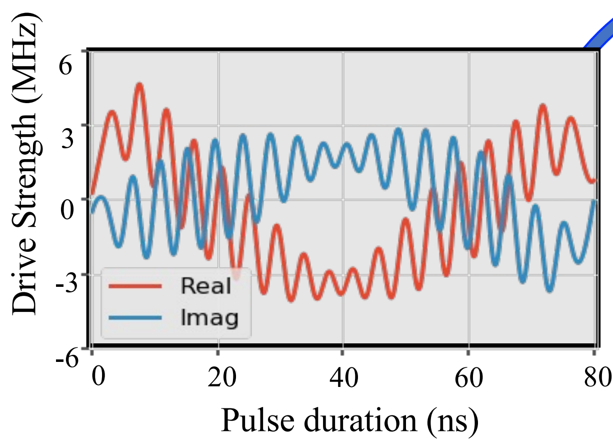
Physically, quantum gates are realized by irradiation with resonant microwave pulses (found by optimization)

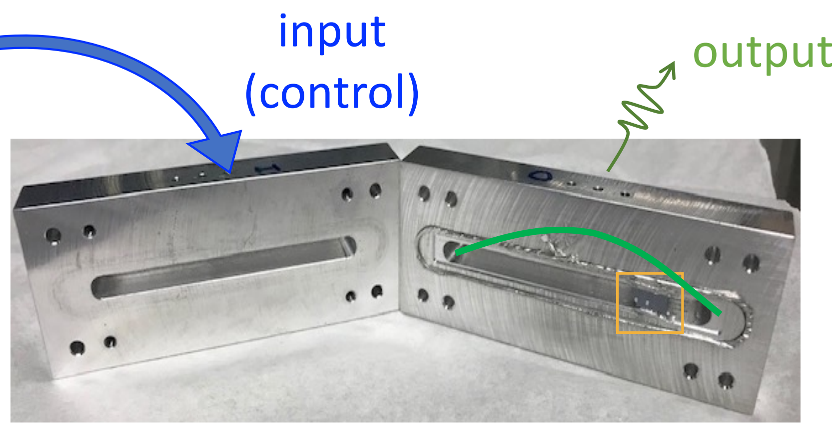


$$U_{targ} \approx U_{opt} = \mathcal{T}exp\left[-\frac{i}{\hbar}\int_0^{T_g}\left(H_0 + \sum_{k=1}^{2n} u_k(t) H_k\right)dt\right]$$

Solve time evolution for quantum device

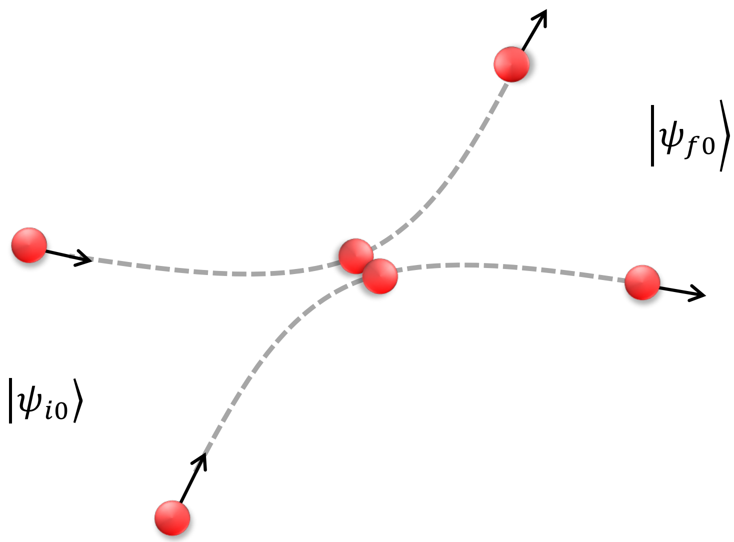
Physically, quantum gates are realized by irradiation with resonant microwave pulses (found by optimization)





$$U_{targ} \approx U_{opt} = \mathcal{T}exp\left[-\frac{i}{\hbar}\int_0^{T_g}[H_0 + u_R(t)(a + a^+) + iu_I(t)(a - a^+)]dt\right]$$

Quantum computing offers a natural framework for simulating time-dependent scattering theory

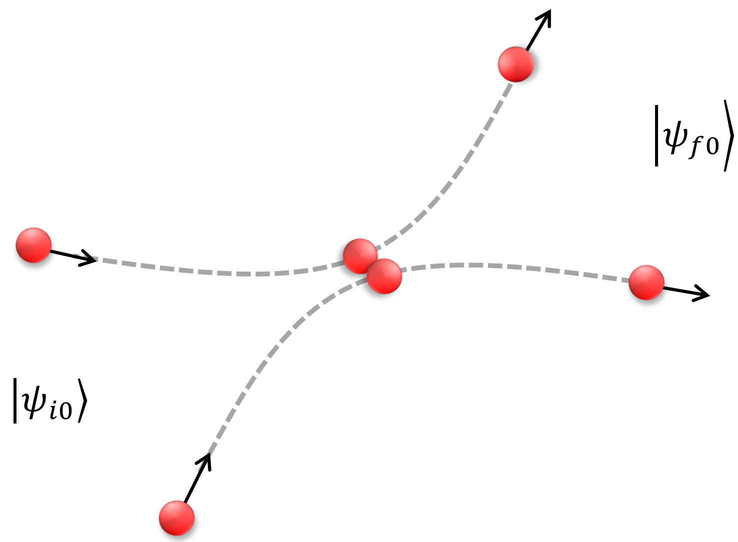


$$P = \left|S_{fi}\right|^2 = \left|\langle\psi_f(0)|\psi_i(0)\rangle\right|^2$$
$$\approx \left|\langle\psi_{f0}(0)\left|\Omega_+^\dagger\Omega_-\right|\psi_{i0}(0)\rangle\right|^2$$

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

Application of unitary transformations (= gates)

Quantum computing offers a natural framework for simulating time-dependent scattering theory



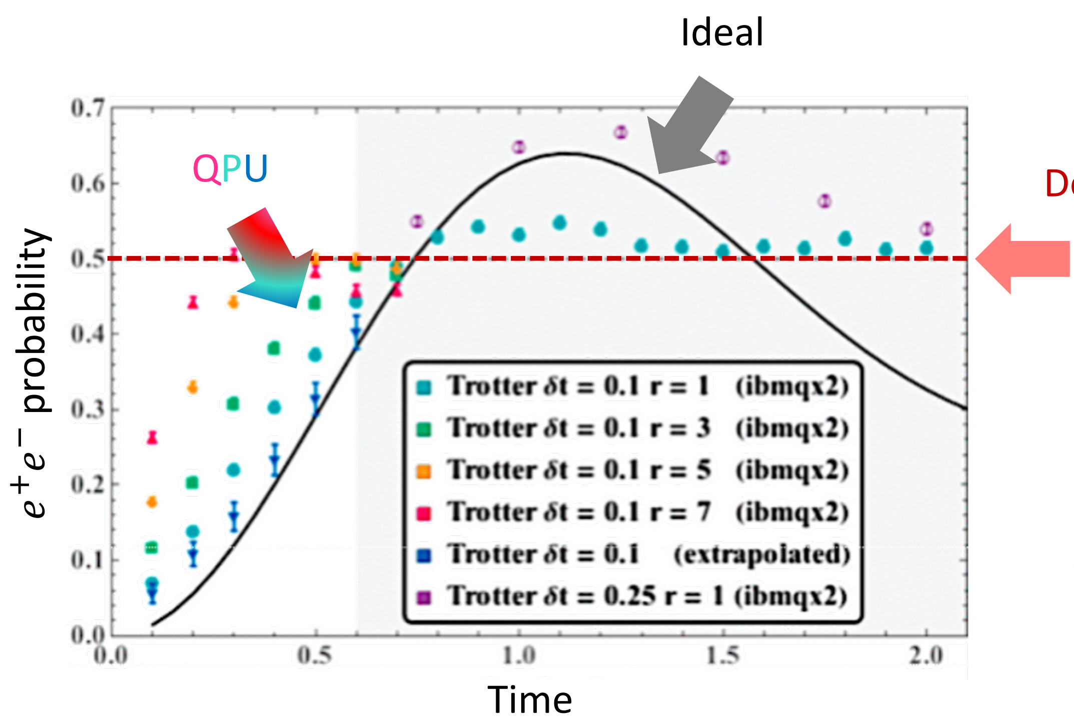
$$P = |S_{fi}|^2 = |\langle \psi_f(0)|\psi_i(0)\rangle|^2$$
$$\approx |\langle \psi_{f0}(t)|e^{-2iHt}|\psi_{i0}(-t)\rangle|^2$$

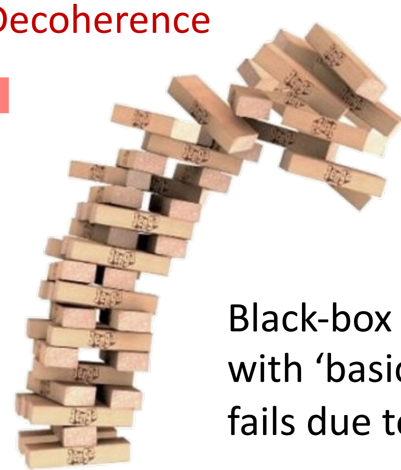
$U(2t)$

Real-time evolution

State preparation

A challenge is to realize useful quantum simulations in this ‘early vacuum tube era’ of quantum computing



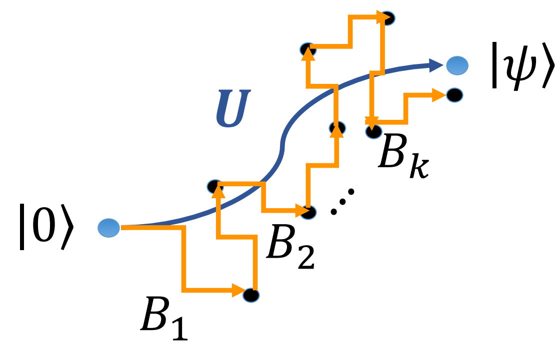


Black-box quantum compilation with ‘basic’ set of quantum gates fails due to accumulation of noise

In the near term, this is a self-inflicted problem!
Can build custom gates for the problem of interest

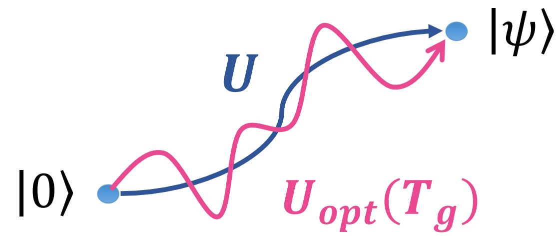
$U \approx B_k \cdots B_2 B_1$

Buildup of noise, error



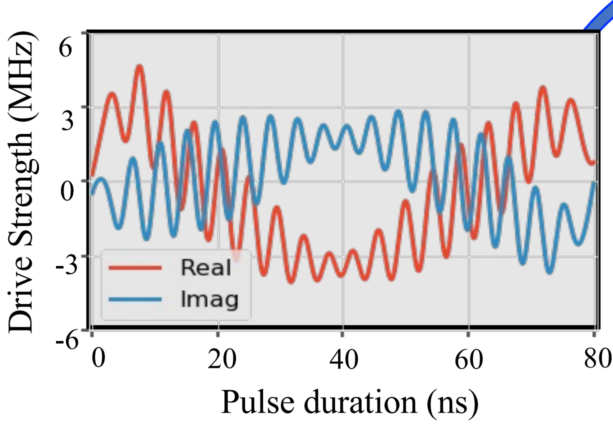
$U \approx U_{opt}(T_g)$

Single gate,
noise resilient



Solution: Noise-resilient quantum compilation through minimal number of custom gates

Optimized pulse = custom gate

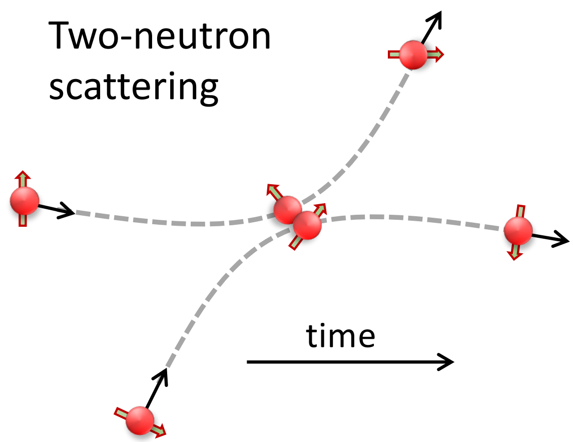


input (control)

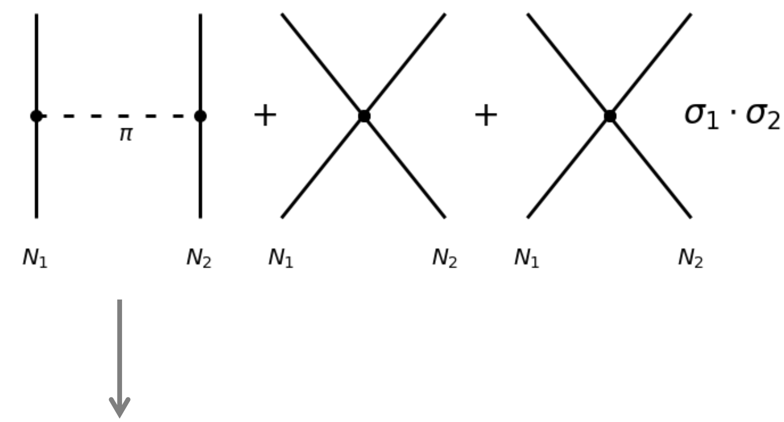
output

analog-digital quantum simulations

Our target problem: evolution of two interacting neutrons

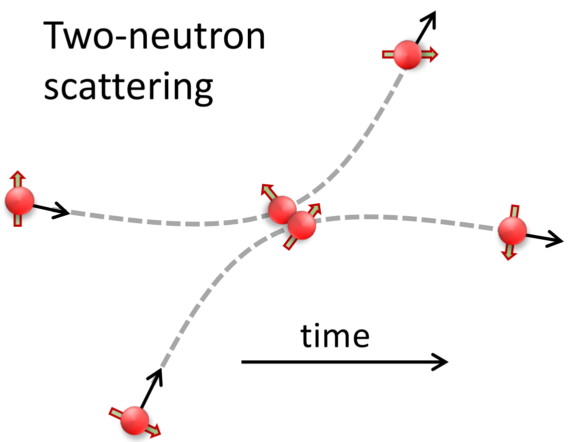


NN force @LO of chiral EFT

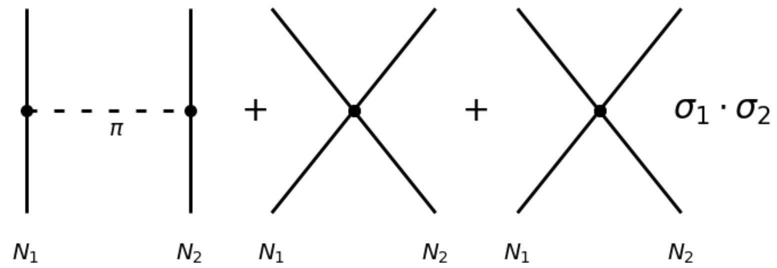


$$S_{12} = 3\left(\vec{\sigma}^1 \cdot \hat{r}\right)\left(\vec{\sigma}^2 \cdot \hat{r}\right) - \vec{\sigma}^1 \cdot \vec{\sigma}^2$$

Our target problem: evolution of two interacting neutrons



NN force @LO of chiral EFT

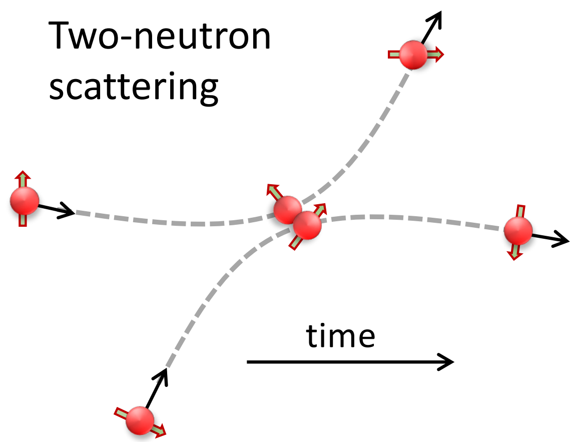


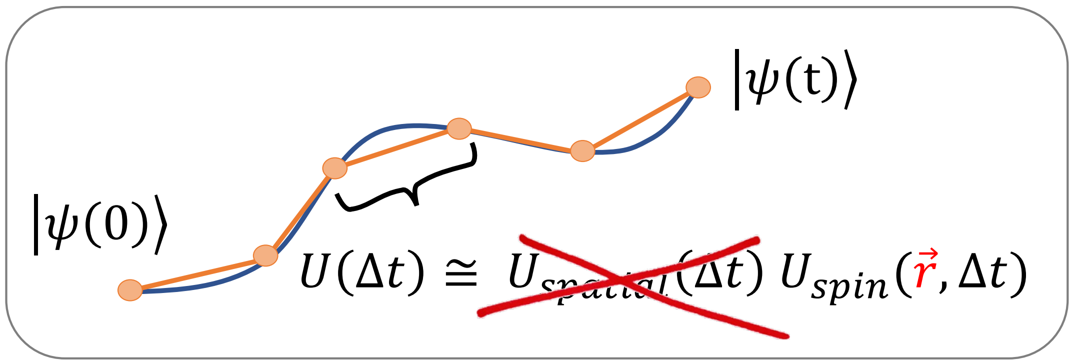
$$H_{LO} = H_{SI} + V_{SD}$$

$$\downarrow$$

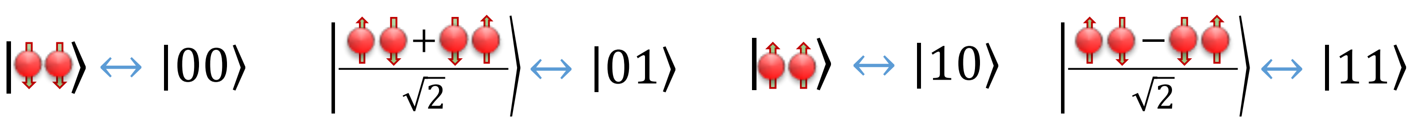
$$U(\Delta t) \cong U_{spatial}(\Delta t)\, U_{spin}(\vec{r}, \Delta t)$$

Our target problem: evolution of two interacting neutrons frozen in space

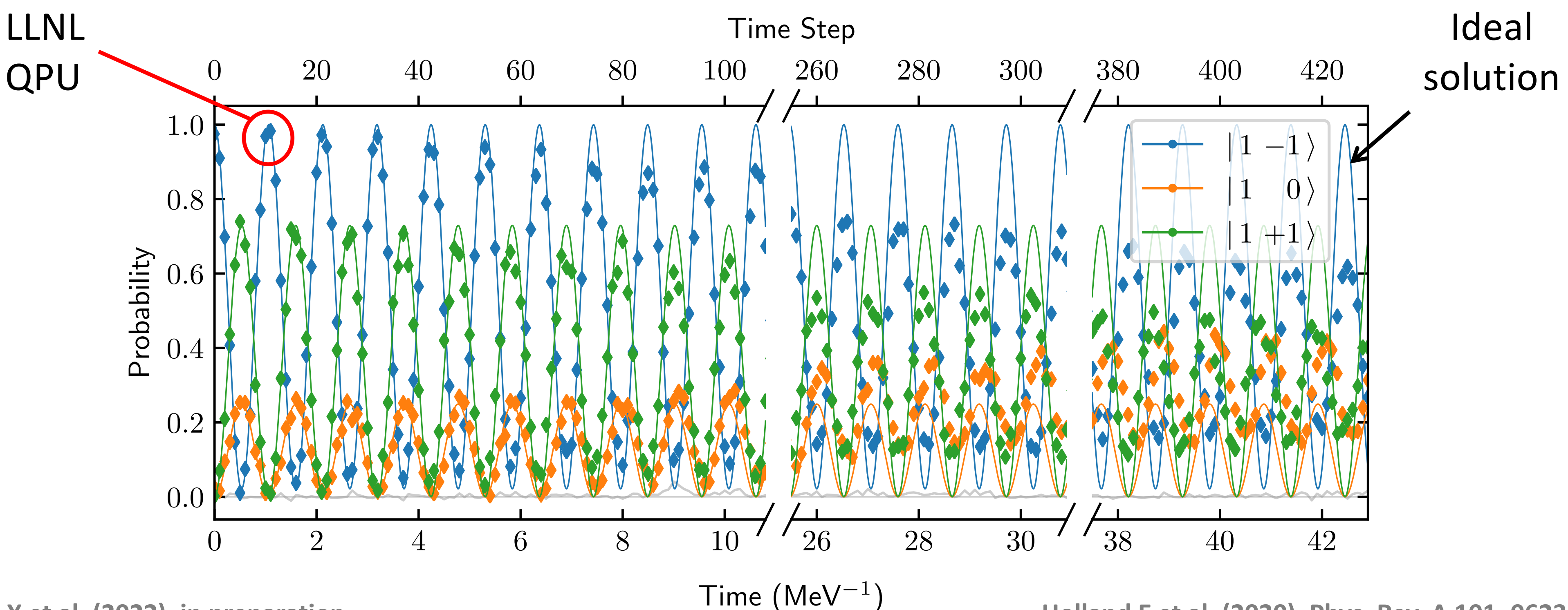




Nuclear ↔ quantum register map:



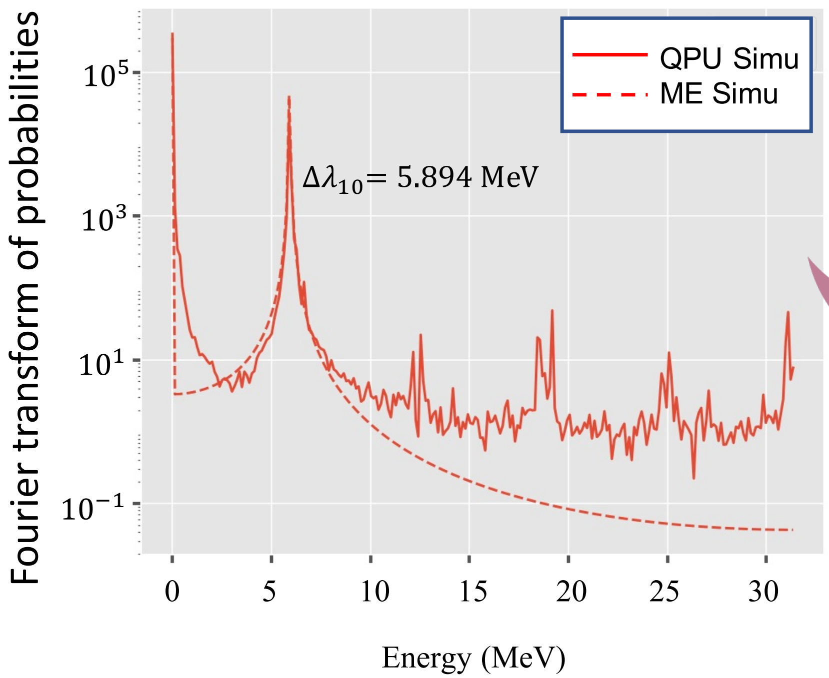
With minimal number of custom gates, we demonstrated >99% fidelity, 10-fold increase in quantum simulation time



Wu X et al. (2022), in preparation

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

We can extract the energy spectrum from the signal because we are able to run the simulation a long time

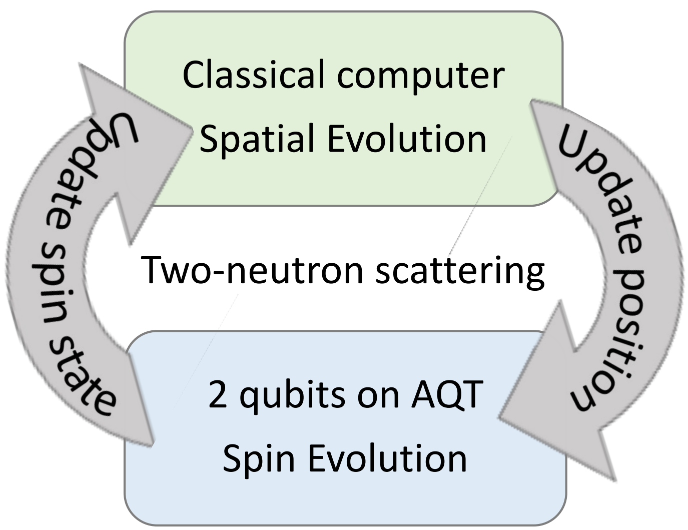


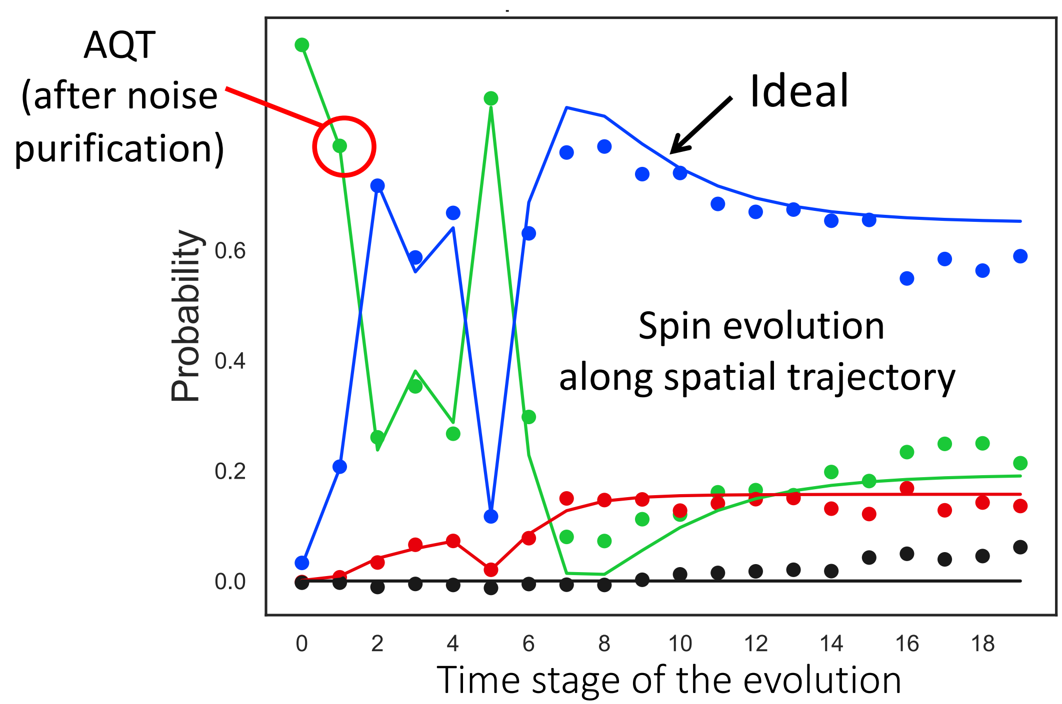
Energies (MeV)

Exact	Quantum Simulation
-2.3289	-2.32(4)
3.5916	3.57(8)

Wu X et al. (2021), in preparation

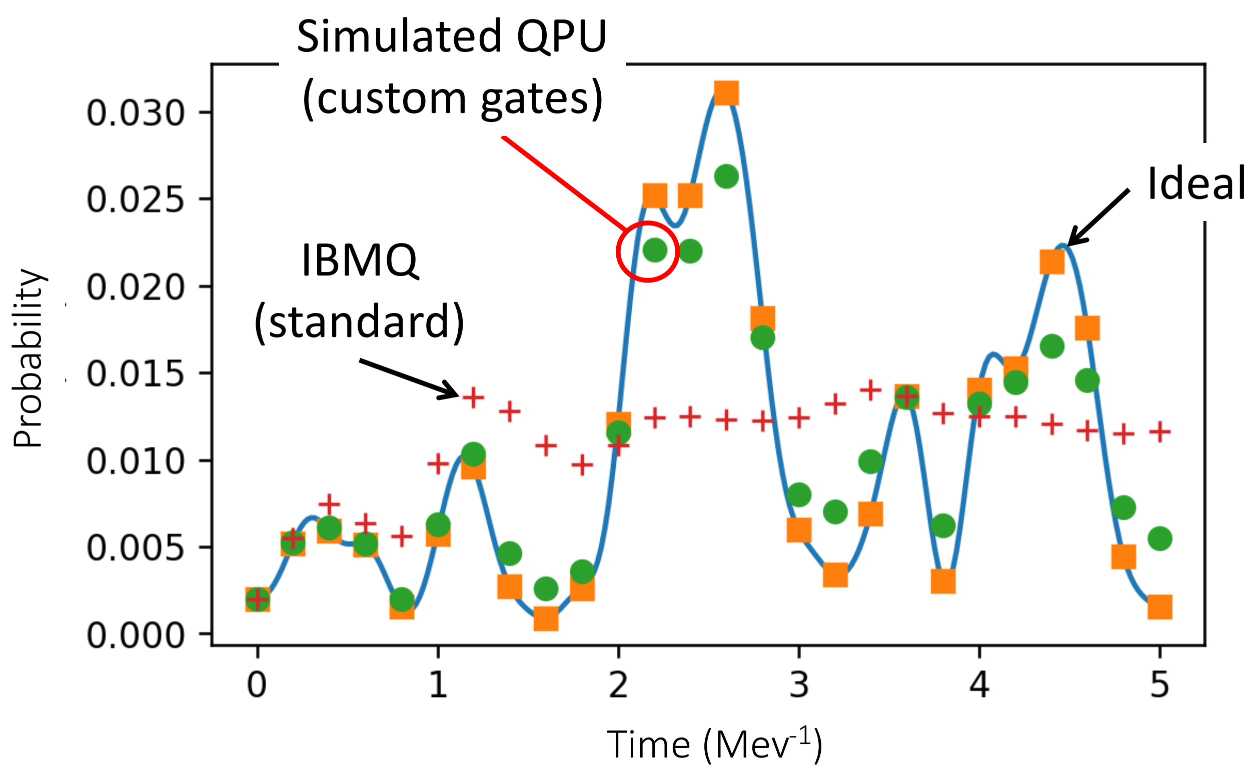
Demonstrated hybrid quantum-classical simulation of nuclear scattering on the Advanced Quantum Testbed

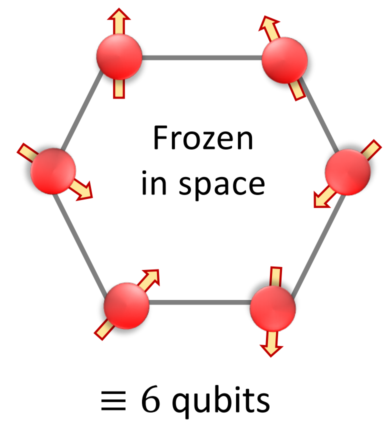




F. Turro, T. Chistolini et. al. (2022), in preparation

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

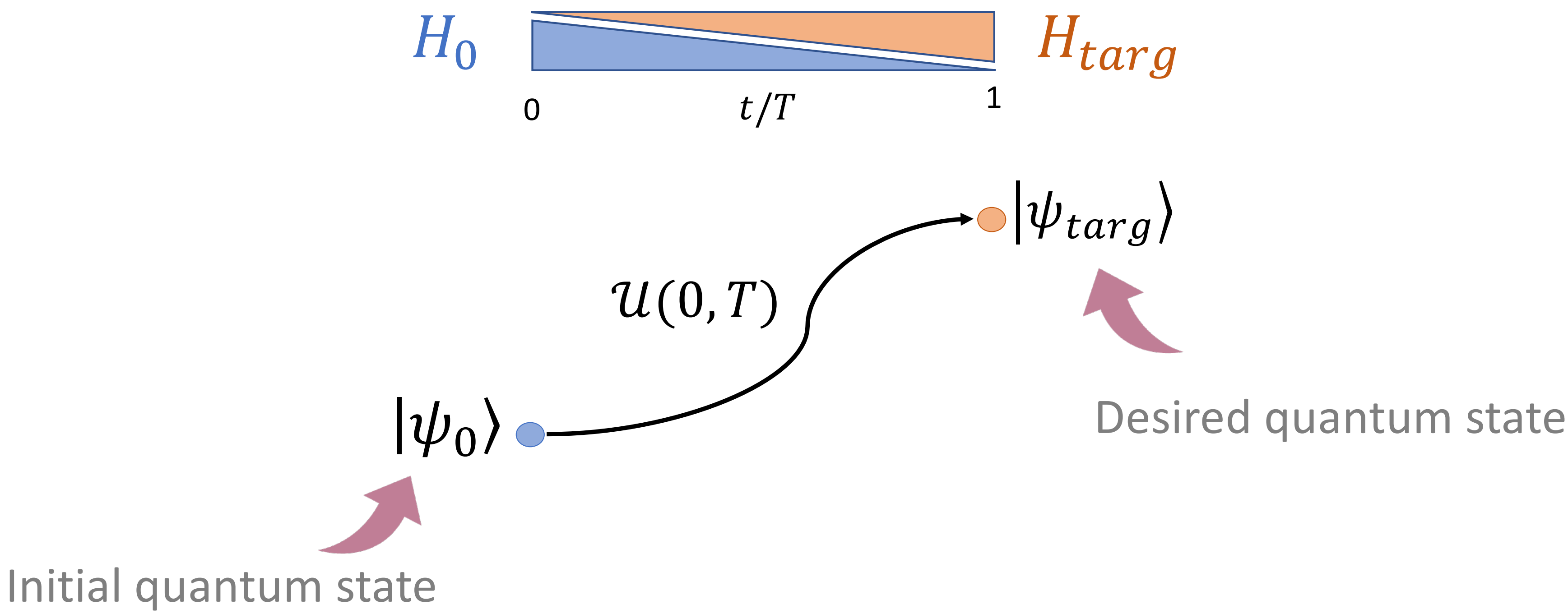




Polynomial scaling
with number of particles

Wendt KA et al, in progress

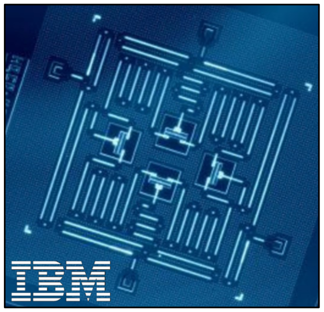
To simulate scattering also need
state preparation approach, e.g., adiabatic evolution



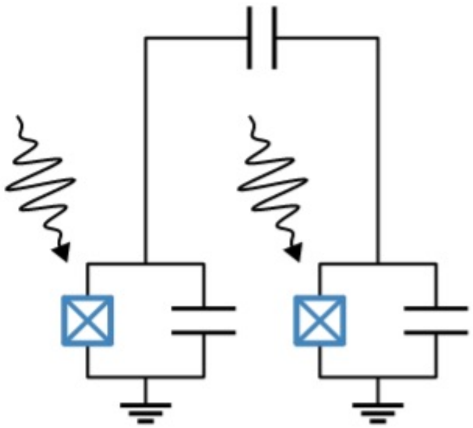
We consider two strategies:
1) gate-based approach; and 2) custom gates approach

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

1) Experimental quantum simulations



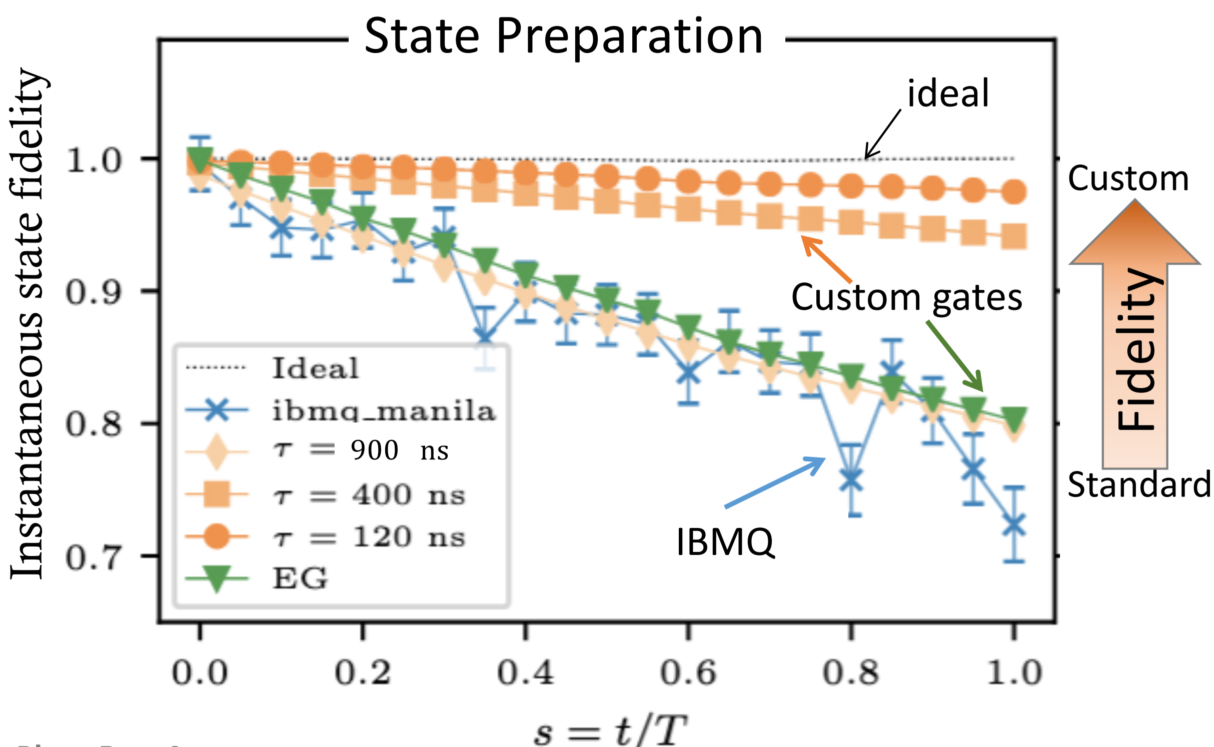
2) Classical device-level simulations



Custom gates enable major performance improvements for state preparation, broader class of problems

Any long sequence of arbitrary operations

Can be realized on IBMQ using pulse control



E.A. Coello-Perz, J. Bonitati et al (2022), submitted to Phys. Rev. A

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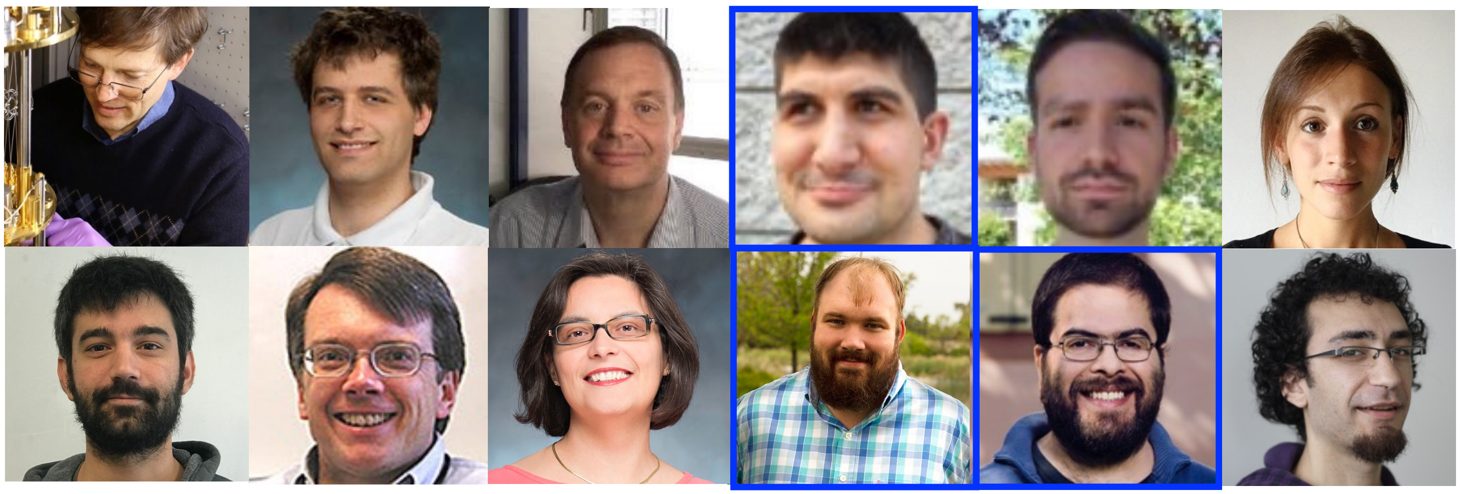

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The APS Topical Group On Few-Body Systems and Multiparticle Dynamics

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