FIRST BABY-STEPS TOWARDS THE QUANTUM SIMULATION OF NUCLEAR REACTIONS

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OUTLINE

- A few words about Quantum Computing
- Real time propagation with realistic nuclear Hamiltonians
- Approximate time evolution of two interacting neutrons: simulations and actual quantum calculations on the LLNL and AQT testbeds

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More products:

Imaginary time propagation (F. Turro, A. Roggero, V. Amitrano, P. Luchi, K. A. Wendt, J. L. Dubois, S. Quaglioni, and FP PRA **105**, 022440 (2022), Neutrinos (V.Amitrano, A. Roggero et al.), Optimal control for parametric Hamiltonians (P.Luchi, F.Turro et al.)

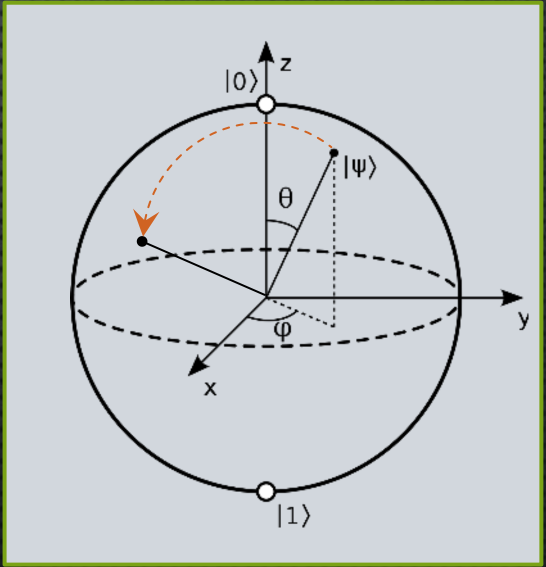
QUBITS

Quantum bit (qubit):
Two orthogonal states that can be reliably initialized for computation. A qubit, contrary to a classical bit, can be found in an arbitrary superposition of |0⟩ and |1⟩:

$$\cos\left(\frac{\theta}{2}\right)|0\rangle + e^{i\phi}\sin\left(\frac{\theta}{2}\right)|1\rangle$$

The states of a qubit can be conveniently represented as the points of a sphere (the "Bloch sphere") parametrized by the angles $0<\theta<\pi$ and $0<\phi<2\pi$.

Bloch Sphere



UNITARY TRANSFORMATIONS

The standard operations we want to perform on qubits are **UNITARY TRANSFORMATIONS.** An example are rotations from one point to another of the Bloch sphere.

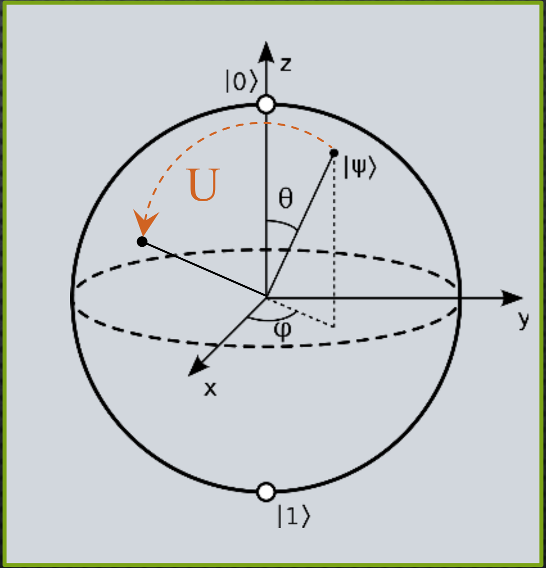
$$R_x(\theta) \equiv e^{-i\frac{\theta}{2}\sigma_x} = \cos\frac{\theta}{2}I - i\sin\frac{\theta}{2}\sigma_x = \begin{bmatrix} \cos(\theta/2) & -i\sin(\theta/2) \\ -i\sin(\theta/2) & \cos(\theta/2) \end{bmatrix}$$

Another example are generic real time propagators:

$$U(t) = \exp(i\frac{H}{\hbar}t)$$

These operations can be performed on *n* qubits.

Bloch Sphere



“UNIVERSAL” QUANTUM COMPUTING

S. Lloyd, Science 273, 1073 (1996)

Universal quantum computing

The quantum computer operates on the qubits by means of unitary transformations, possibly obtained as a combination of a finite ”quantum gates” set. Examples of quantum gates are:

- **Rotations on the Bloch sphere**
- **Hadamard gate:** acts on a single qubit giving a superposition of the 0 and 1 states:

$$H \equiv \frac{1}{\sqrt{2}}\begin{pmatrix} 1 & 1 \\ 1 & -1 \end{pmatrix} \qquad H|0\rangle = \frac{|0\rangle + |1\rangle}{\sqrt{2}} \qquad H|1\rangle = \frac{|0\rangle - |1\rangle}{\sqrt{2}}$$

- **CNOT (controlled NOT):** acts on two qubits flipping the second depending on the state of the first:

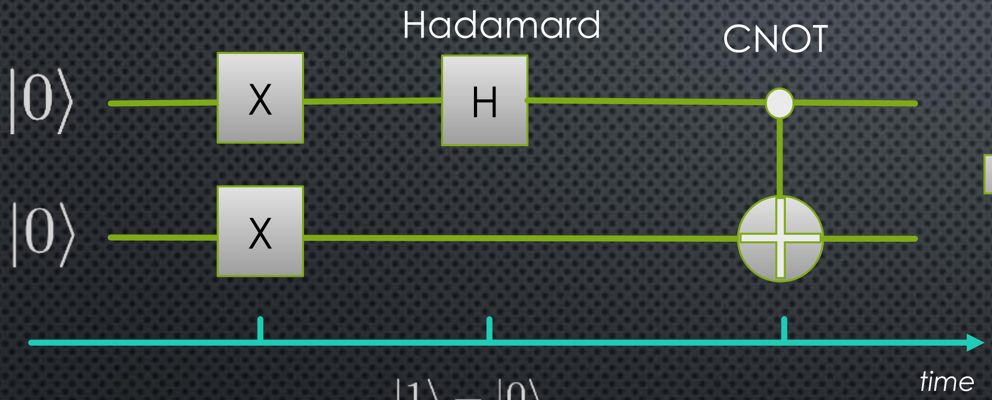
$$CNOT \equiv \begin{array}{c} \begin{array}{cccc} |01\rangle & |00\rangle & |10\rangle & |11\rangle \end{array} \\ \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 \\ 0 & 0 & 1 & 0 \end{pmatrix} \end{array} \begin{array}{c} \\ |00\rangle \\ |01\rangle \\ |10\rangle \\ |11\rangle \end{array} \quad CNOT|01\rangle = |01\rangle \qquad CNOT|11\rangle = |10\rangle$$

$$|00\rangle = \begin{pmatrix} 1 \\ 0 \\ 0 \\ 0 \end{pmatrix} \qquad |10\rangle = \begin{pmatrix} 0 \\ 0 \\ 1 \\ 0 \end{pmatrix}$$

$$|01\rangle = \begin{pmatrix} 0 \\ 1 \\ 0 \\ 0 \end{pmatrix} \qquad |11\rangle = \begin{pmatrix} 0 \\ 0 \\ 0 \\ 1 \end{pmatrix}$$

A SIMPLE CIRCUIT ENTANGLING TWO STATES

Problem: Design a "Quantum circuit" to generate an entangled state of two qubits



$$\frac{|1\rangle \otimes |0\rangle - |0\rangle \otimes |1\rangle}{\sqrt{2}}$$

$|0\rangle \otimes |0\rangle$ $\quad |1\rangle \otimes |1\rangle$ $\quad \frac{|1\rangle - |0\rangle}{\sqrt{2}} \otimes |1\rangle$

Parallel single qubit operations

Single qubit operation

Two qubit operation

$$\mathrm{X} \equiv R_x(\pi) = -i \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}$$

Circuit of *depth* 3 (number of time steps)

flips the qubit state within a global phase

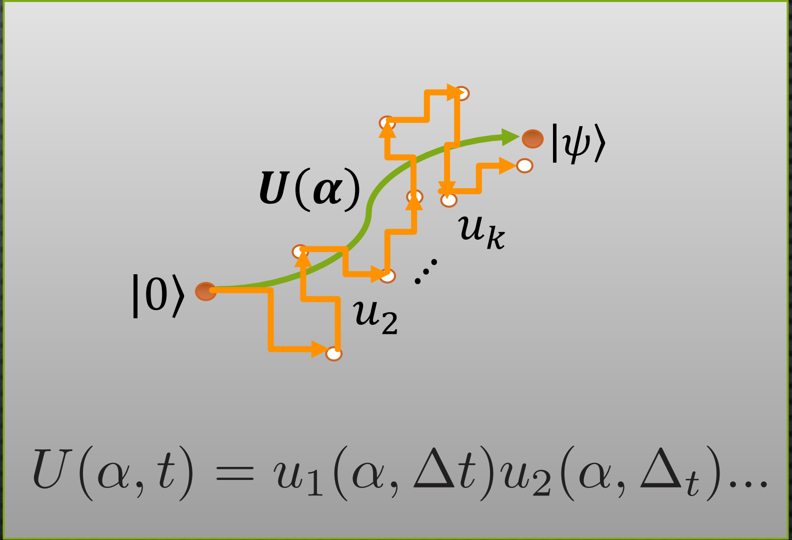
Potential advantage, but algorithms need to be deeply re-thought

UNIVERSAL QUANTUM COMPUTING

Useful theorem (Solovay-Kitaev)

Given an Hilbert space $\mathscr{H}$, any unitary transformation $U \in U(\mathscr{H})$ can be approximated with arbitrary precision δ by a circuit of size $poly(1/\delta)$ over the standard gates basis, possibly using ancillary qubits (i.e there exists a

This guarantees that we can approximate for instance an arbitrary time evolution under a Hamiltonian H with a circuit depth that will increase at most a polinomially with the required accuracy.



THIS THEOREM IS AT THE BASIS OF UNIVERSAL QC SCHEME

WARNING: other problems like decoherence (thermal effects) and dissipation

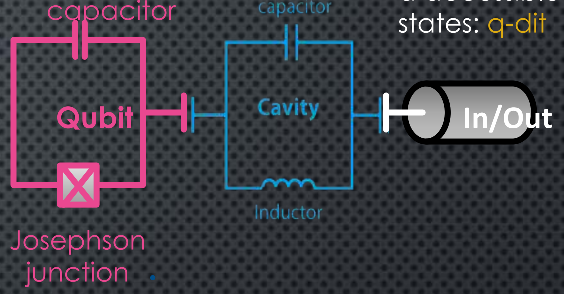
"CONTROL-CENTRIC" APPROACH TO QUANTUM COMPUTATION

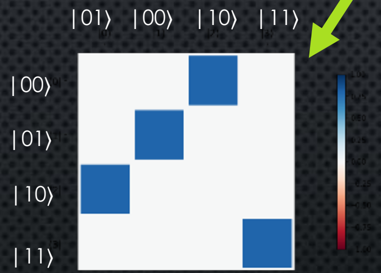
Given some control parameterization $f(t,\alpha) = \sum_k \alpha_k \phi_k(t)$

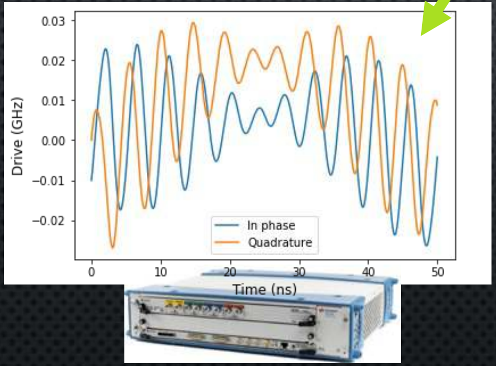
all unitary transformations in time T can be expressed as

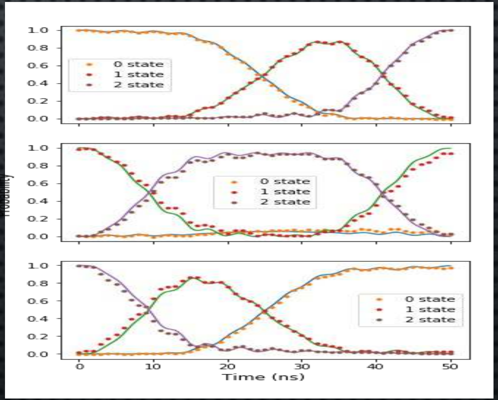
$$U(t,\alpha) = \mathcal{T} e^{-i \int_0^t dt' [\hat{H}_0 + f(t',\alpha)\hat{H}_c]}$$

Device with d accessible states: q-dit





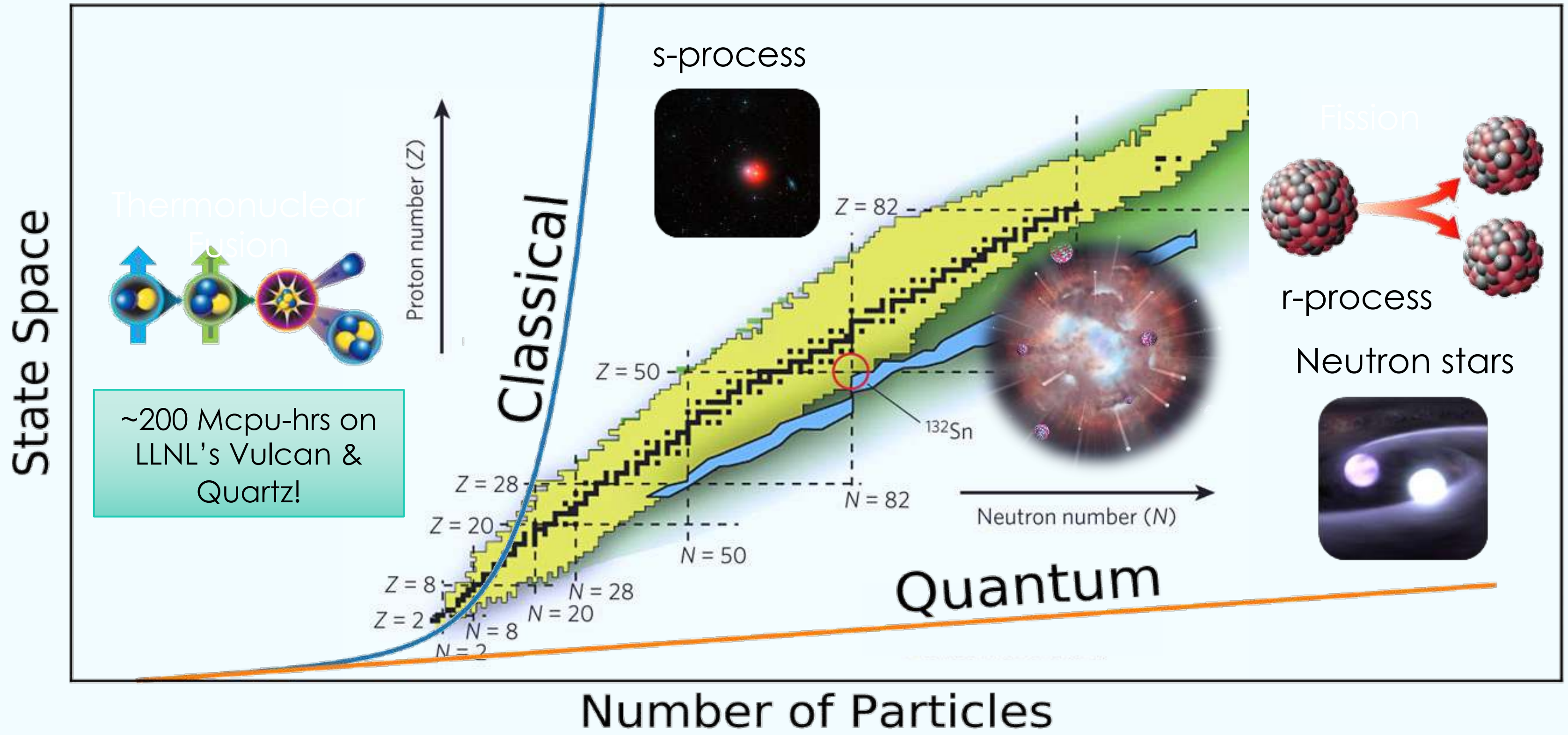




See e.g. S. Schirmer, "Hamiltonian Engineering for Quantum Systems." , Proceedings of the 7th International Conference on Cooperative Control and Optimization (2007)

Optimization methods, machine learning (Q@Tn ML-QFORGE project (Jonathan Dubois, Kyle Wendt (LLNL), Simone Taioli, Paolo Trevisanutto (ECT*-LISC), FP, Piero Luchi, (UNITN)) – PRA 101, 062307 (2020)

THE DREAM.....



State Space
Number of Particles
Classical
Quantum
s-process
r-process
Neutron stars
Thermonuclear Fusion
Fission
~200 Mcpu-hrs on LLNL's Vulcan & Quartz!
Proton number (Z)
Neutron number (N)
Z = 82
Z = 50
Z = 28
Z = 20
Z = 8
Z = 2
N = 82
N = 50
N = 28
N = 20
N = 8
N = 2
132Sn

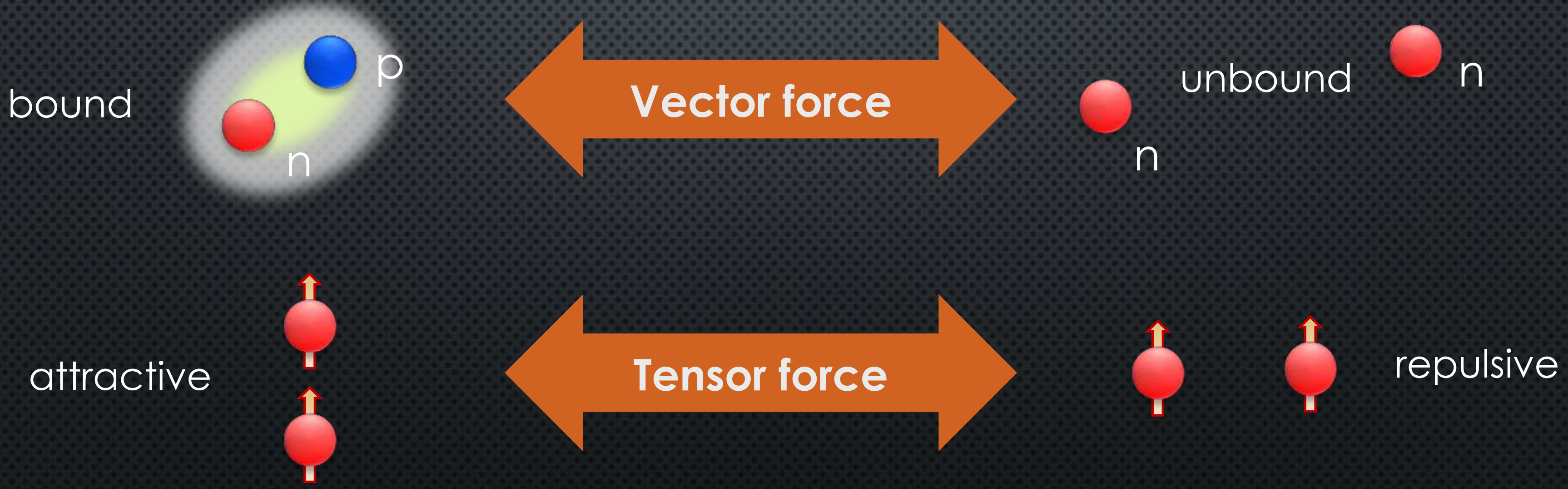
REALITY: A SIMPLE, YET NON-TRIVIAL, NUCLEAR PHYSICS PROBLEM…

Describe how two neutrons evolve in time under the effect of their mutual interaction

- Interaction at leading-order (LO) of chiral effective field theory (spin tensor!)
- Implementation of real-time evolution of the system of 2 neutrons
- Realistic device-level simulations gauged on LLNL's QPU without/with measured noise
- Measurements/calculations on the LLNL testbed
- A simple extension on a digital machine (AQT testbed @ LBL) including some kind of evolution of the coordinates

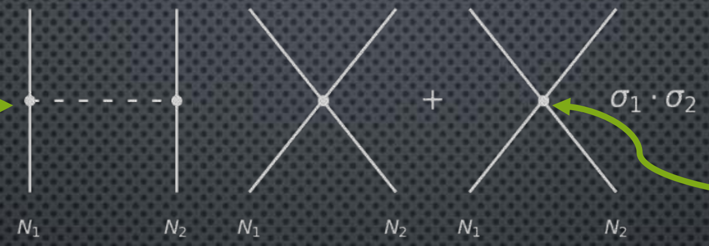
THE STRONG NUCLEAR INTERACTION HAS A NON-TRIVIAL DEPENDENCE ON THE QUANTUM STATE OF THE NUCLEONS

- One of the main features of the nucleon-nucleon interaction is its spin/isospin dependence. This dependence accounts for some very basic phenomenology.



NUCLEON NUCLEON INTERACTION (LO)

One-pion exchange (OPE)



Regularized contact (cutoff in momentum)

$$H_{\rm int}^{\rm LO} = V_{\rm OPE}\left[1 - \delta_{R_0}(\vec{r})\right] + \left[C_0 + C_1\,\vec{\sigma}^1 \cdot \vec{\sigma}^2\right] \delta_{R_0}(\vec{r})$$

regulator function

$$V_{\rm OPE} = \frac{f_\pi^2 m_\pi}{12\pi}\left[T_\pi(r)\,S_{12} - \left(Y_\pi(r) - \frac{4\pi}{m_\pi^3}\,\delta(\vec{r})\right)\vec{\sigma}^1 \cdot \vec{\sigma}^2\right]\vec{\tau}^1 \cdot \vec{\tau}^2$$

Spin independent

Spin dependent

TIME PROPAGATION

Formal solution of the time-dependent Schroedinger equation:

$$\exp\left(-\frac{i}{\hbar}\hat{H}t\right) = \exp\left[-\frac{i}{\hbar}\left(\hat{T}+\hat{V}_{SI}+\hat{V}_{SD}\right)t\right]$$

- V_{SI}: **SPIN-INDEPENDENT** part of the interaction
- V_{SD}: **SPIN-DEPENDENT** part of the interaction

In the short-time limit, we can separate the terms depending on V_{SI} and V_{SD}:

$$\exp\left[-\frac{i}{\hbar}\left(\hat{T}+\hat{V}_{SI}\right)\delta t\right]\exp\left[-\frac{i}{\hbar}\hat{V}_{SD}\delta t\right]+o(\delta t^2)$$

TIME PROPAGATION

First application: "frozen" nucleons → Spin/isospin Hamiltonian only

$$\exp\left[-\frac{i}{\hbar}\hat{V}_{SD}\delta t\right] = \exp\left[-\frac{i}{\hbar}\left(\sum_{i,j=1}^{A}\sum_{\alpha,\beta=x,y,z}\sigma_{i\alpha}A(r_{ij})_{ij;\alpha\beta}\sigma_{j\beta}\right)\delta t\right]$$

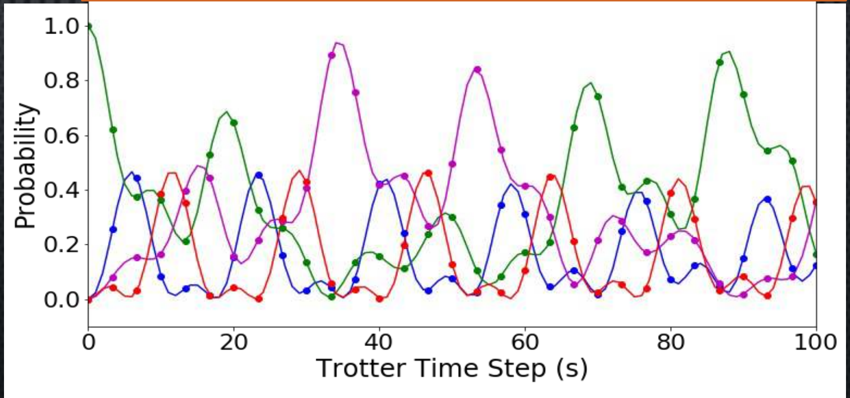
coordinates appear as "parameters"

Computer simulation of the actual device

Lines: analytic results
Circles: synthetic data: probability of measuring state $|\alpha\rangle$ after a time t (obtained by repeating the process over and over)

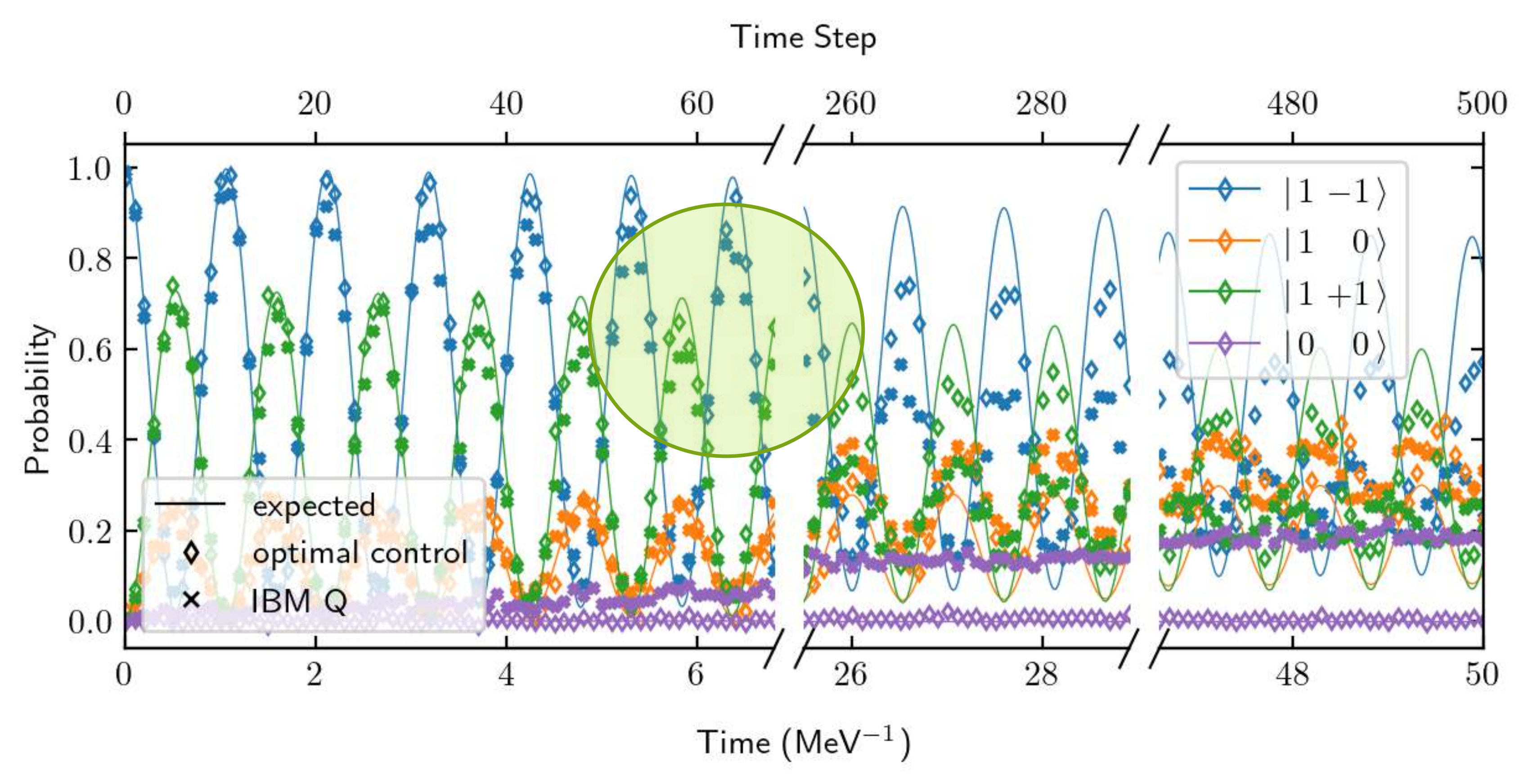
The time evolution with a tensor Hamiltonian introduces spin-parallel components

Occupation probability



$|0\rangle = |\uparrow\uparrow\rangle$ $|1\rangle = |\uparrow\downarrow\rangle$ $|2\rangle = |\downarrow\uparrow\rangle$ $|3\rangle = |\downarrow\downarrow\rangle$

RESULTS ON LLNL TEST BED SIMULATION



"COPROCESSING" SCHEME FOR FULL TIME EVOLUTION

$$\exp\left(-\frac{i}{\hbar}\hat{H}t\right) = \exp\left[-\frac{i}{\hbar}\left(\hat{T}+\hat{V}_{SI}+\hat{V}_{SD}\right)t\right]$$

As a first step in the direction of simulating the full dynamical evolution of a scattering process, we employed a mixed scheme in which the coordinates are evolved classically.

Remind that:

$$\exp\left[-\frac{i}{\hbar}\left(\hat{T}+\hat{V}_{SI}\right)\delta t\right]\exp\left[-\frac{i}{\hbar}\hat{V}_{SD}\delta t\right]+o(\delta t^2)$$

With T. Chistolini, A. Hashim, Y. Kim, W. Livingston, D. Santiago, I. Siddiq @LBLi

We can make the (very crude) approximation of evolving the coordinates of the nucleons classically (using V_{SI}), and evolving the spin of the nucleons with the second factor in the propagator. Since the coordinates are evolved on a classical computer, we call this "coprocessing" scheme.

"COPROCESSING" SCHEME FOR FULL TIME EVOLUTION

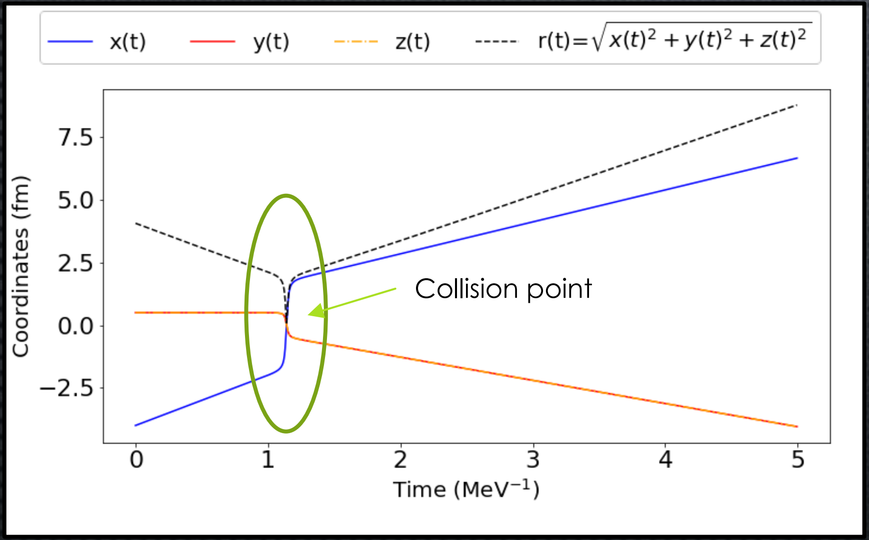
This approach has severe limits. In particular:

- The true space evolution is obviously not classical
- while there is feedback of the special evolution on the spin evolution, the opposite does not happen. This could be fixed in several ways.

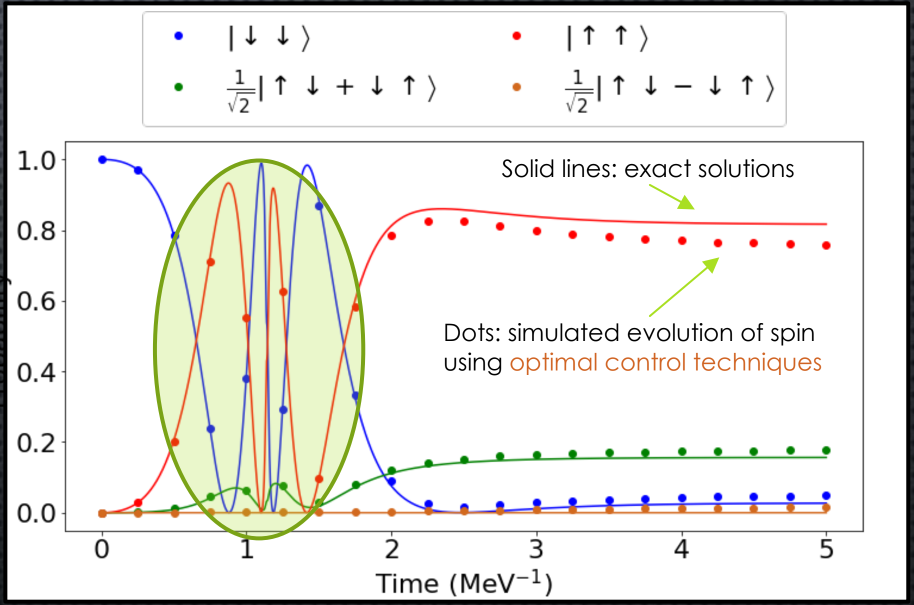
For the moment the aim is essentially to study the stability of a quantum computation in which the Hamiltonian has a heavy parametric dependence on time dependent quantities.

Essentially, one is studying the evolution of a state of a time-dependent Hamiltonian (which is one of the important features of the propagator when we use the Trotter decomposition)

TIME EVOLUTION OF SPIN (IDEAL CASE)

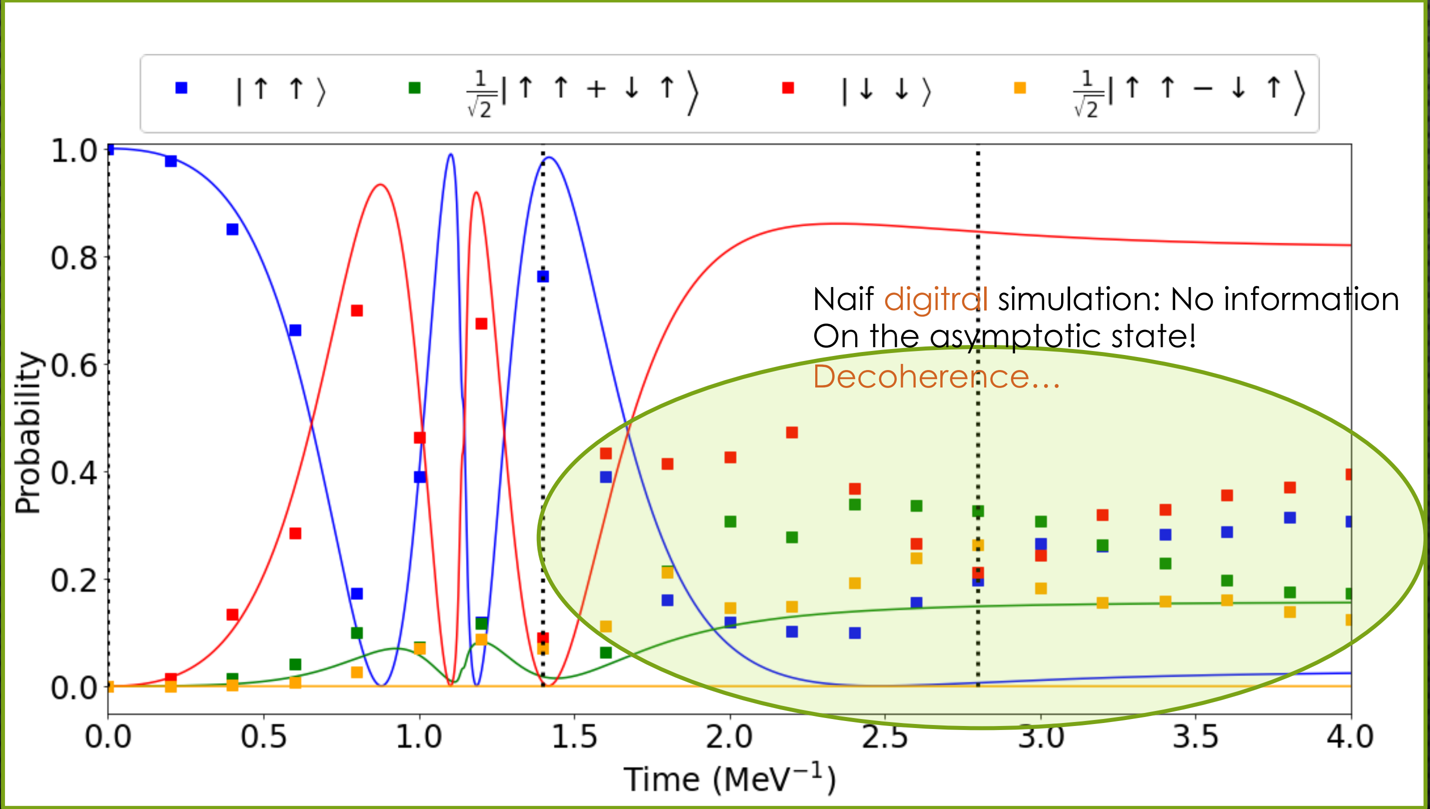


Evolution of the relative coordinate

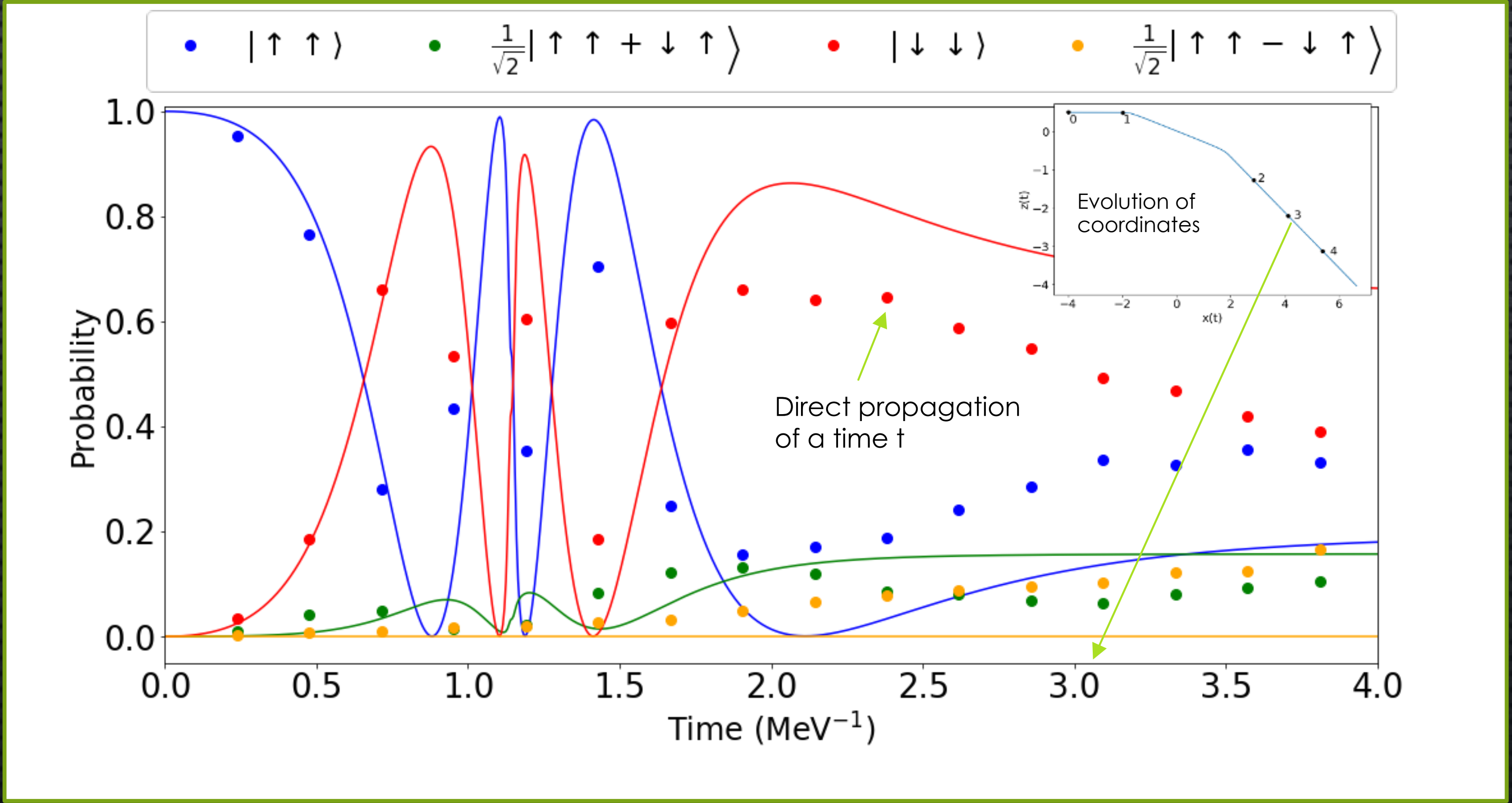


Evolution of the spin state (simulated, Optimal control)

TIME EVOLUTION OF SPIN (AQT@LBL)

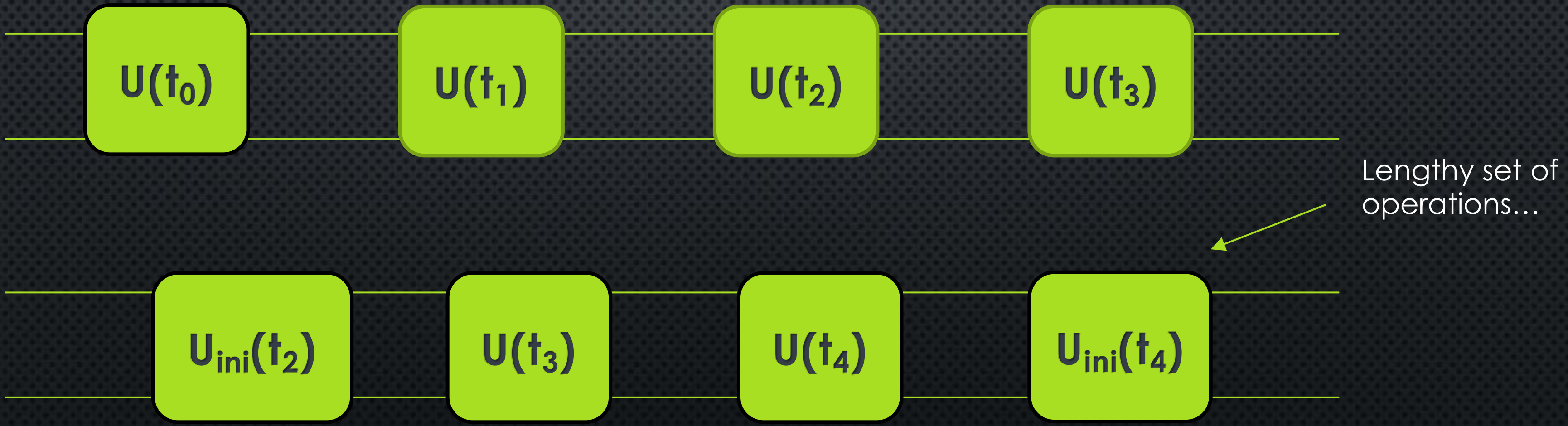


"LONG TIME" PROPAGATOR



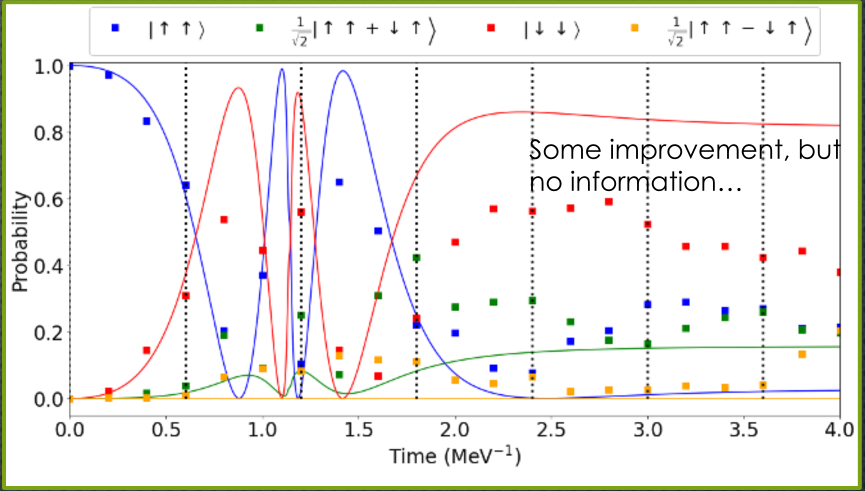
REINIZIALIZATION

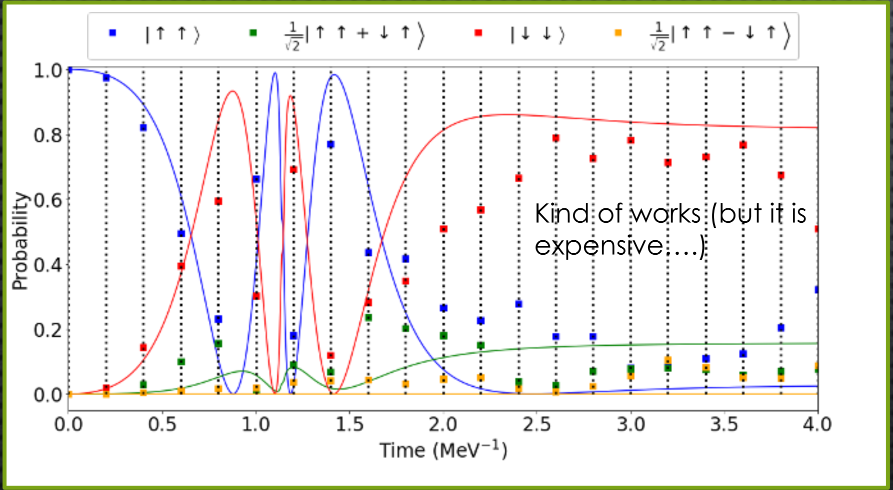
A possible, non scalable, approach consists of re-initializing the state at each time-step. Of course this requires STATE TOMOGRAPHY, followed by a circuit (set of (controlled) rotations) giving back the required state.



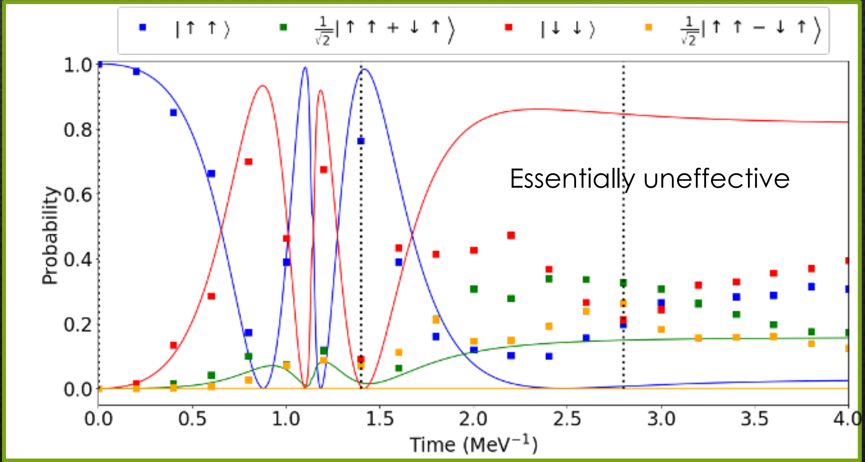
REINIZIALIZATION

Every 3 time steps



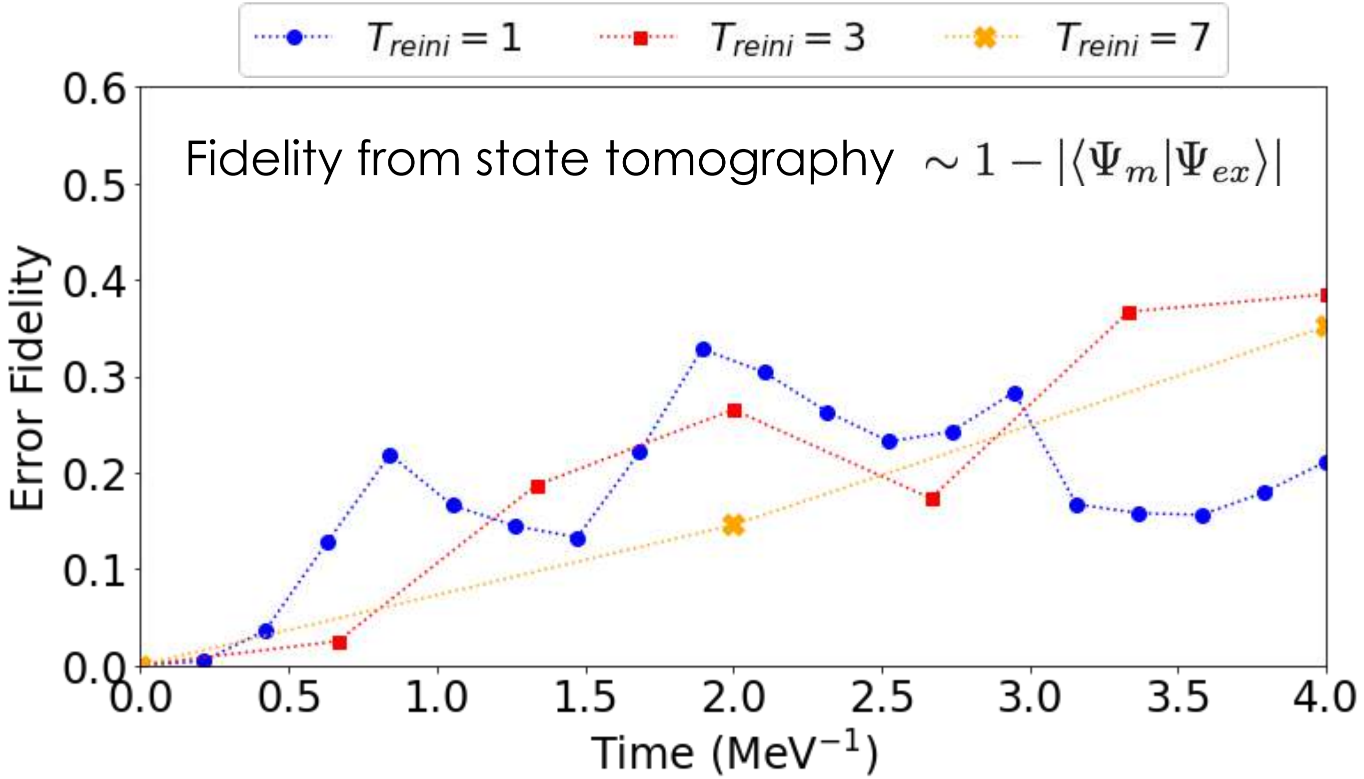


Every time step

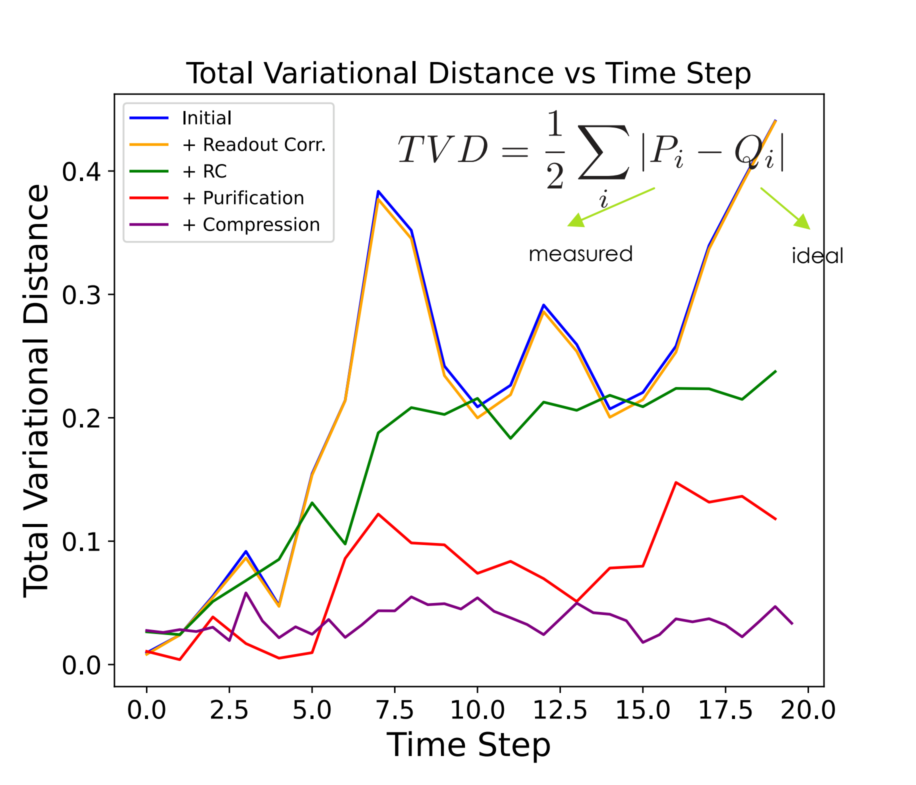


Every 7 time steps

FIDELITY IN THE REINIZIALIZATION PROCEDURE



FURTHER IMPROVEMENTS



The results shown for the reinizialization strategy were obtained without implementing any error correction procedures. These might help to increase the time interval between successive reinizializations.

CONCLUSIONS

- Optimal control techniques can definitely help to realize proofs of concept for quantum algorithms that need to be robust over time (as for the case of scattering studies)

- A path for the study of nuclear reactions with realistic interactions is visible. However, there are still many open problems (like a more accurate implementation of space propagators with a reasonable scaling) which still need to be addressed.

- Digital QC requires a more elaborated circuit optimization, but some interesting demonstration might not be too far.

- In both cases, it is very important to have access to low level optimization -> work in strict cooperation with the experimental groups!

THANK YOU!