UNIVERSITÀ DI TRENTO

Istituto Nazionale di Fisica Nucleare

Trento Institute for Fundamental Physics and Applications

Quantum Science and Technology in Trento

Lawrence Livermore National Laboratory

Nuclear Simulations on Quantum Computers with Optimal Control

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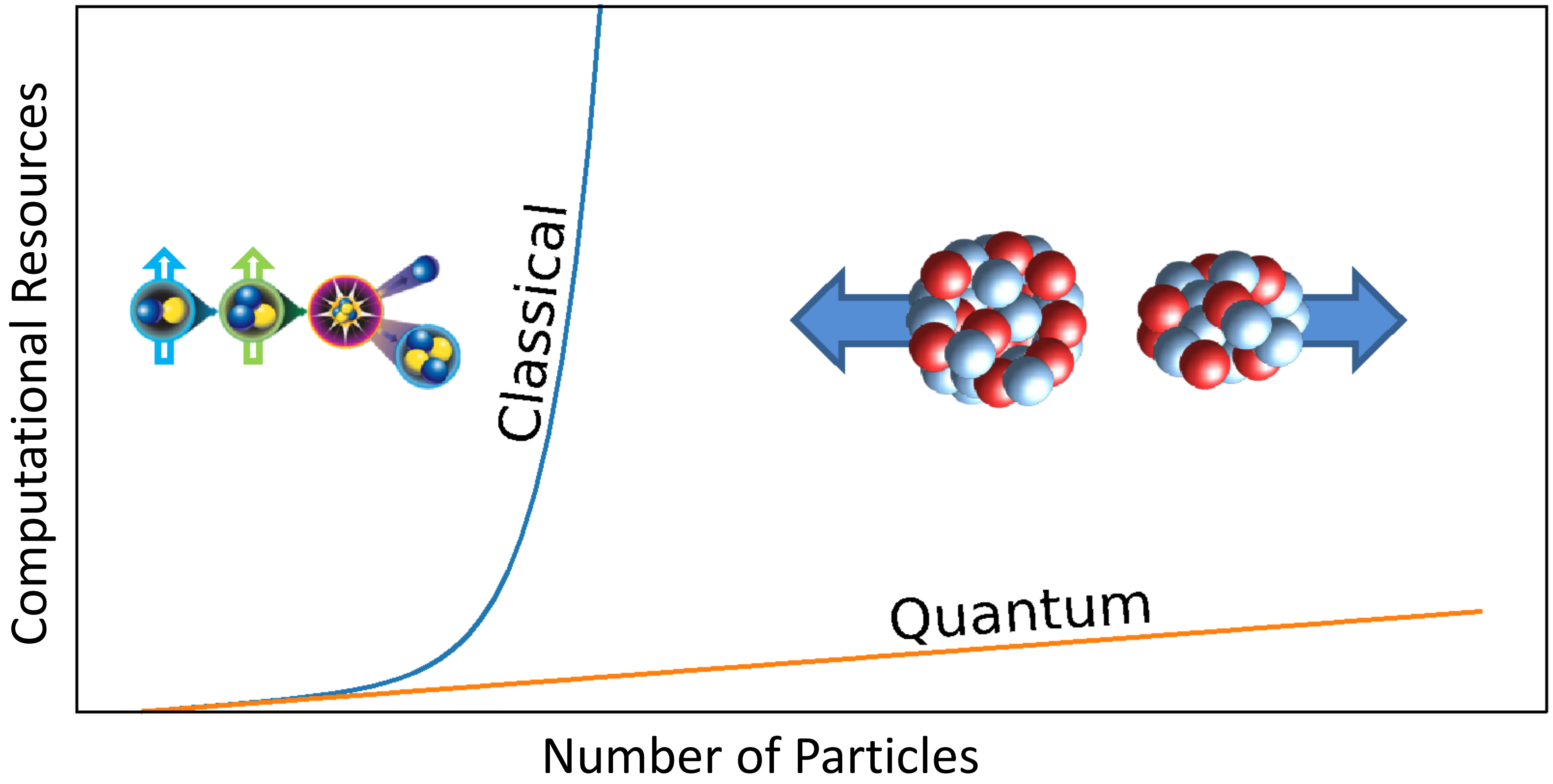
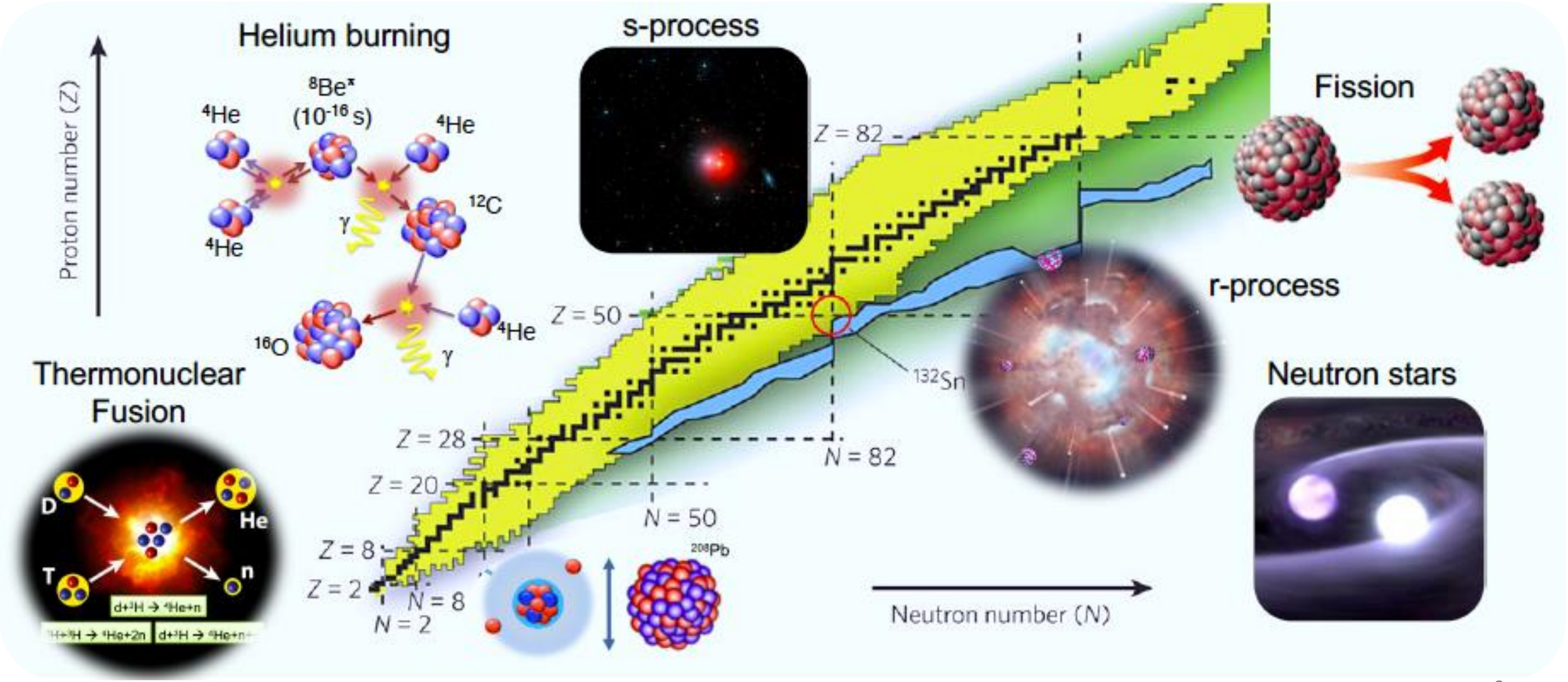
Quantum Computing @ INFN

14-15 November 2022

Computational effort: classical vs quantum

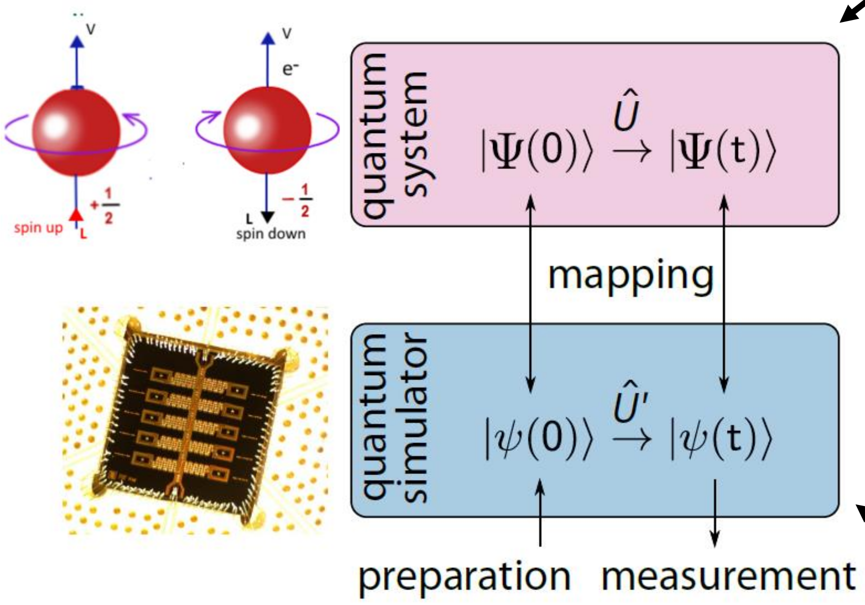


Goal: studying dynamical processes in nuclear systems



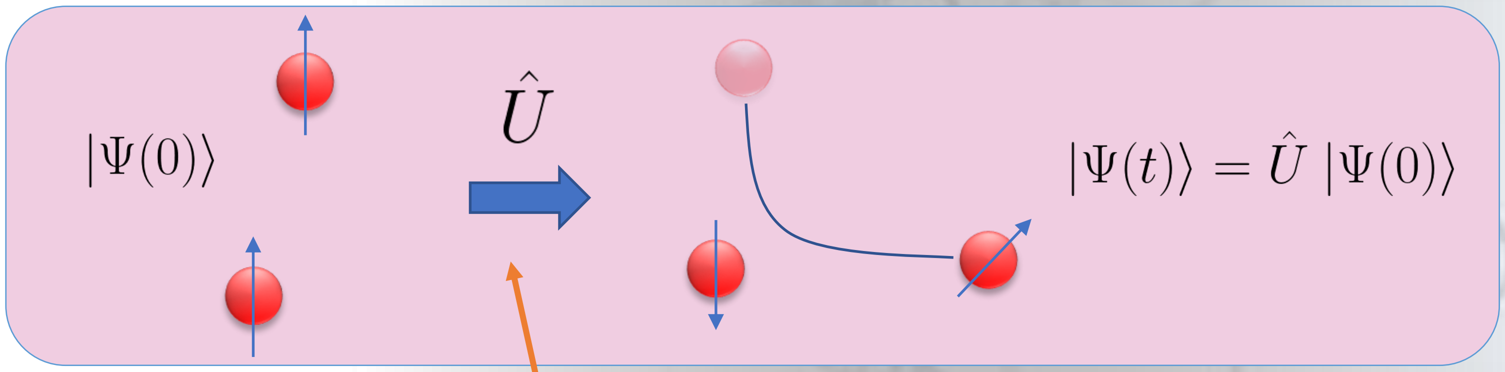
How does it works?

- Mapping



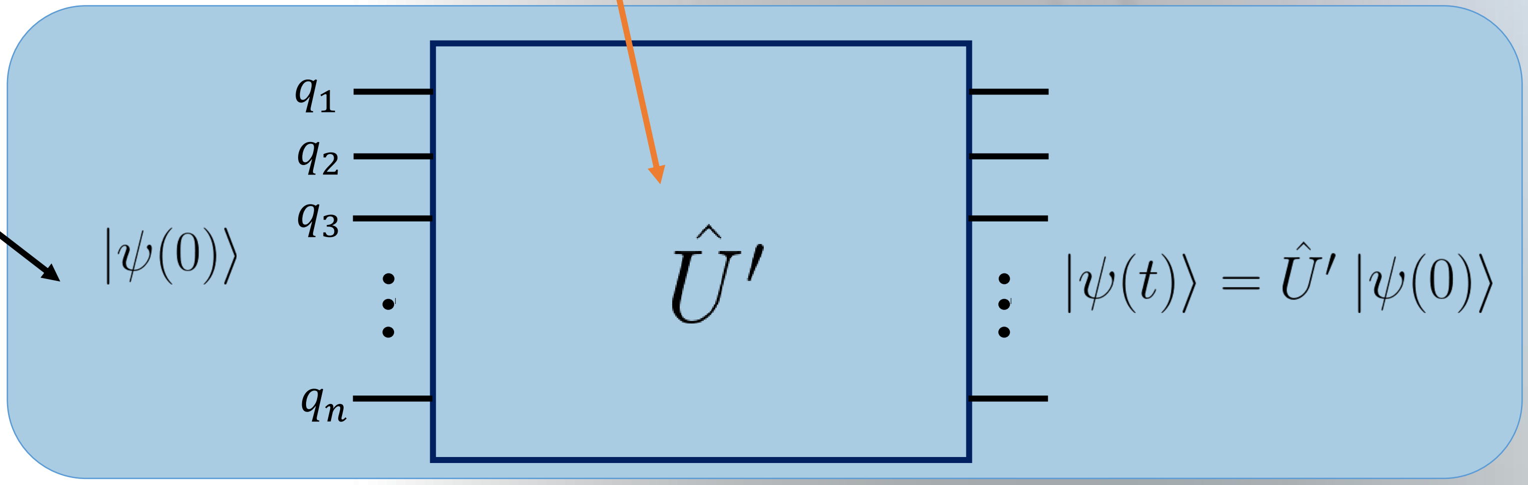
Holland, E. T., Wendt, K. A., et al. (2020) *Physical Review A*, *101*(6), 062307.

Real system: Not directly controllable



- Unitary transformation implementation

Qubit: "Two-level quantum system that can be controlled and measured"



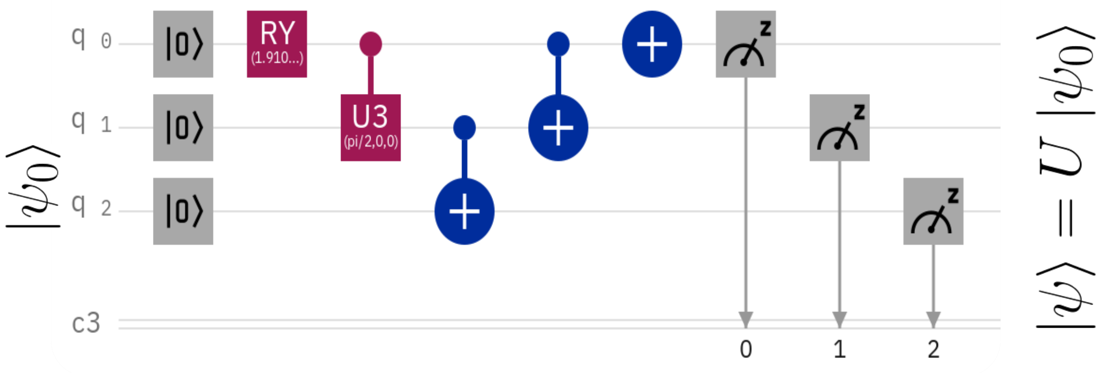
Quantum device: controllable and measurable

Quantum Gates

(Differences between QC setups)

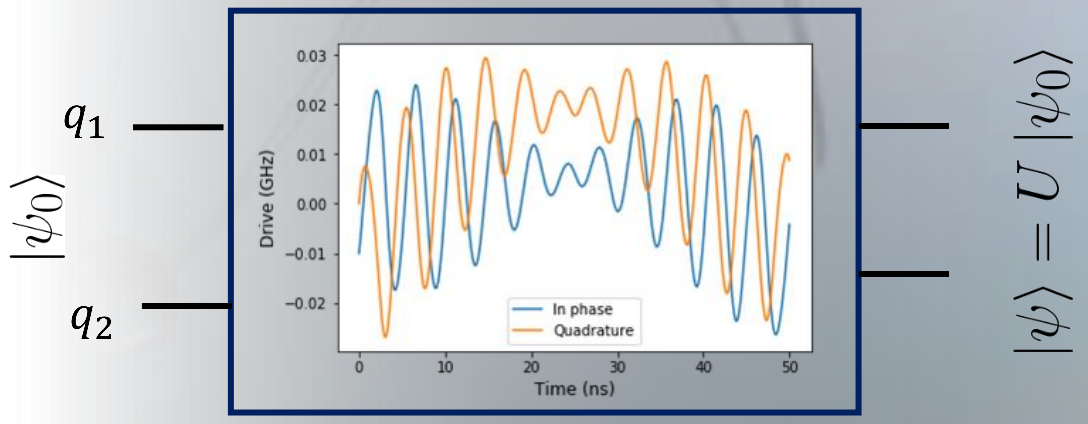
Standard (discrete gate sets)

- Discrete, finite predetermined set of quantum logical operations (gates)
- Many-body dynamics to be simulated implemented through a circuit involving multiple gates



Optimal control-based

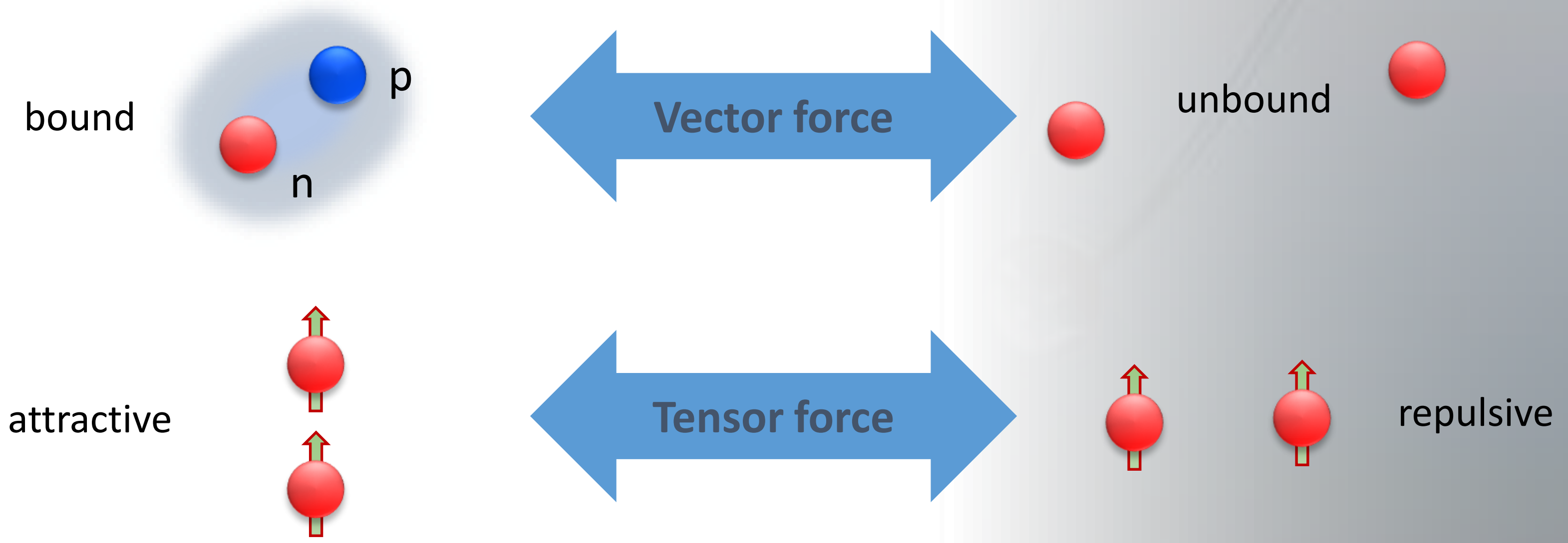
- Software reconfigurable, continuous unitary transformation (gate)
- Many-body dynamics to be simulated implemented with a single gate
- Microwave pulse to control the qubit



Two Nucleon Dynamics

- Nuclear dynamics relies on the expansion of the interaction between nucleons (coming from QCD) by means of effective field theories (EFT).

- Resulting nuclear force presents non-trivial dependence on the relative spin/isospin state of pairs/triplets of nucleons.



See e.g. J.E. Lynn et al. Phys. Rev. C 96, 054007 (2017)

Two Nucleons Dynamics

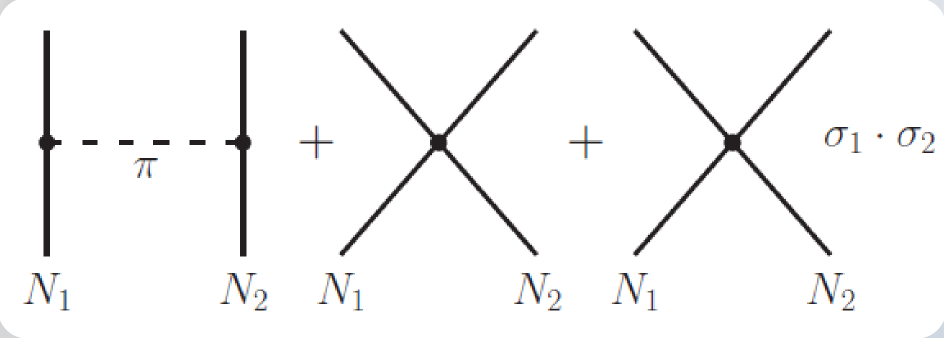
- Characteristic features of the nucleon-nucleon interaction are captured by the leading order (LO) in the EFT expansion.

- Hamiltonian $\widehat{H}_{int}^{LO} = \widehat{\mathrm{T}} + \widehat{\mathrm{V}}^{\mathrm{SI}} + \widehat{\mathrm{V}}^{\mathrm{SD}}$

- The propagator is:

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

  - V_{SI}: **spin-independent** part of the interaction
  - V_{SD}: **spin-dependent** part of the interaction



Schematic description of interaction:
single pion exchange +
spin-independent contact term +
spin-dependent contact term

Two Nucleons Dynamics

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

- Approximation: treat neutron as frozen in space for the duration of the spin-dependent part of the propagation.

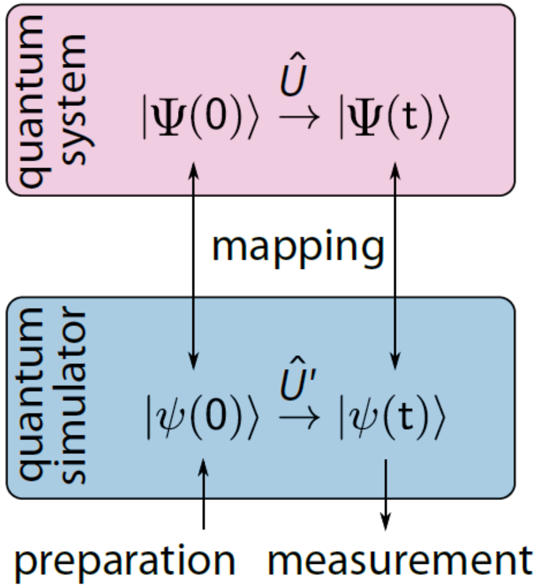
- **Quantum-classical coprocessing protocol**:

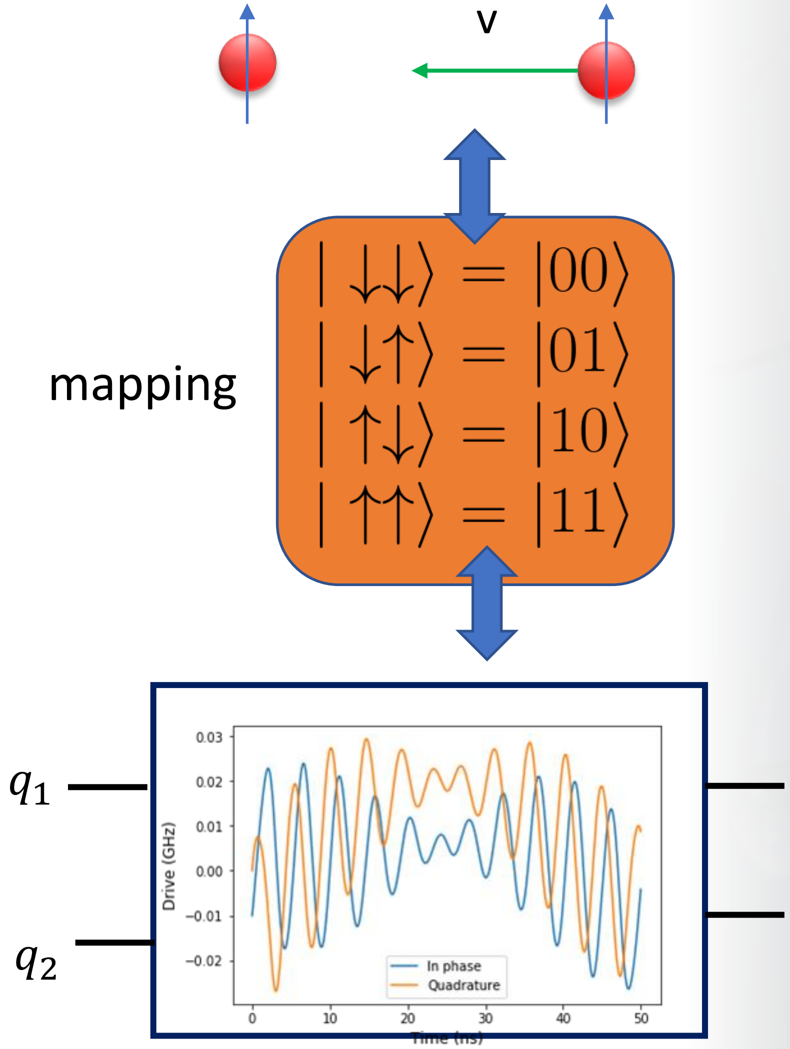
  For a small time step δt:

  1. Advance the spin part with the **quantum computer**: $$\hat{U}_{SD}=\exp\left[-\frac{i}{\hbar}\hat{V}_{SD}\delta t\right]$$
  2. Advance the spatial part with a **classical computer**: $$\hat{U}_{SI}=\exp\left[-\frac{i}{\hbar}\left(\hat{T}+\hat{V}_{SI}\right)\delta t\right]$$
  3. Repeat

Obviously the correct approach is to expand the Hamiltonian on a basis set and map all the system onto the QC but this would require an great number of qubits

Example: Two neutrons dynamics:



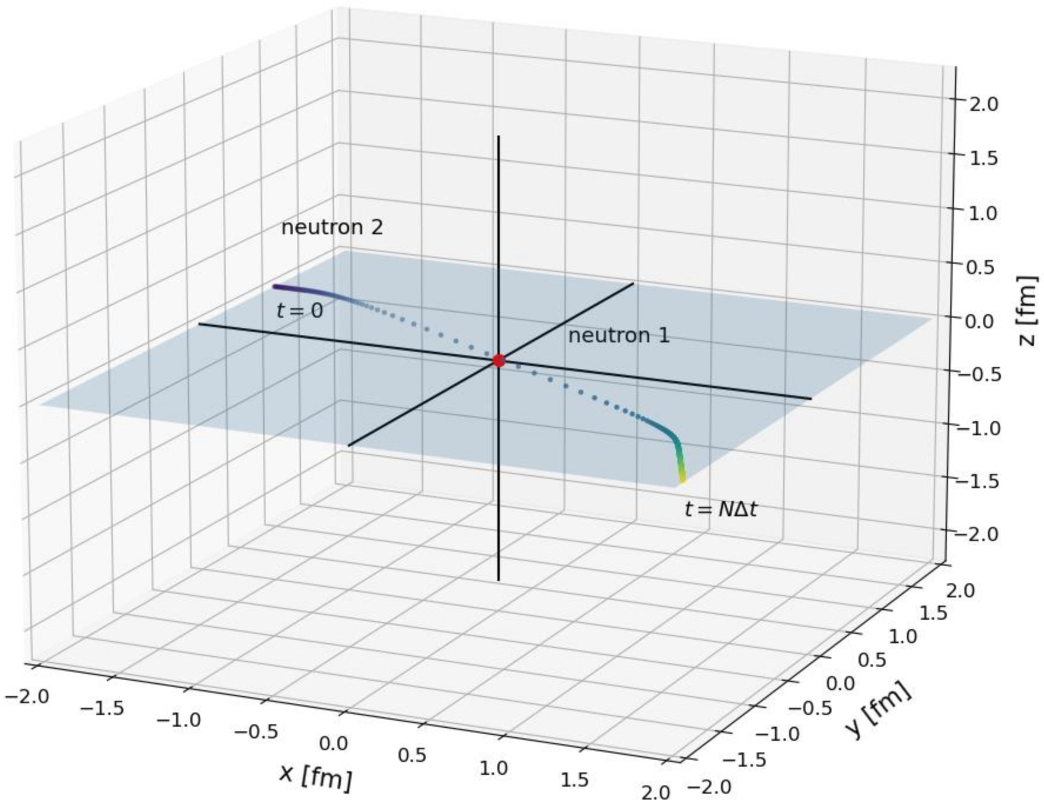


$$\hat{U}_{SD} = \exp\left[-\frac{i}{\hbar}\hat{V}_{SD}\delta t\right]$$

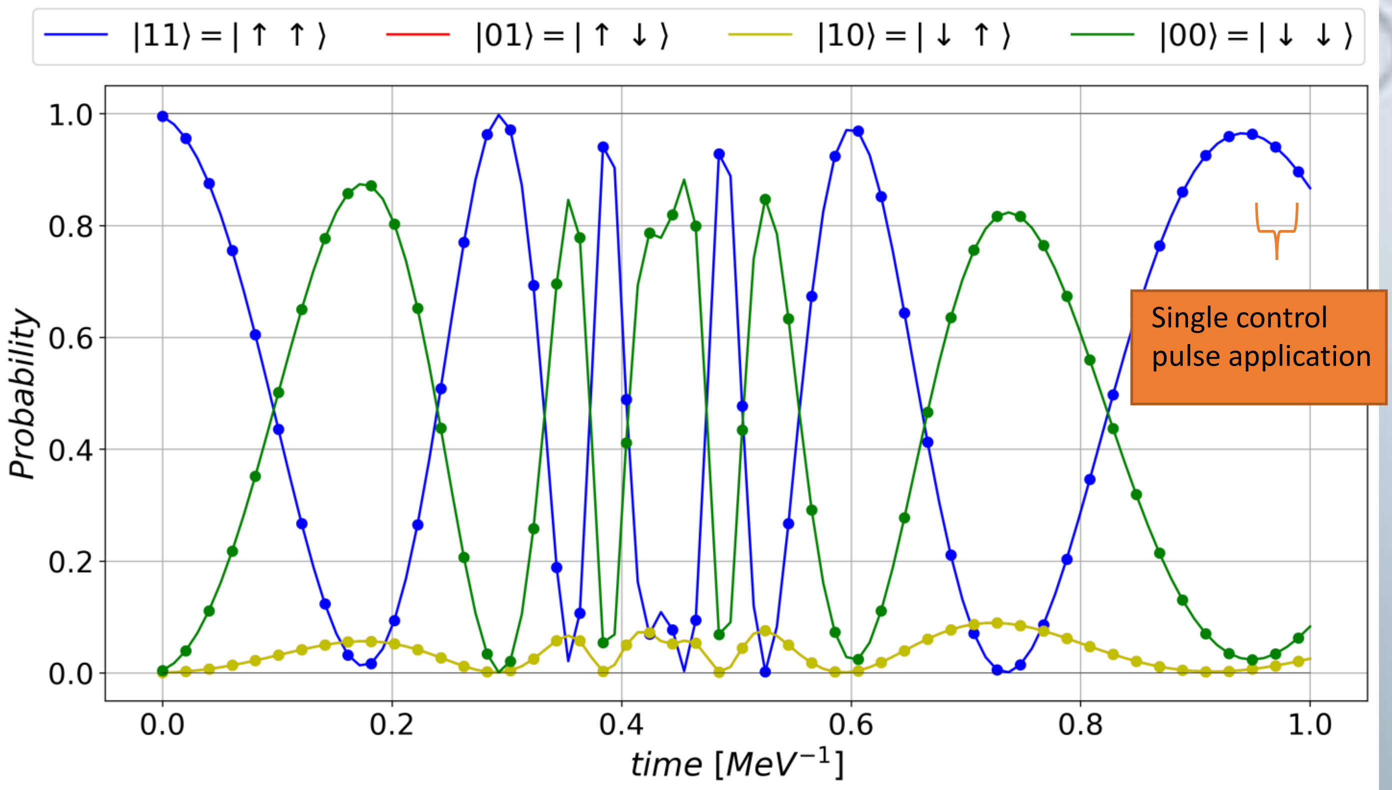
Implementation of unitary transformation

$$\hat{U}'_{SD} = \exp\left[-\frac{i}{\hbar}\int_0^{\tau} H_{qubits} + H_c(t)dt\right]$$

Example: Two neutrons dynamics:



Spatial Trajectory



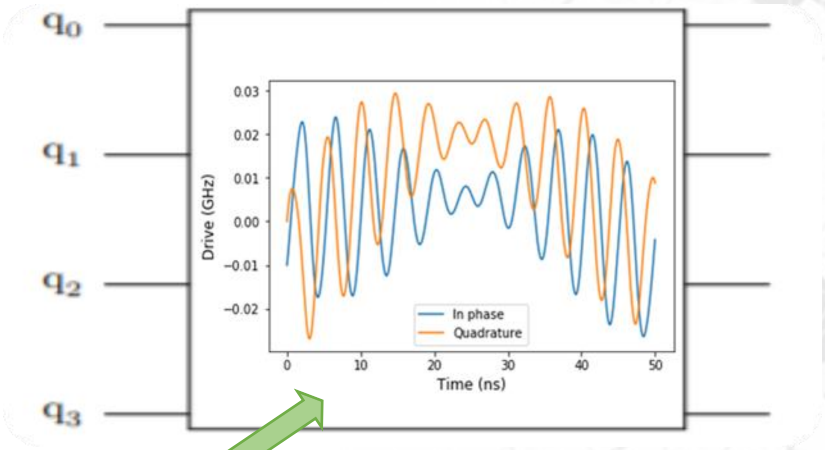
Spin dynamics: Occupation probability.
(Solid: exact dynamics
Points: dynamics obtained with application of the propagator.)

Quantum Control Interpolation

Optimal Control Reconstruction

- Quantum gate optimization :

$$\hat{U}_{SD}(\vec{r}_1 - \vec{r}_2) \cong$$



Controls optimization: bottle-neck of the analysis

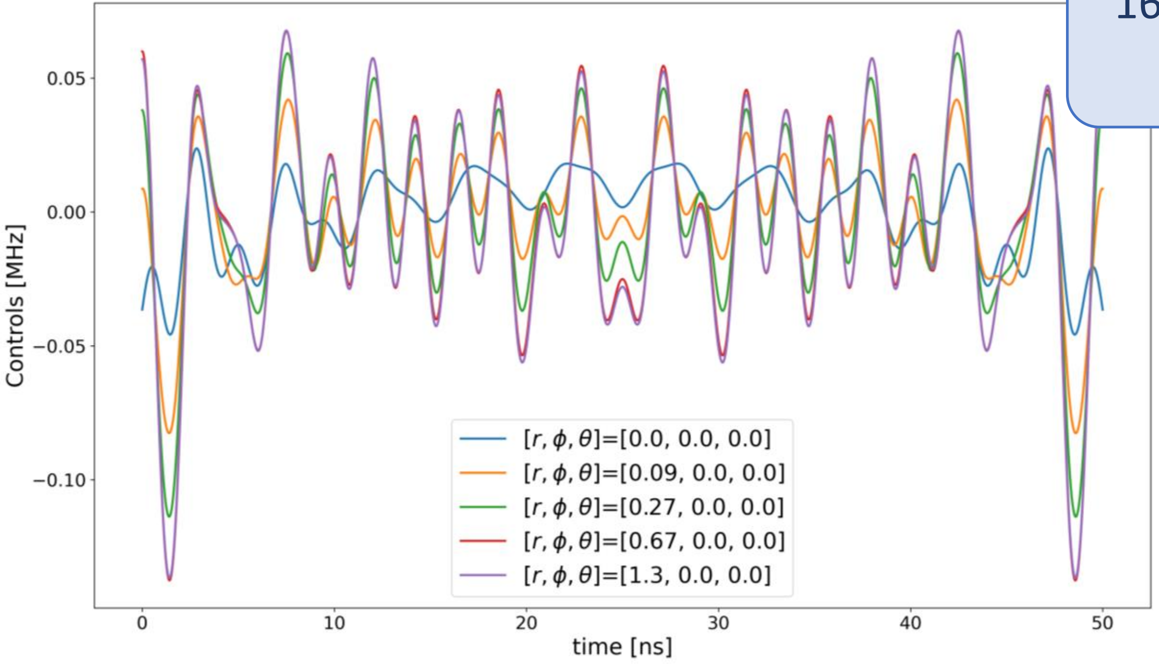
- Slow (especially for many qubits) → **Time consuming**
- The Hamiltonian could be dependent on parameters (e.g neutrons relative position) that change during the simulation → **Need to calculate the controls at every time-step**

Possible solution: <u>try to find a mathematical relation that can reconstruct the controls corresponding to given parameters values, without using the optimization algorithm.</u>

Controls Reconstructing Method

See: Luchi, Piero, et al. *arXiv preprint arXiv:2102.12316* (2021).

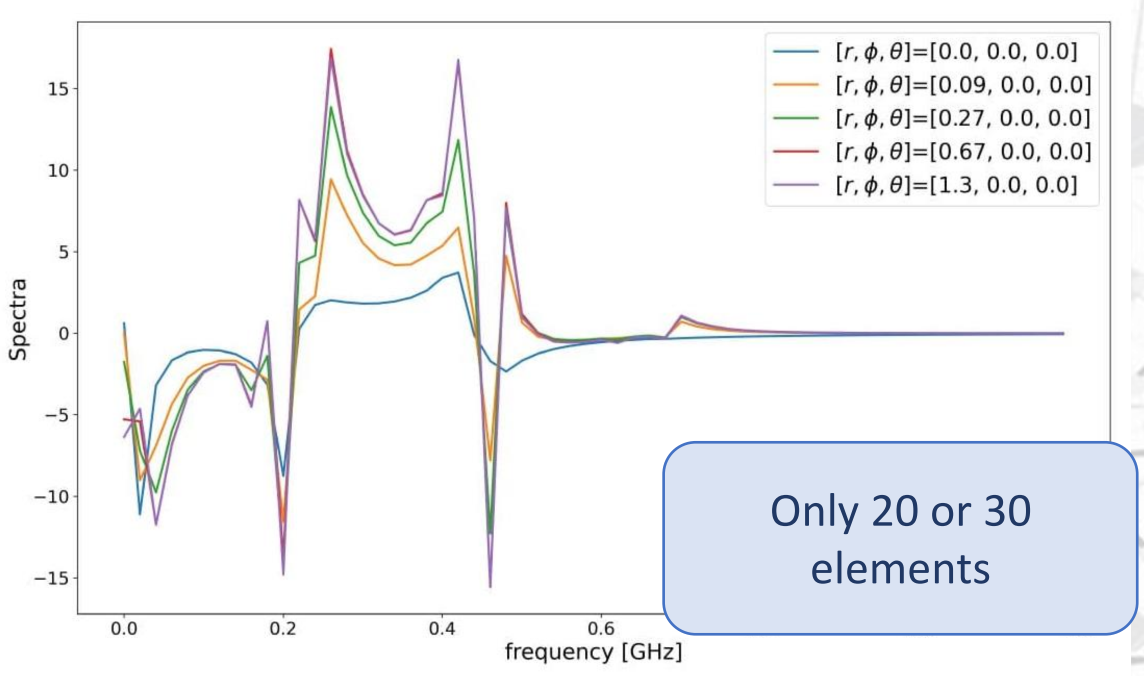
Fourier Transform Method



1600 time-steps for each control

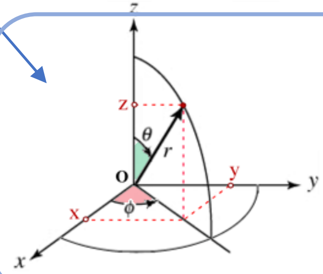
Fourier transform

Corresponding set of spectra



Only 20 or 30 elements

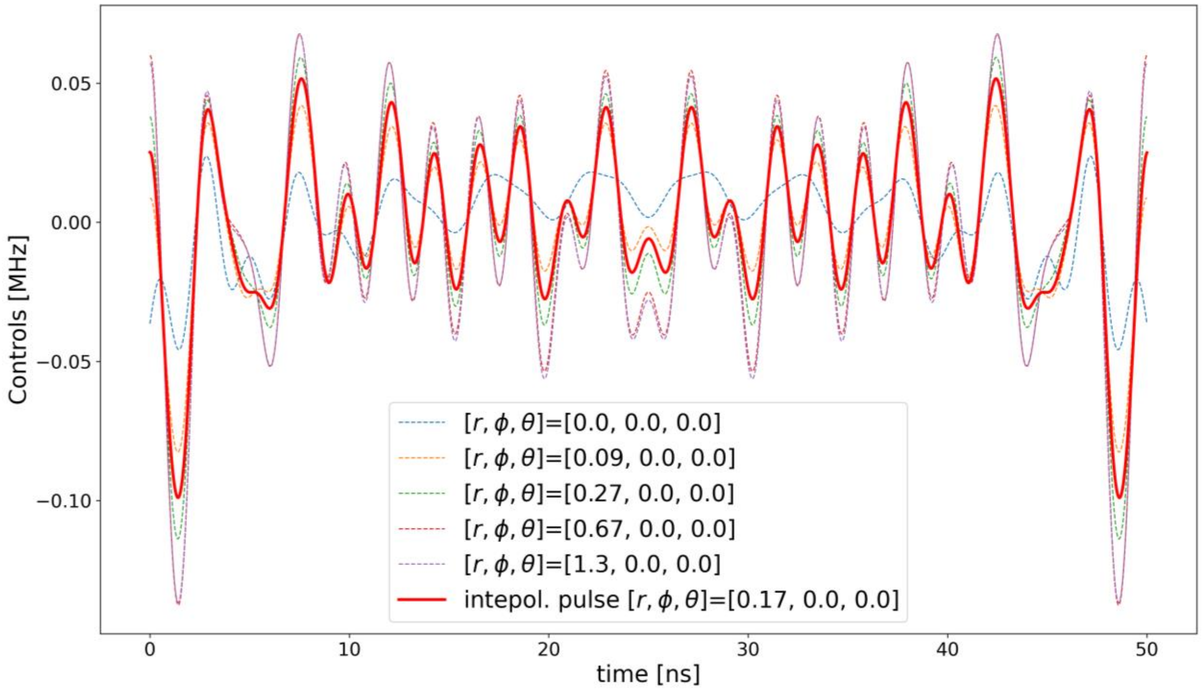
Compute and store (with the optimization procedure) a set of controls corresponding to a grid of (r, φ, θ) values.



Neutrons relative position in spherical coordinate

Controls Reconstructing Method

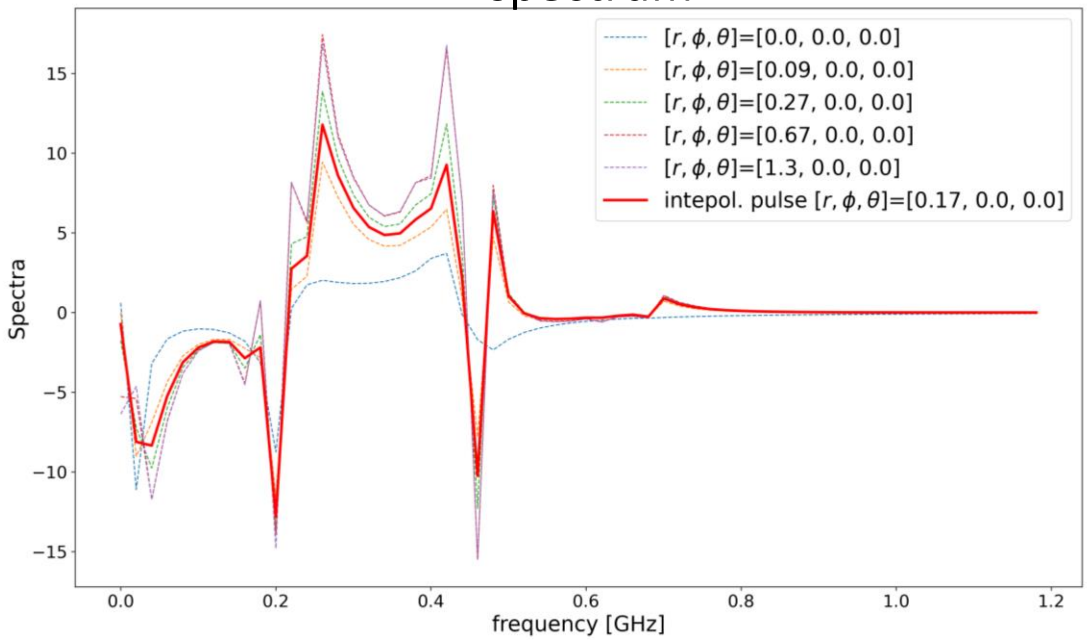
Fourier Transform Method



New control for the quantum computer

2] Inverse Fourier transform and obtain a new control

1] Choose $(r_{new}, \varphi_{new}, \theta_{new})$ and Interpolate a new spectrum

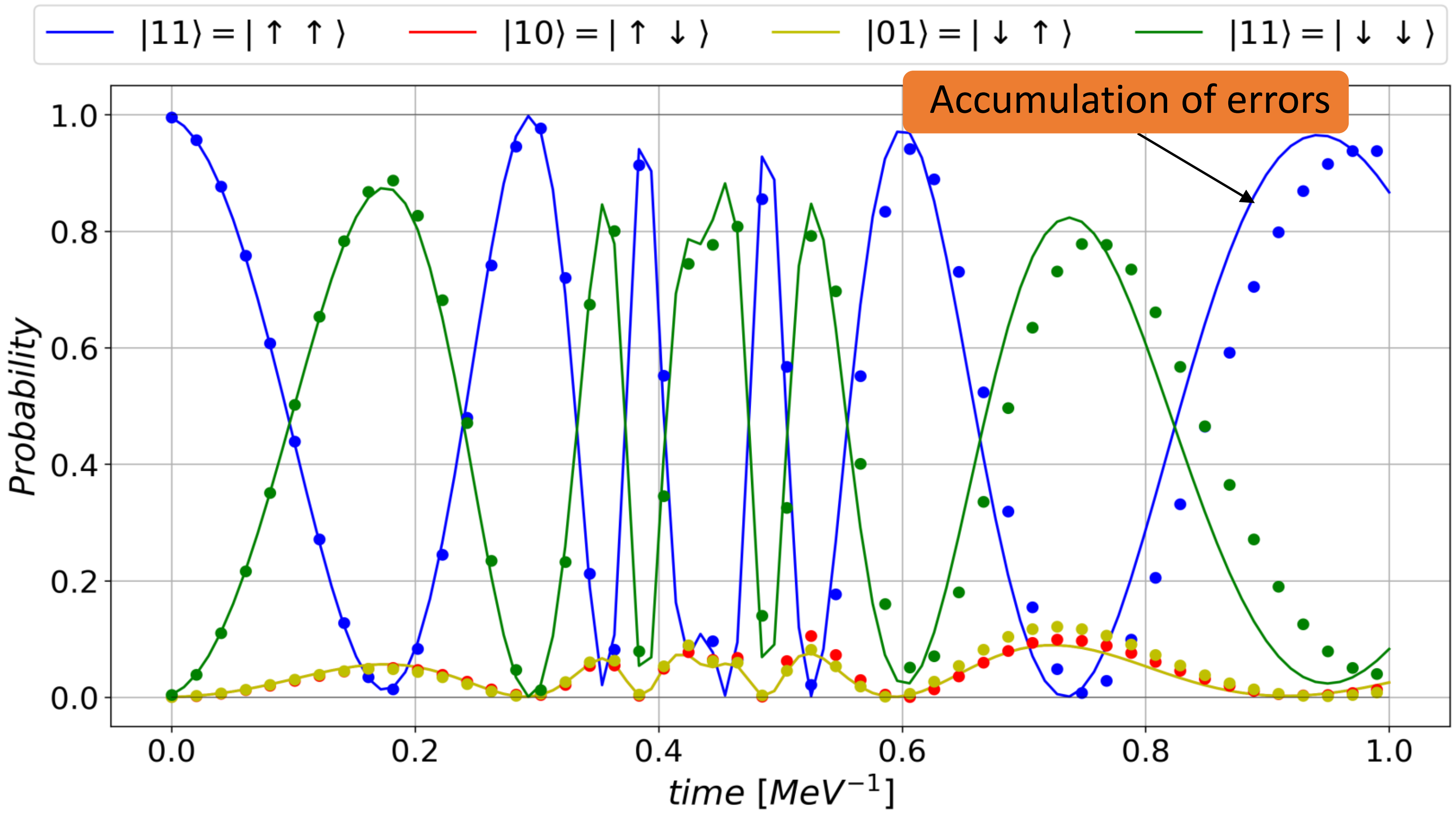


<u>After the computation of a (possibly small) set of controls in advance, we can obtain an infinite number of them at a low computational cost</u>

Controls Reconstructing Method

Fourier Transform Method

Simulation of the spin dynamics of the neutron-neutron system along a trajectory



Average accuracy reconstruction: 99,99%

5-10 times faster than the optimization based procedure

Conclusions

- QC are a promising device to perform realistic nuclear simulations
- A simple but non-trivial example of two neutrons interaction has been shown.
- The implementation of $\widehat{U}$ can be improved with some interpolation techniques.

Thank you for your attention

Supplementary Information

Controls Reconstructing Method

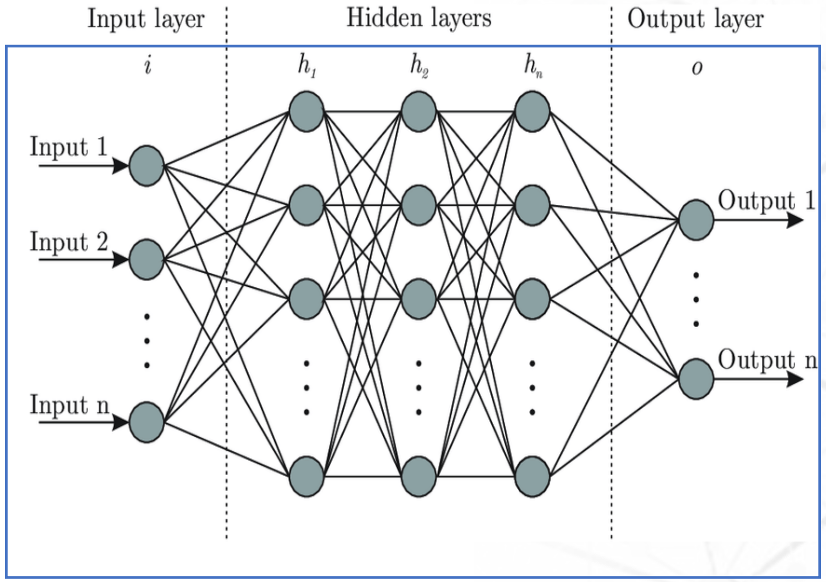
Neural Network Method

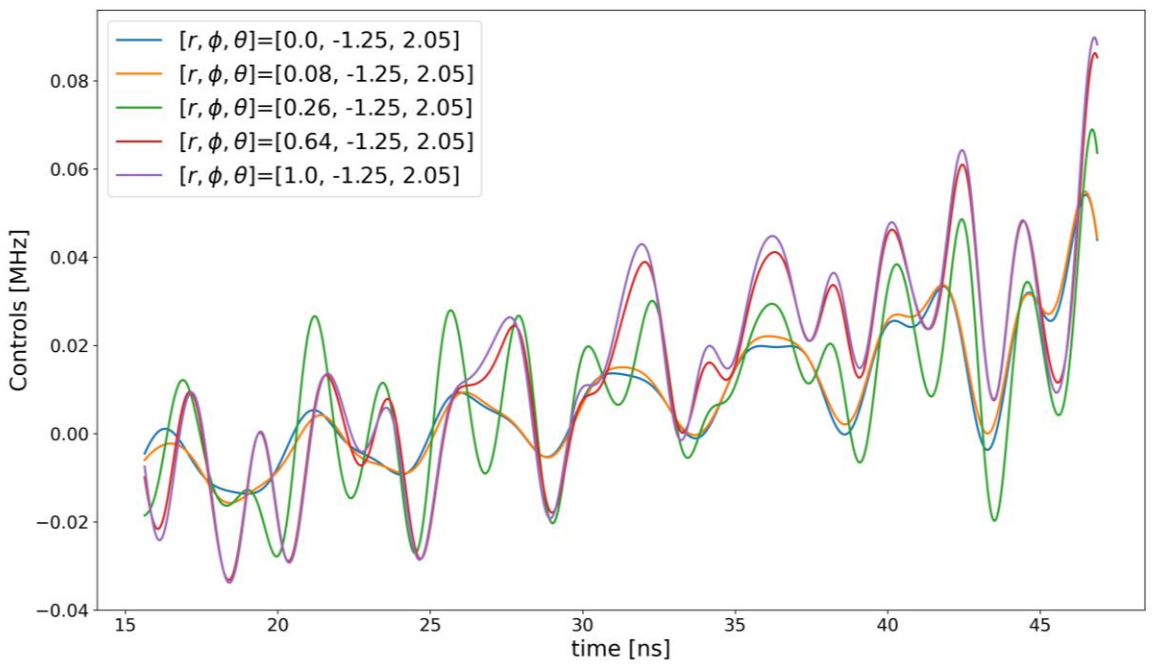
- Train

Set of controls corresponding to a grid of (r, φ, θ) values

Set of propagators for a a grid of (r, φ, θ) values

$$U_{SD}$$

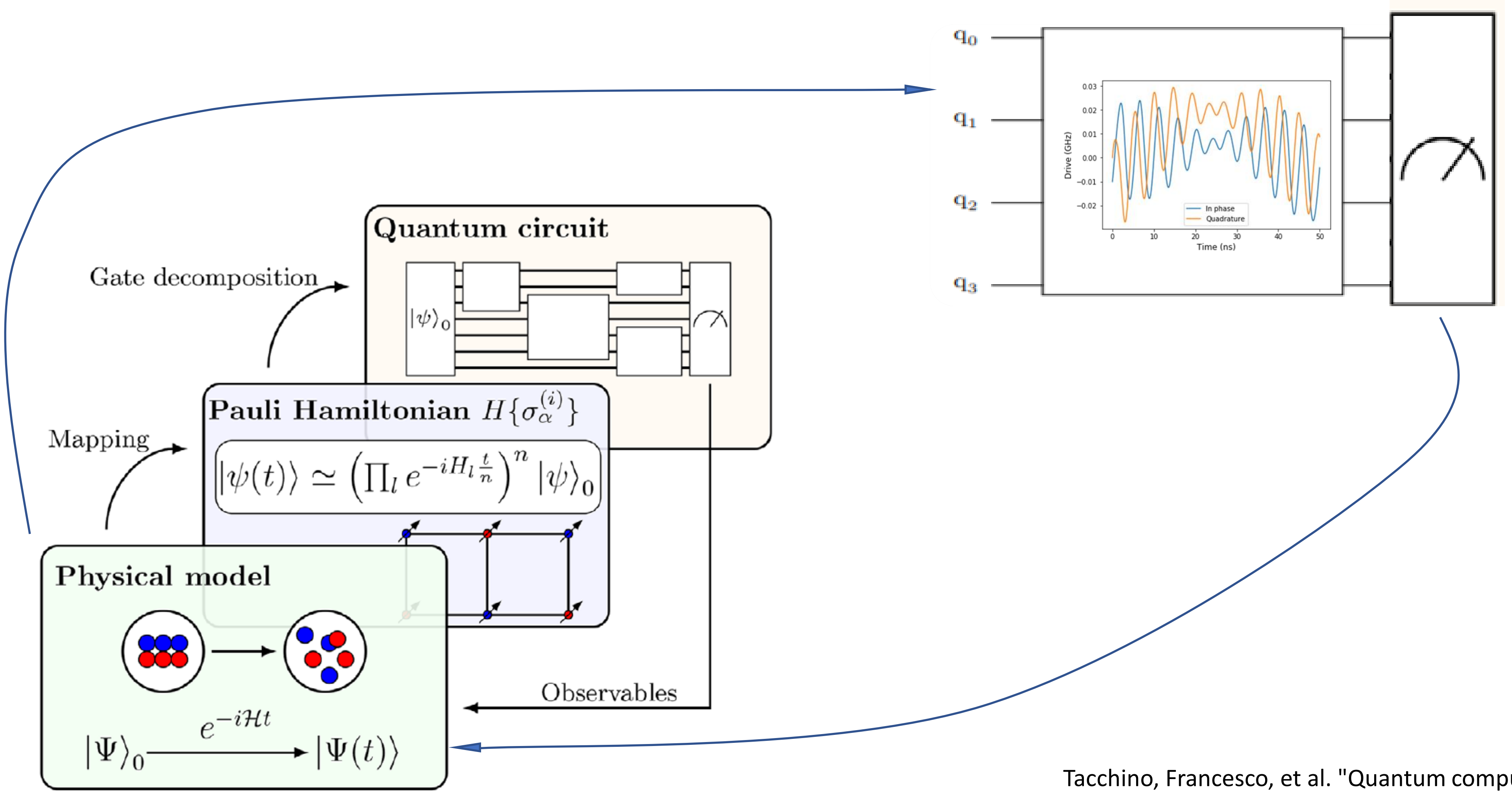




$$U_{SD} = \exp\left[-\frac{i}{\hbar}\hat{V}_{SD}\delta t\right] = \exp\left[-\frac{i}{\hbar}\left(\sum_{i,j=1}^{A}\sum_{\alpha,\beta=x,y,z}\sigma_{i\alpha}A(r_{ij})_{ij;\alpha\beta}\sigma_{j\beta}\right)\delta t\right]$$

Quantum Gates

(Differences between QG approaches)

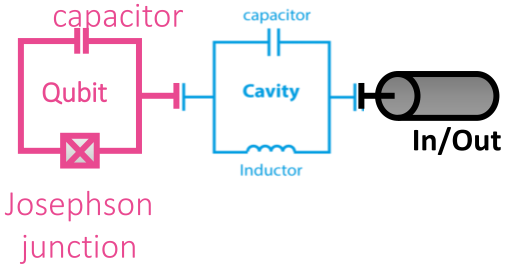


Tacchino, Francesco, et al. "Quantum computers as universal quantum Simulators: state-of-the-art and perspectives." *Advanced Quantum Technologies* 3.3 (2020): 1900052.

Physical implementation: Control-based Gates

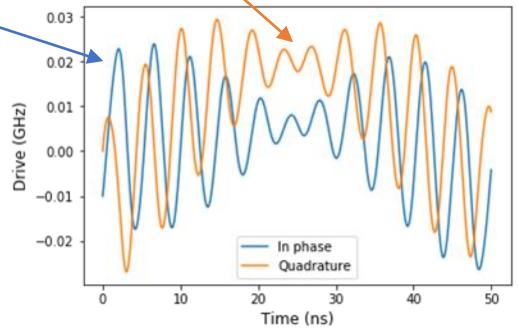
General Hamiltonian for a transmon coupled with the readout cavity:

$$\hat{H}_d = \hbar\omega_T \hat{a}_T^\dagger \hat{a}_T + \hbar\omega_R \hat{a}_R^\dagger \hat{a}_R - E_J \left[\cos(\hat{\phi}_j) + \frac{1}{2}\hat{\phi}_j^2\right]$$



Time-dependent drive in the frame of the transmon is:

$$\hat{H}_c = \hbar\varepsilon_I(t)(\hat{a}_T^\dagger + \hat{a}_T) + i\hbar\varepsilon_Q(t)(\hat{a}_T^\dagger - \hat{a}_T)$$



$$U_{targ} \simeq \mathcal{T} \exp\left\{-\frac{i}{\hbar}\int_0^{\tau}\left[\hat{H}_d + \hat{H}_c(\tau')\right] d\tau'\right\}$$

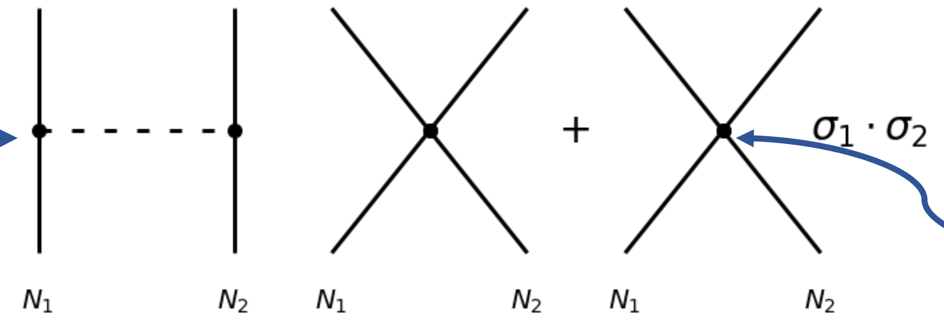
Optimise the control sequence $\varepsilon_I, \varepsilon_Q$ such that they satisfies, within an acceptable error, this relation (using GRAPE algorithm):

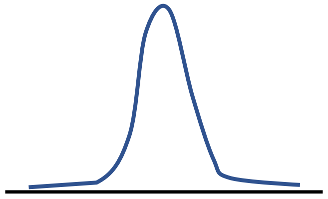
The computational cost of this **grows exponentially** in the number of effective qubits controlled

[1] Holland, E. T., Wendt, K. A., Kravvaris, K., Wu, X., Ormand, W. E., DuBois, J. L., ... & Pederiva, F. (2019). Optimal Control for the Quantum Simulation of Nuclear Dynamics. *arXiv preprint arXiv:1908.08222*.

Example: Local chiral EFT potential at leading order

One-pion exchange (OPE)





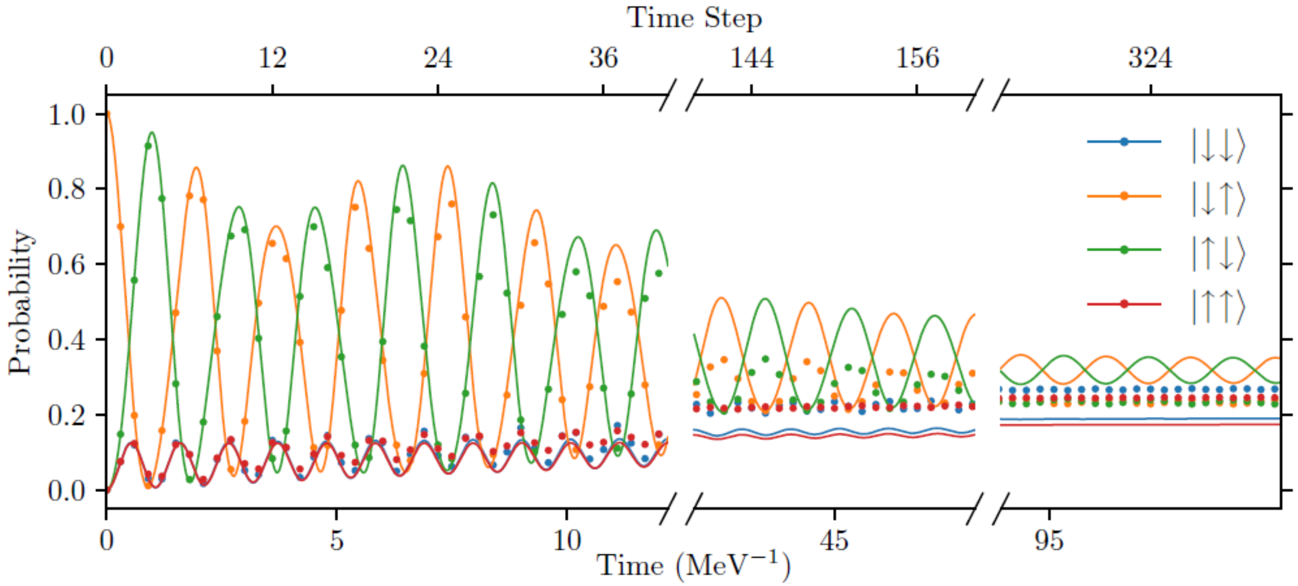
Regularized contact (cutoff in momentum)

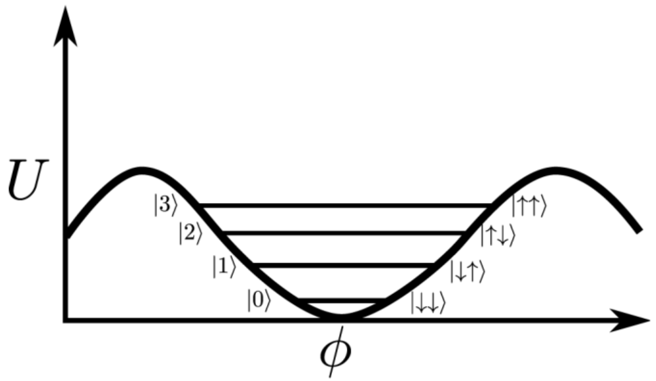
$$H_{\text{int}}^{\text{LO}} = V_{\text{OPE}} \left[1 - \delta_{R_0}(\vec{r})\right] + \left[C_0 + C_1 \vec{\sigma}^1 \cdot \vec{\sigma}^2\right] \delta_{R_0}(\vec{r})$$

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

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

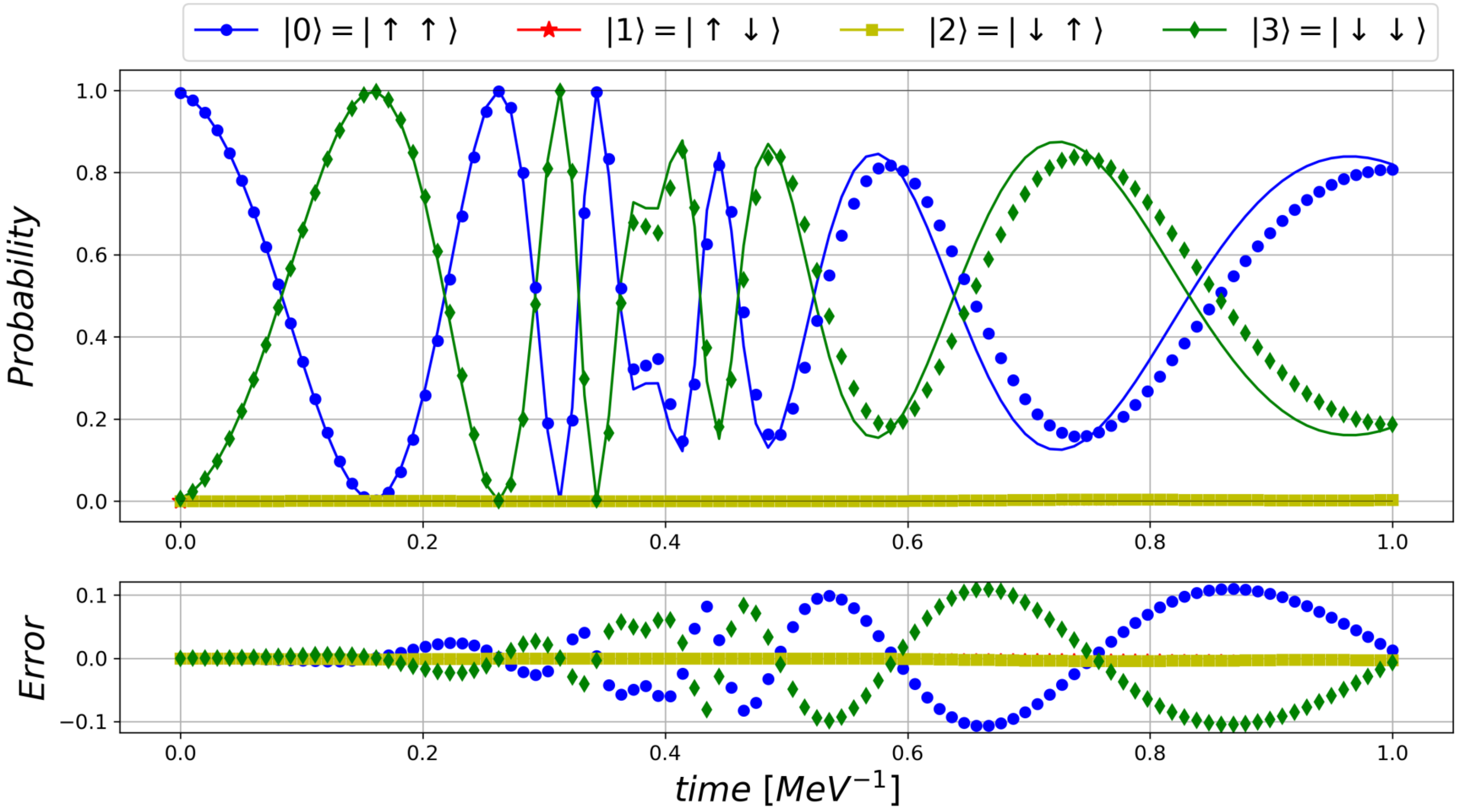
See e.g. J.E. Lynn et al. Phys. Rev. C 96, 054007 (2017)





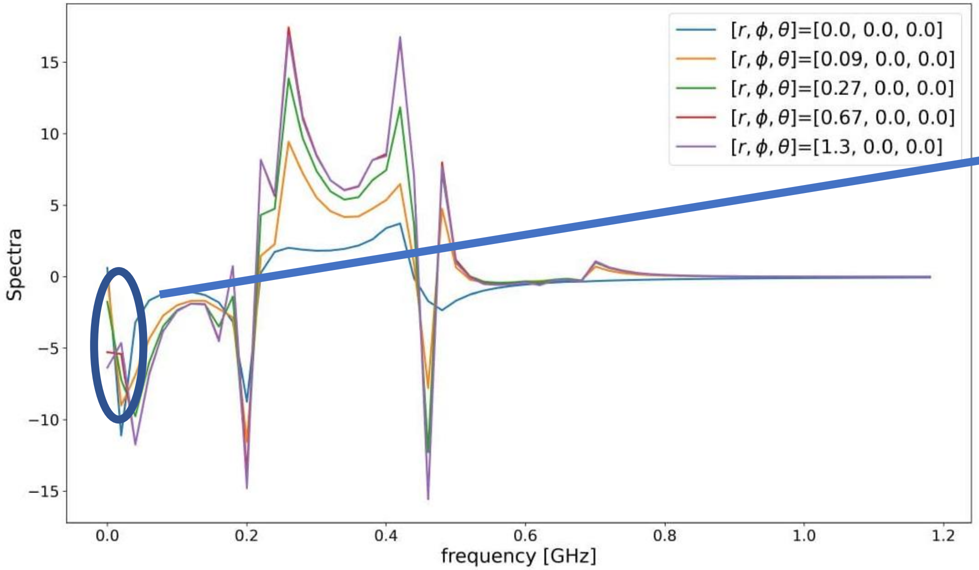
mapping

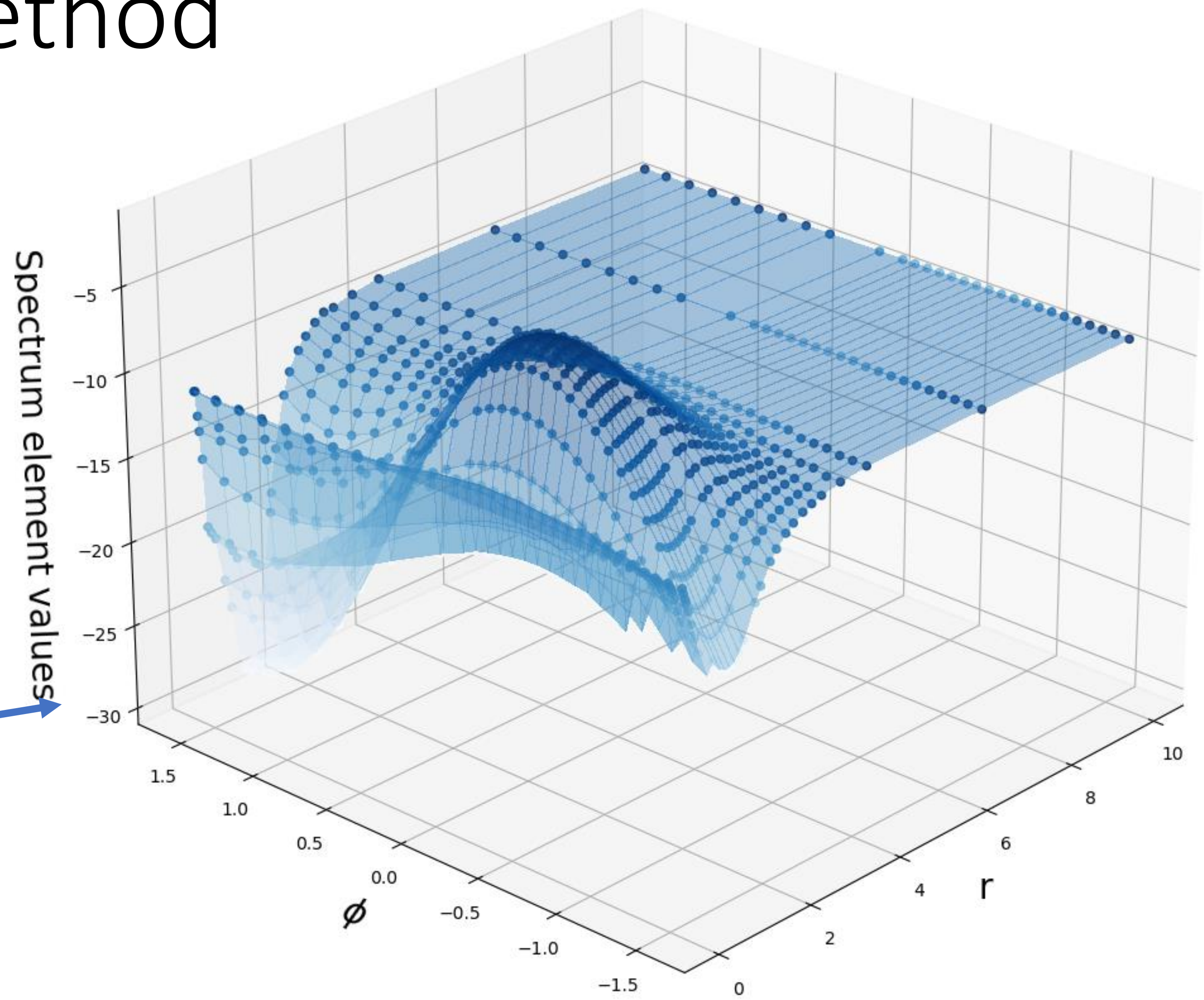
See: Holland, Eric T., et al. "Optimal control for the quantum simulation of nuclear dynamics." *Physical Review A* 101.6 (2020): 062307.


$|0\rangle = |\uparrow\ \uparrow\rangle$
$|1\rangle = |\uparrow\ \downarrow\rangle$
$|2\rangle = |\downarrow\ \uparrow\rangle$
$|3\rangle = |\downarrow\ \downarrow\rangle$
Probability
Error
time [MeV^{-1}]
1.0
0.8
0.6
0.4
0.2
0.0
0.1
0.0
−0.1
0.0
0.2
0.4
0.6
0.8
1.0

Fourier Transform method

- For each element of the spectrum we interpolate with cubic between r, phi and theta



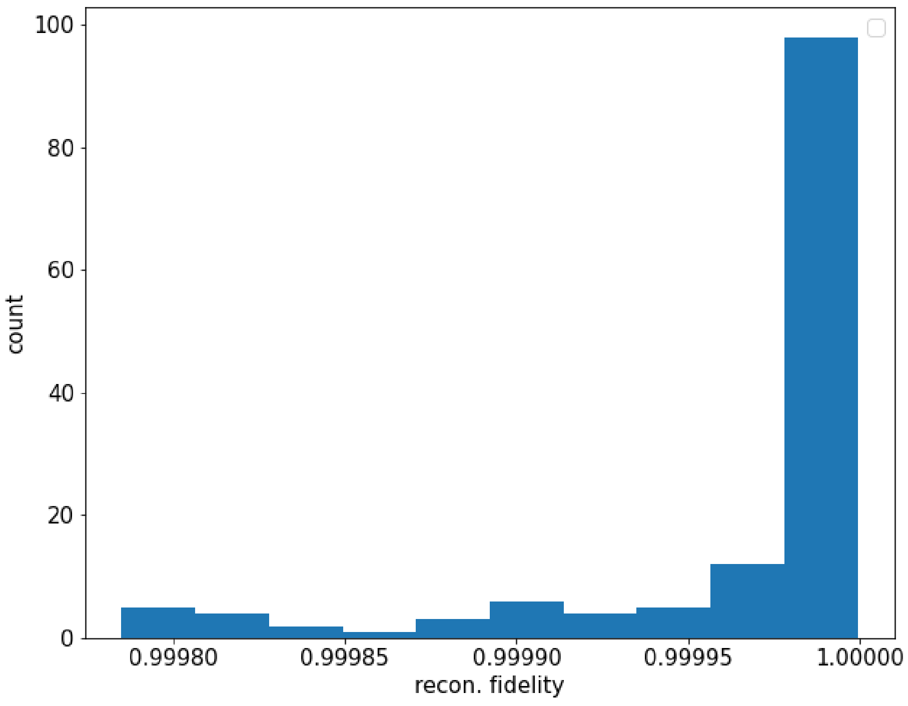


2D representation only with r and phi

Errors for Fourier transform method

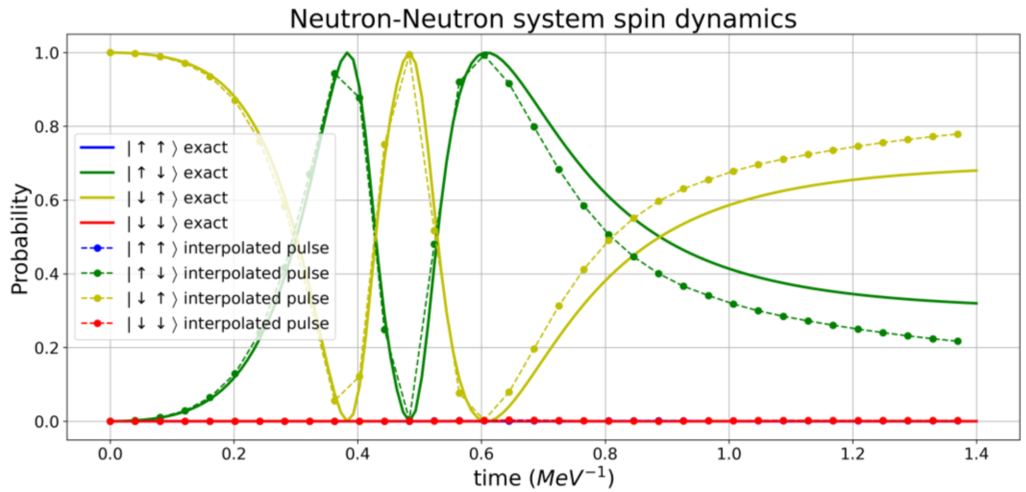
- **Fidelity** : metric to quantify the similarity between two matrices

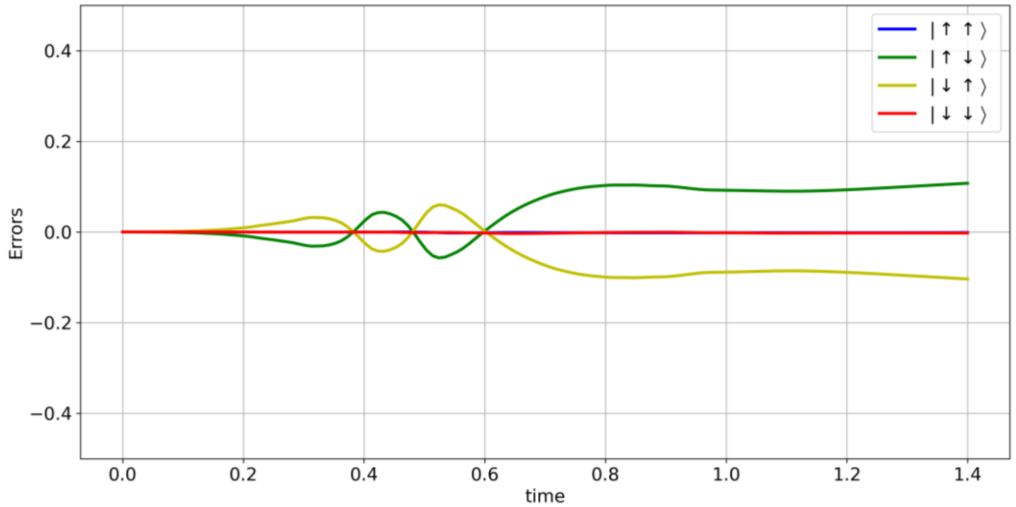
$$f(U_{recon}, U_{exact}) = \mathrm{Tr}\left(\sqrt{U_{recon}^{1/2} U_{exact} U_{recon}^{1/2}}\right)^2$$



Reconstruction fidelity

Accumulation of errors

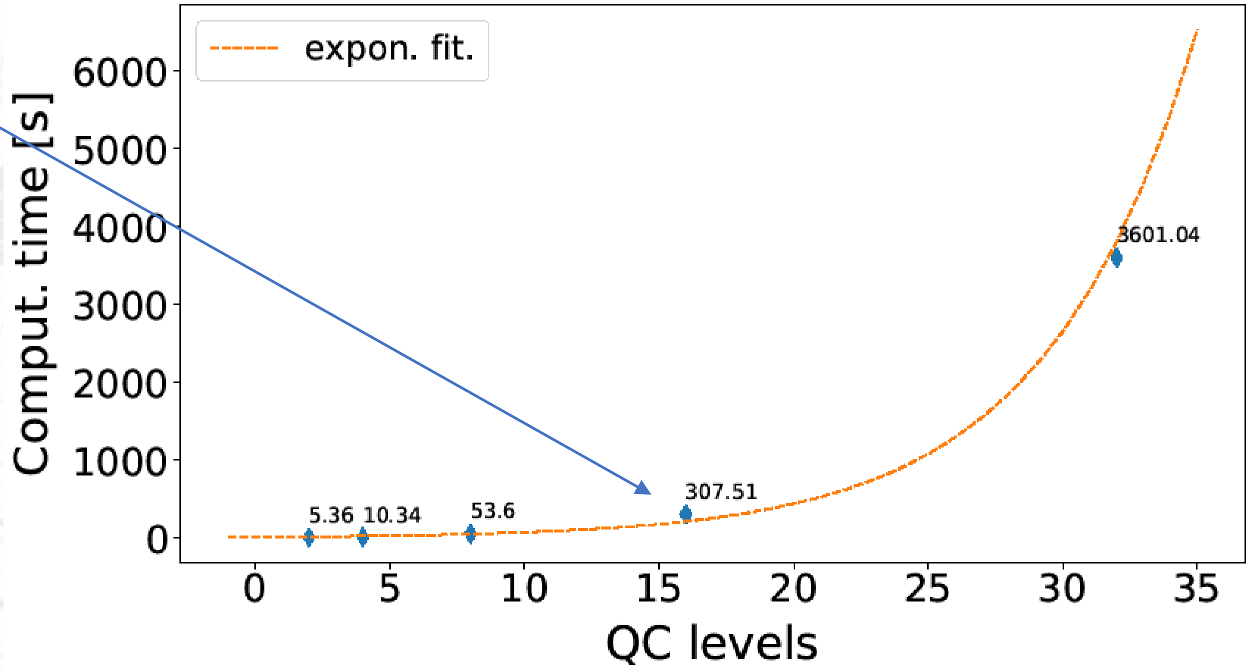




Controls Reconstructing Method

Fourier Transform Method

- Average time to obtain a single control:
  - Classical Optimization: [see table]
  - Reconstructing method: 800 ms
- The advantage of this method is high if the number of needed controls are grater than the set computed in advance.



Controls Reconstructing Method

Neural Network Method

- Test

$(r_{new}, \varphi_{new}, \theta_{new})$

U_{SD}