Nuclear Simulations on Quantum Computers with Optimal Control

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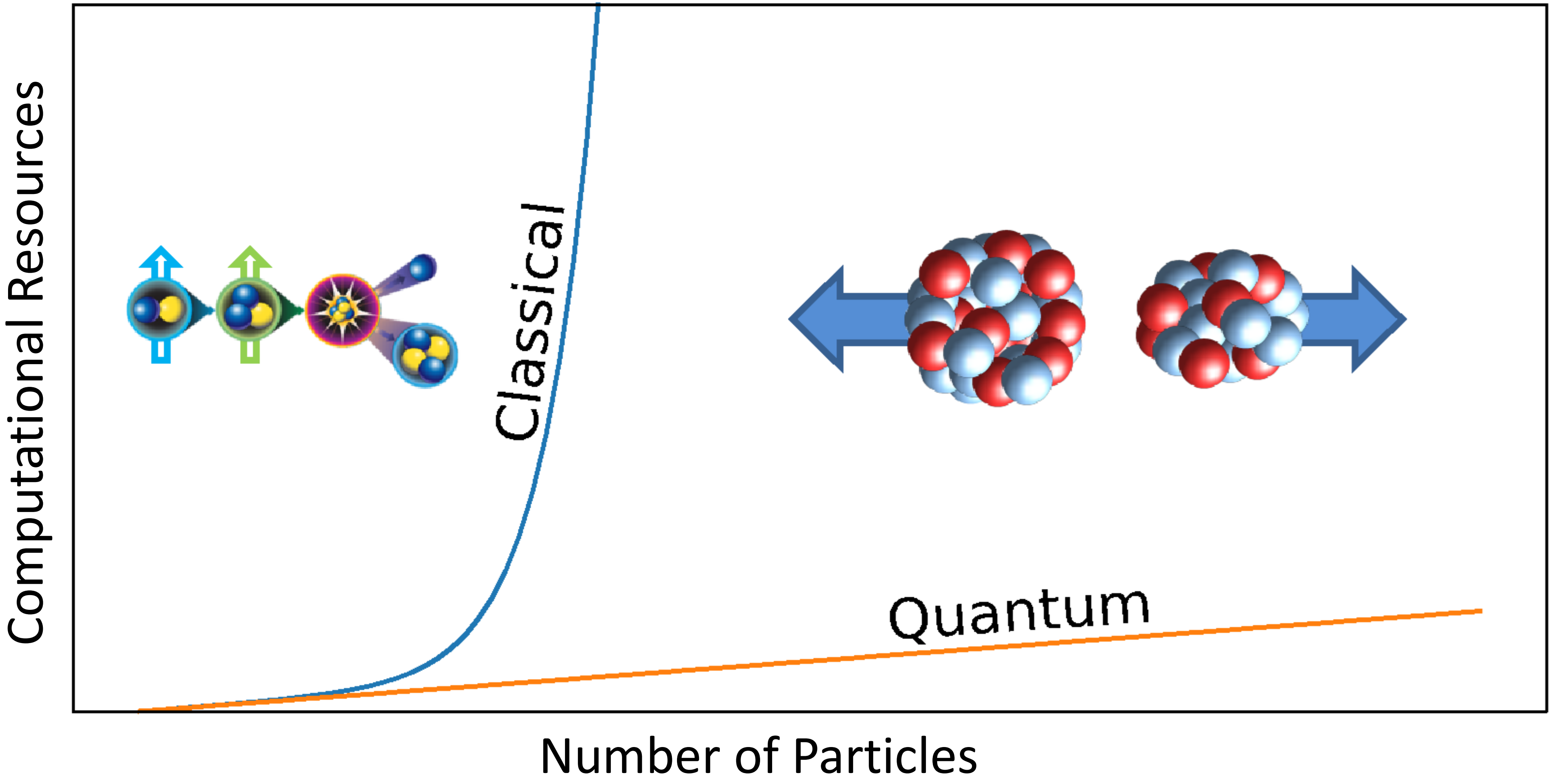
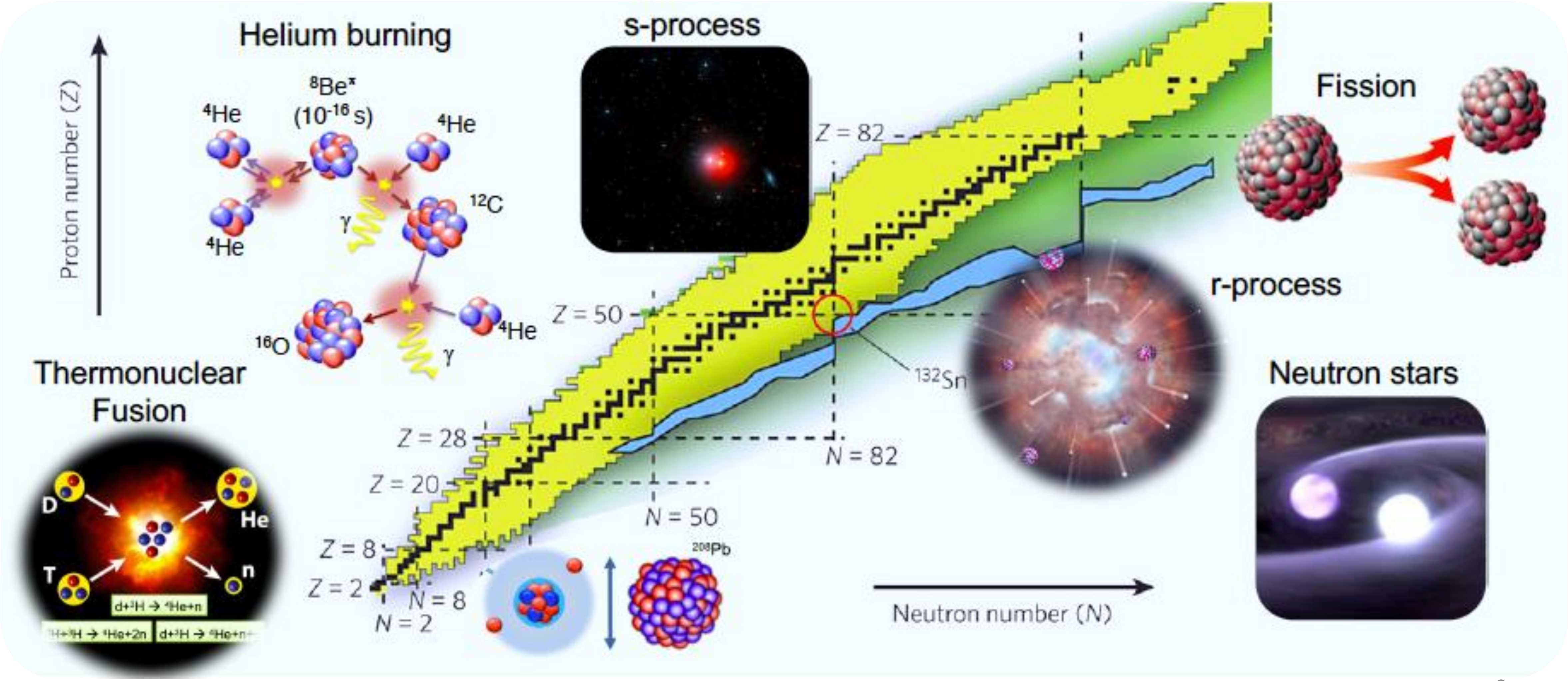
Quinto Incontro Nazionale di Fisica Nucleare INFN 2022

Computational effort: classical vs quantum

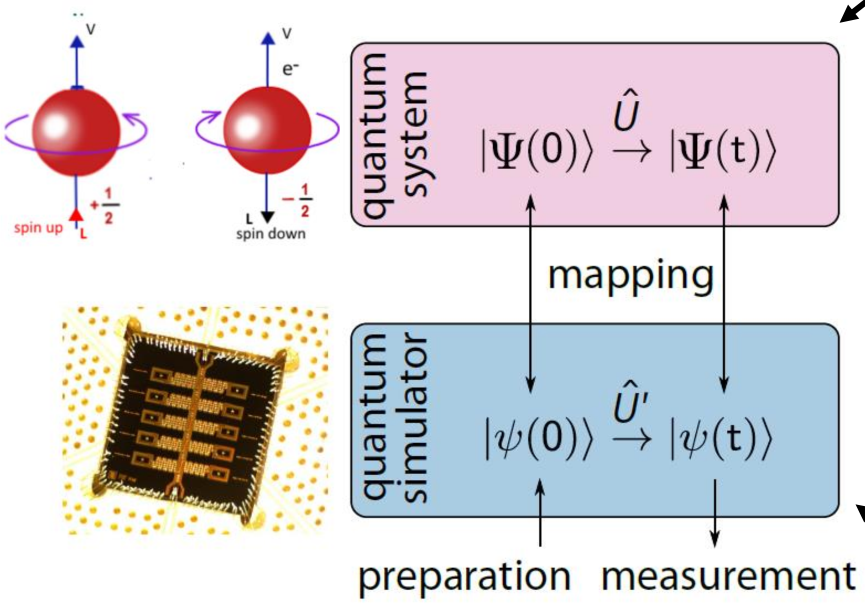


Goal: studying dynamical processes in nuclear systems

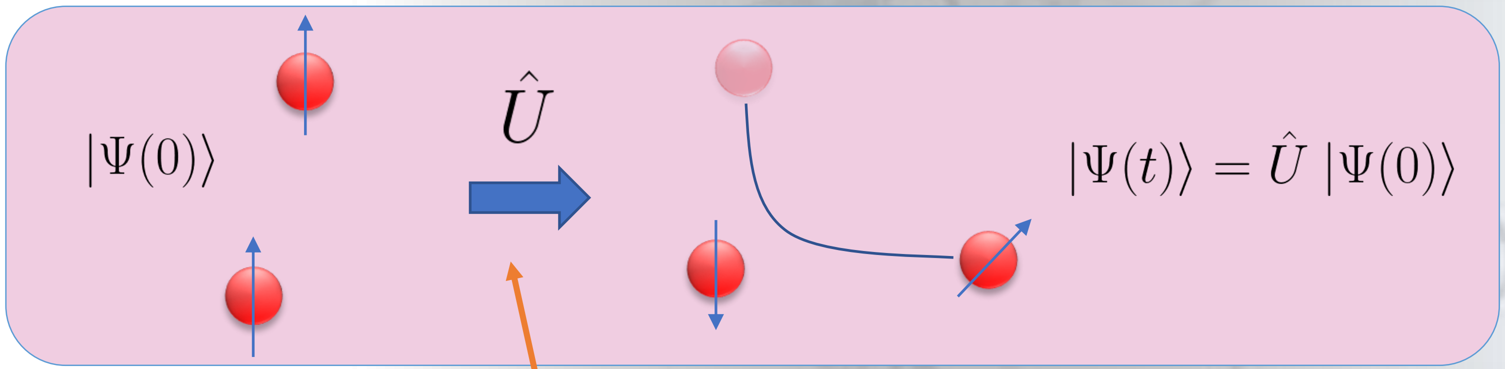


How does it works?

- Mapping

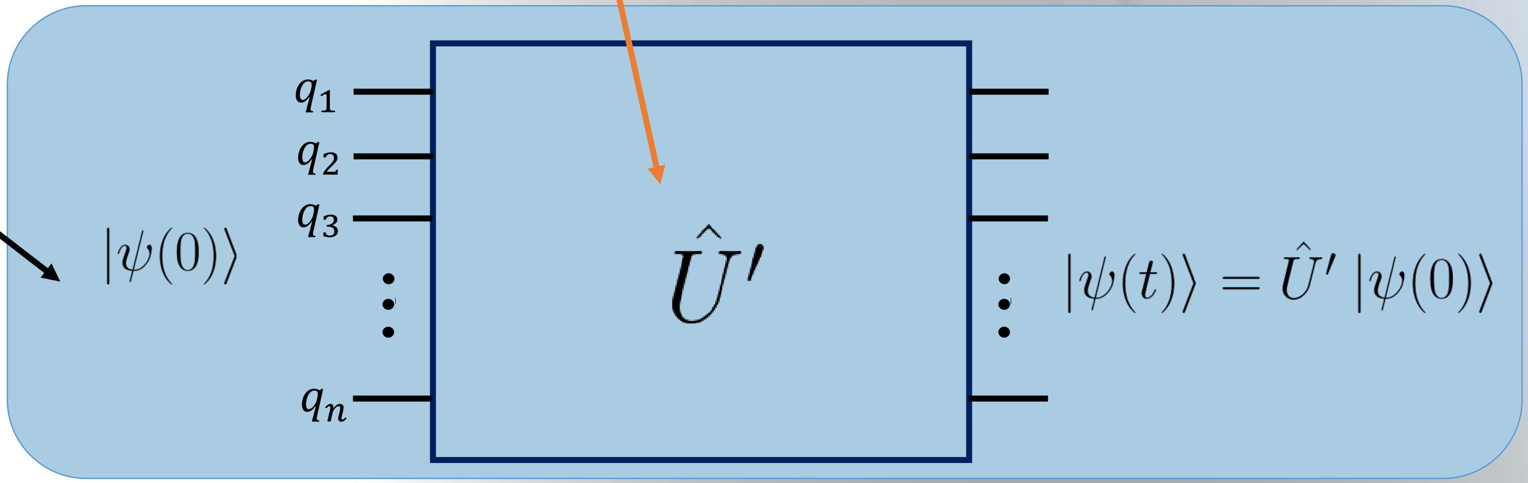


Real system: Not directly controllable



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

- Unitary transformation implementation



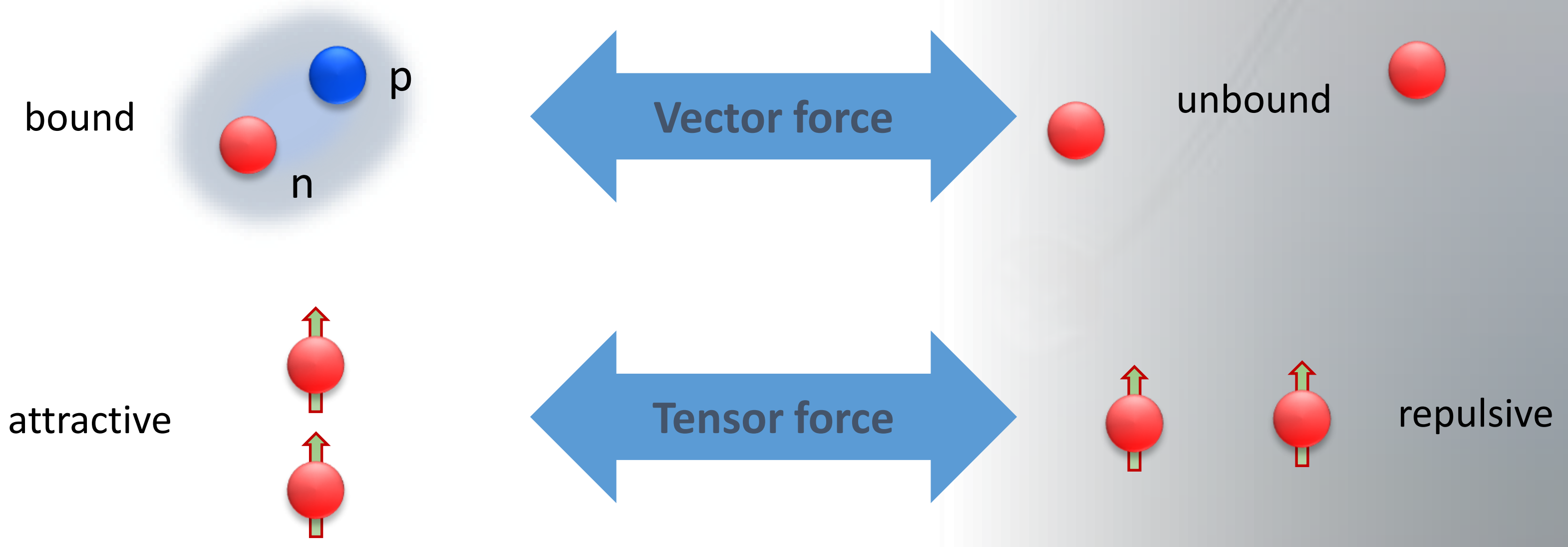
Quantum device: controllable and measurable

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

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

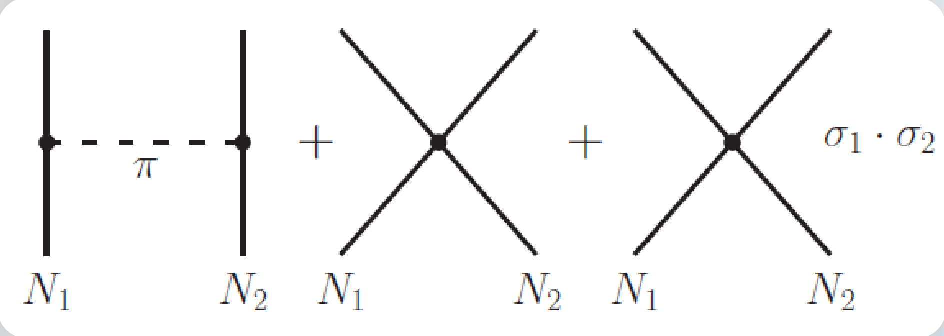
- Characteristic features of the nucleon-nucleon interaction are captured by the leading order (LO) in the EFT expansion.

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

- 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.

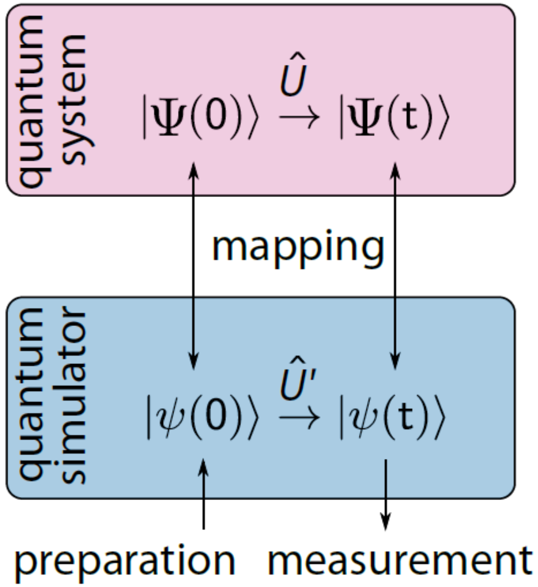
- **Quantum-classical coprocessing protocol**:

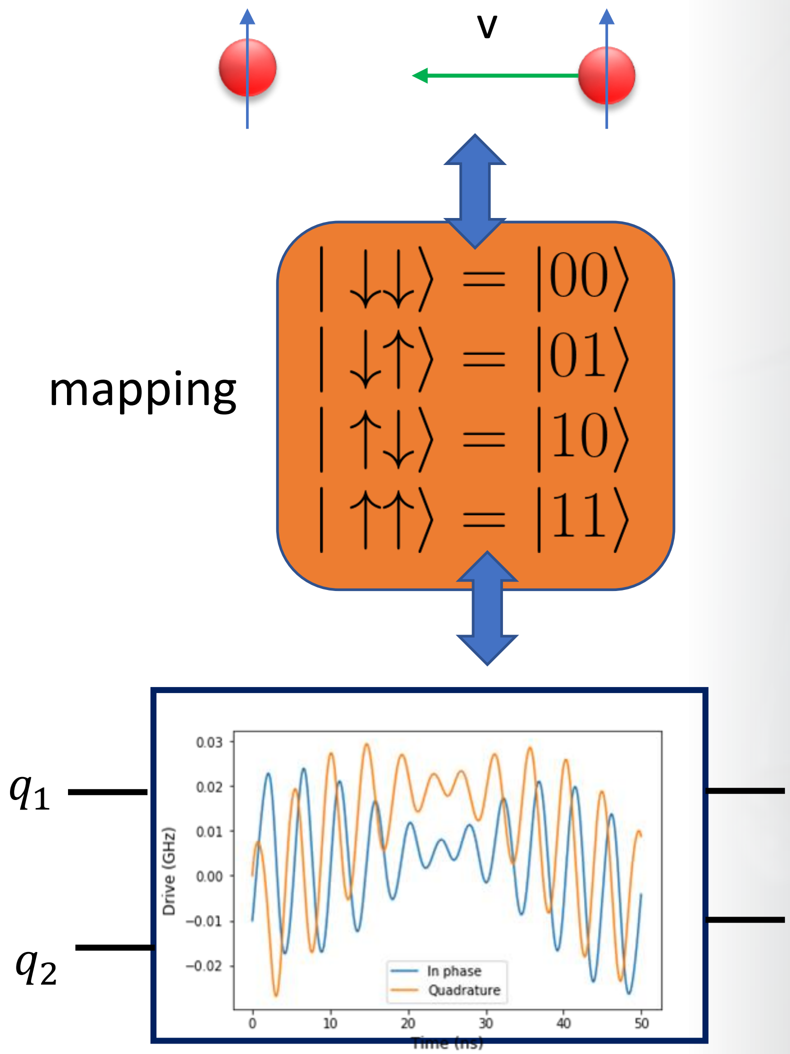
  For a small time step δt:

  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:



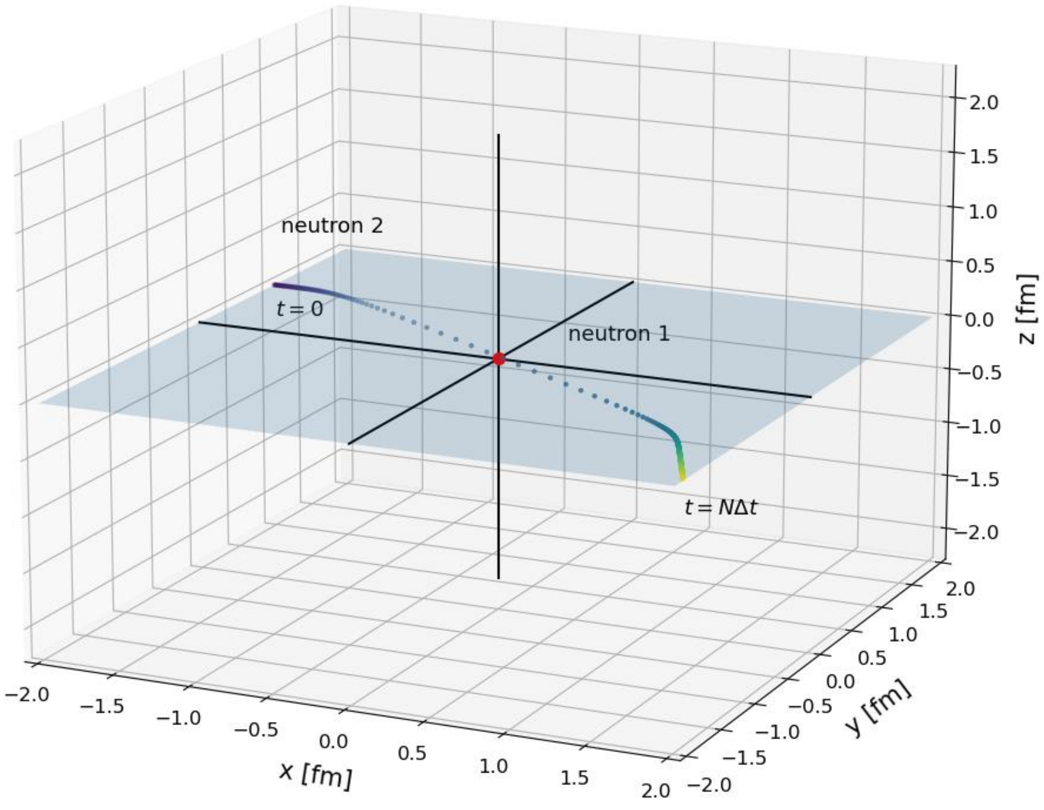


$$\hat{U}_{SD} = \exp\left[-\frac{i}{\hbar}\hat{V}_{SD}\delta t\right]$$

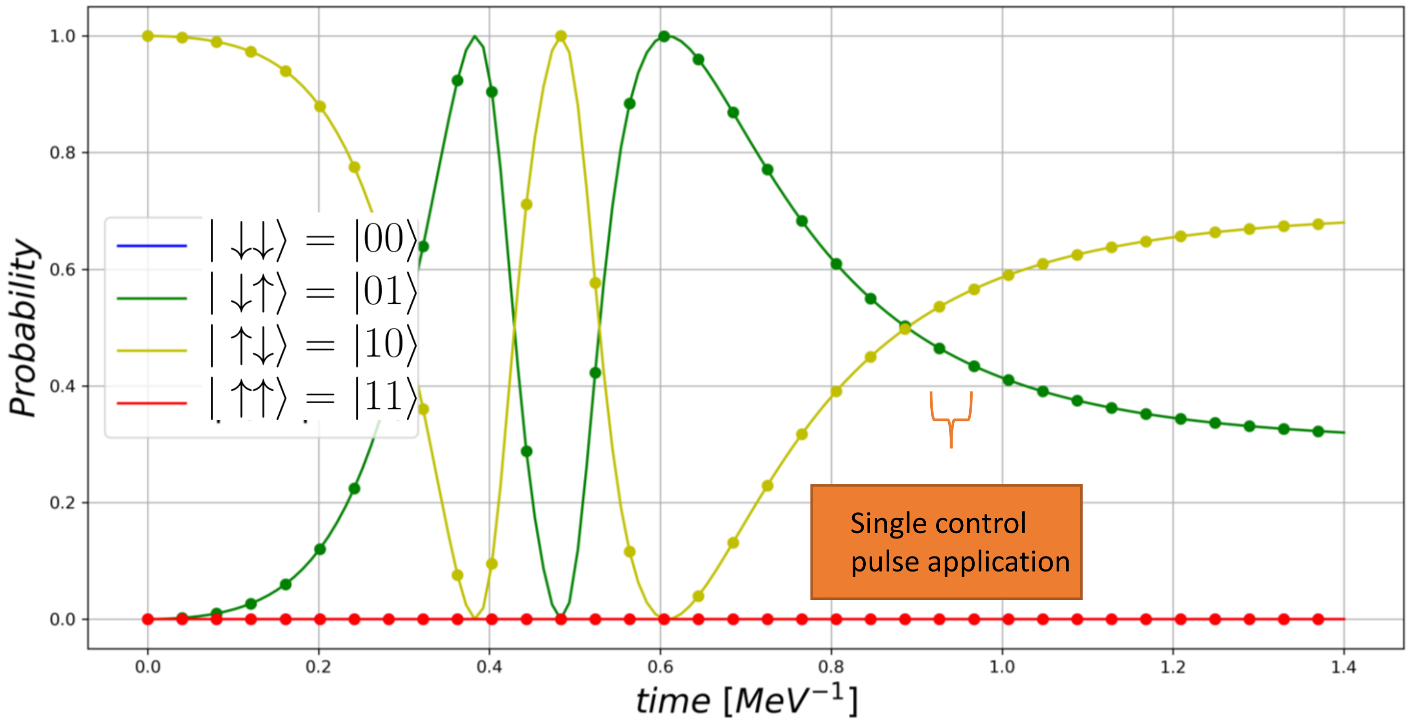
Implementation of unitary transformation

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

Example: Two neutrons dynamics:



Spatial Trajectory



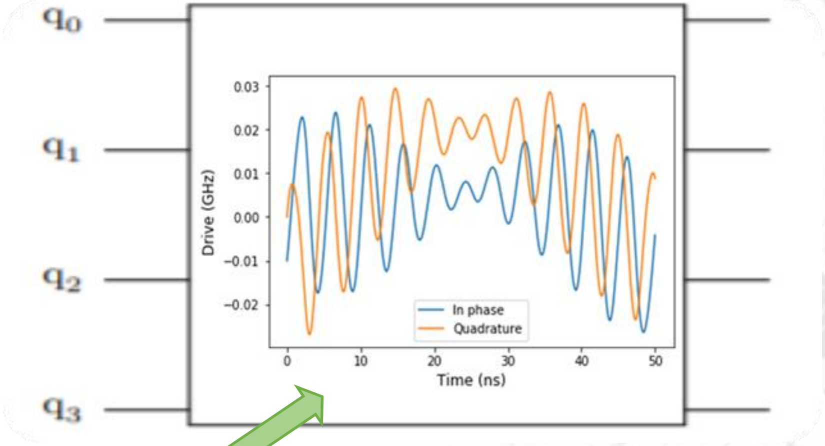
Spin dynamics: Occupation probability.
(Solid: exact dynamics
Points: dynamics obtained with application of the propagator.)

Quantum Control Interpolation

Quantum Gate Control Reconstruction

- Quantum gate optimization :

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



Controls optimization: bottle-neck of the analysis

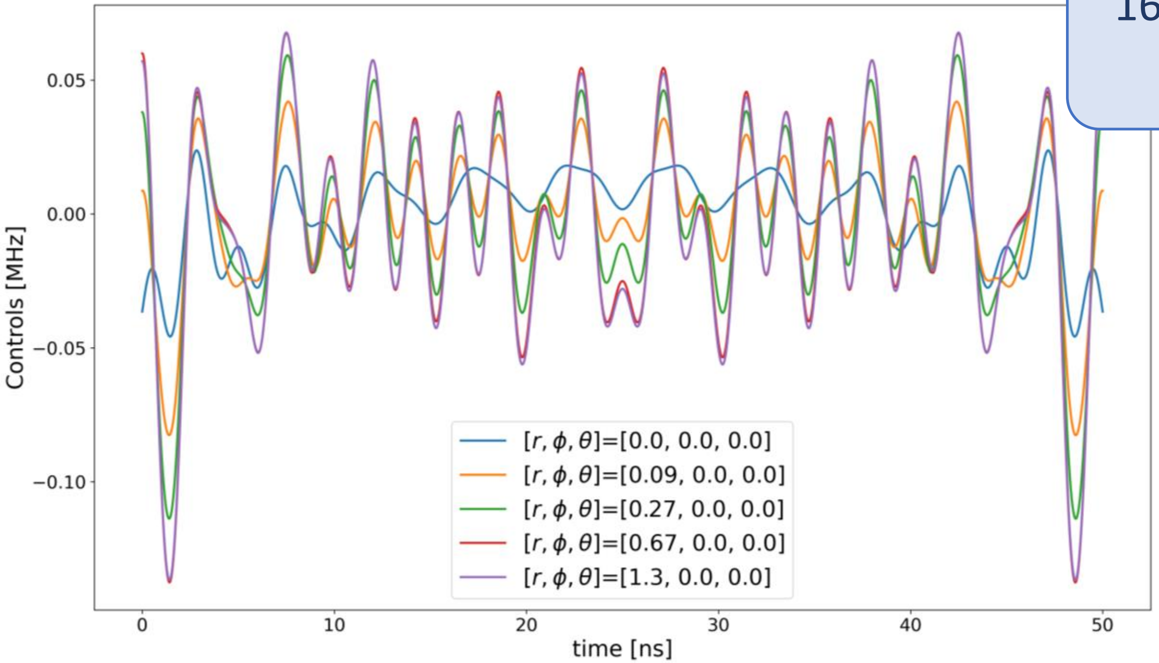
- Slow (especially for many qubits) → **Time consuming**
- The Hamiltonian could be dependent on parameters (e.g neutrons relative position) that change during the simulation → **Need to calculate the controls at every time-step**

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).

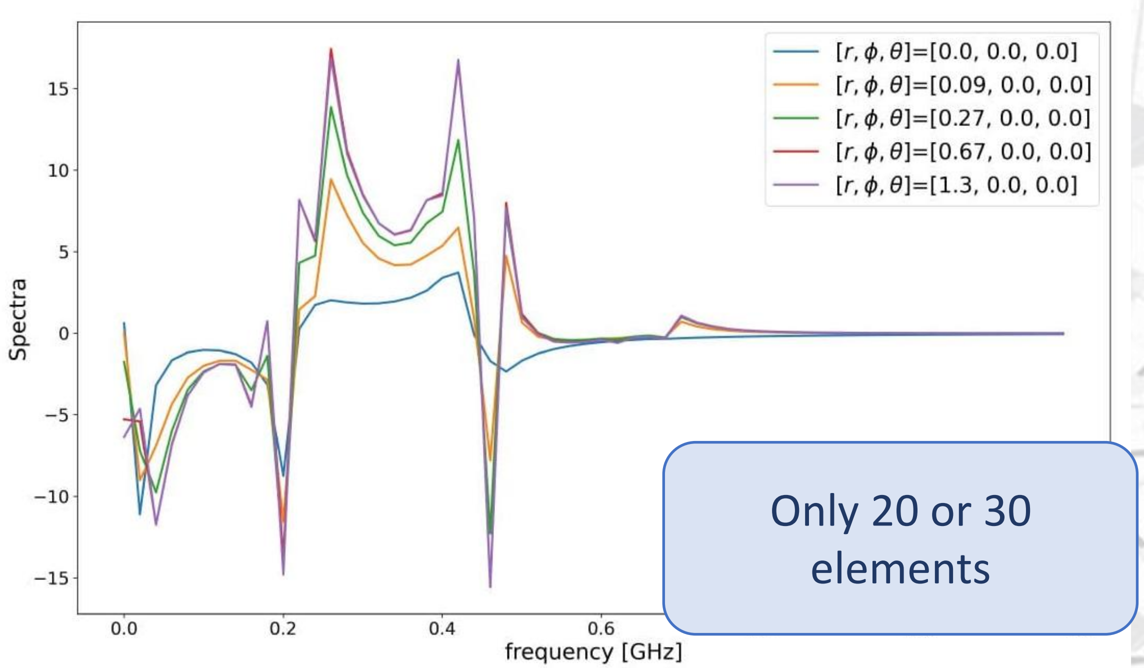
Fourier Transform Method



1600 time-steps for each control

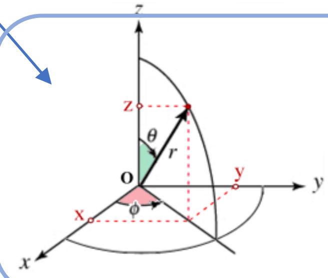
Fourier transform

Corresponding set of spectra



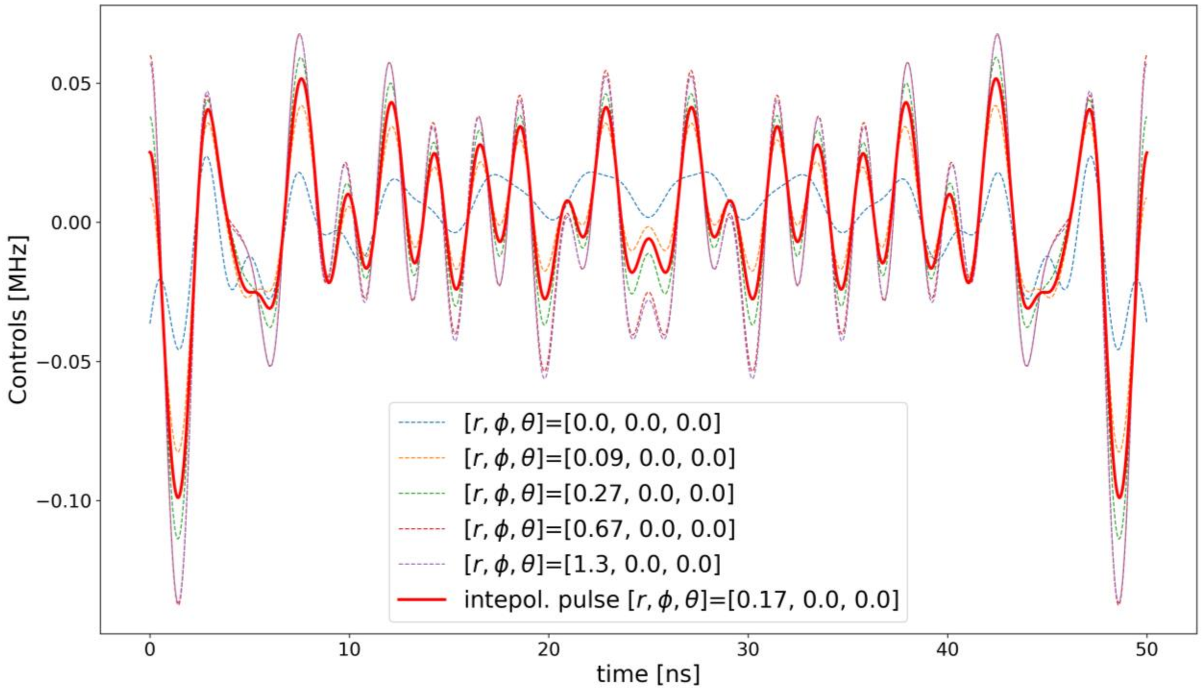
Only 20 or 30 elements

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

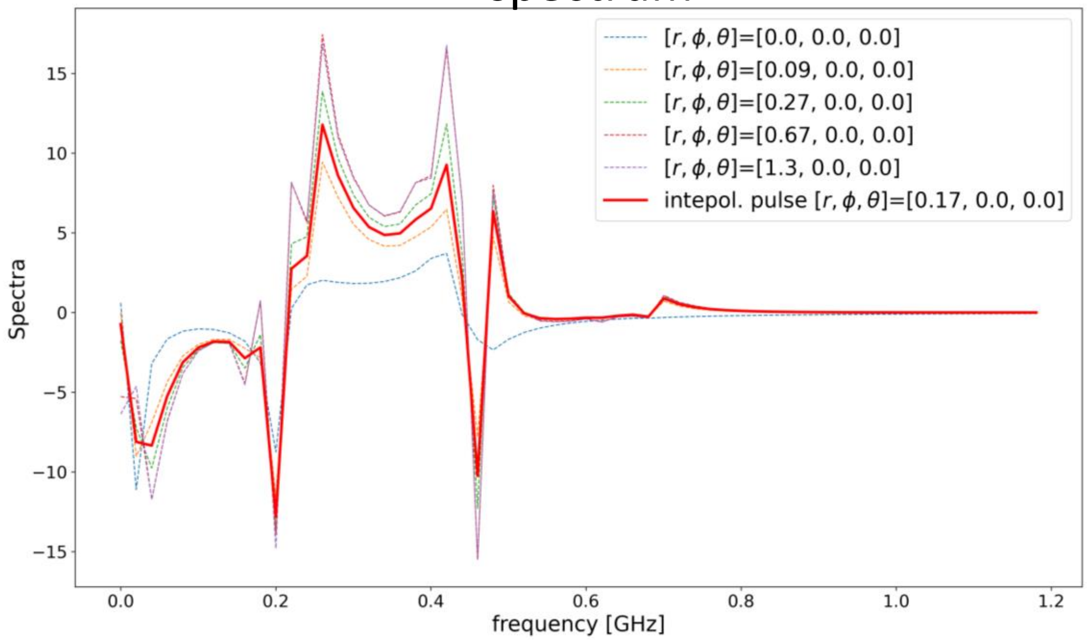
Controls Reconstructing Method
Fourier Transform Method



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

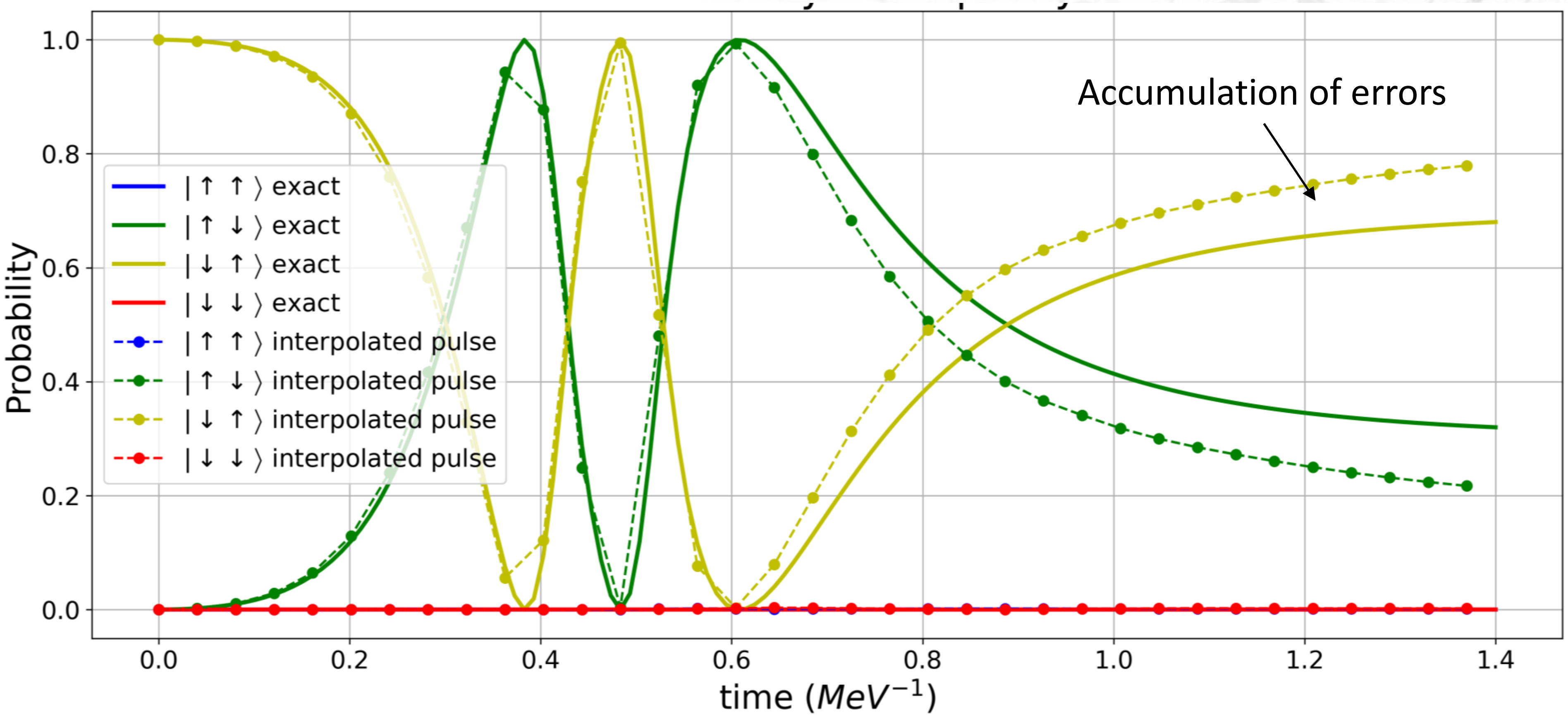


<u>After the computation of a (possibly small) set of controls in advance, we can obtain an infinite number of them at a low computational cost</u>

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

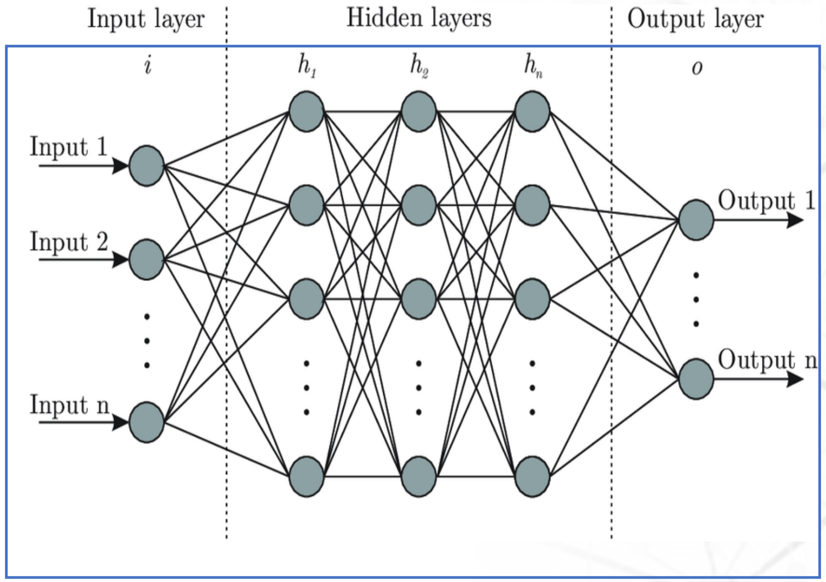
Neural Network Method

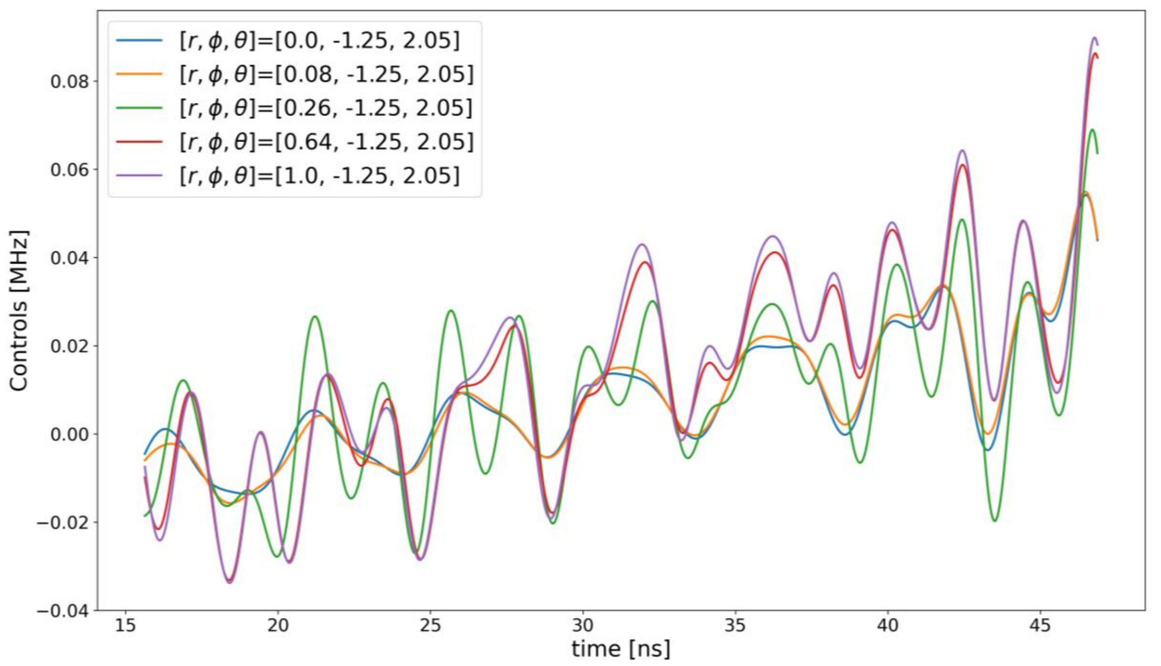
- Train

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

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

$$U_{SD}$$

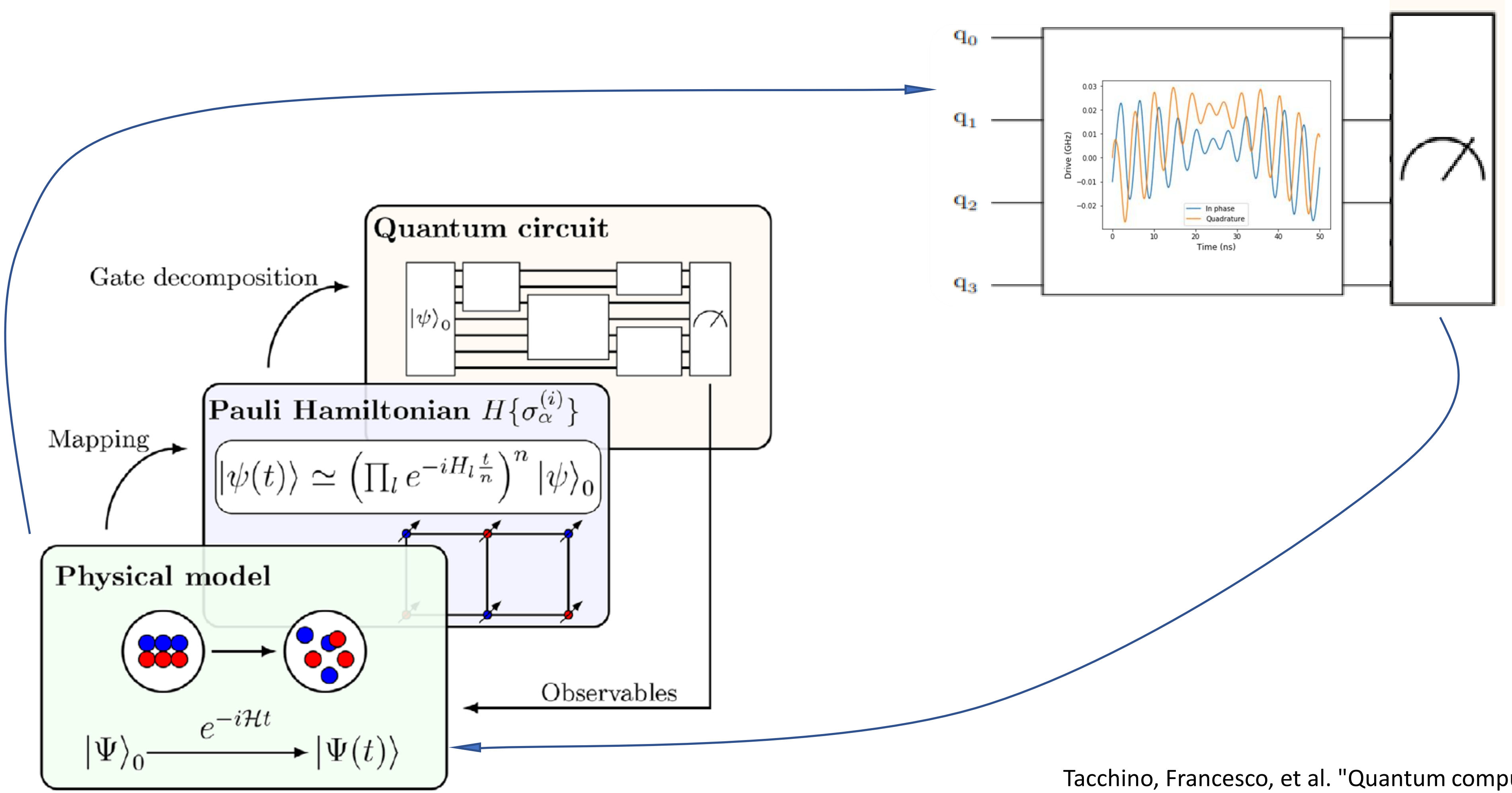




$$U_{SD} = \exp\left[-\frac{i}{\hbar}\hat{V}_{SD}\delta t\right] = \exp\left[-\frac{i}{\hbar}\left(\sum_{i,j=1}^{A}\sum_{\alpha,\beta=x,y,z}\sigma_{i\alpha}A(r_{ij})_{ij;\alpha\beta}\sigma_{j\beta}\right)\delta t\right]$$

Quantum Gates

(Differences between QG approaches)

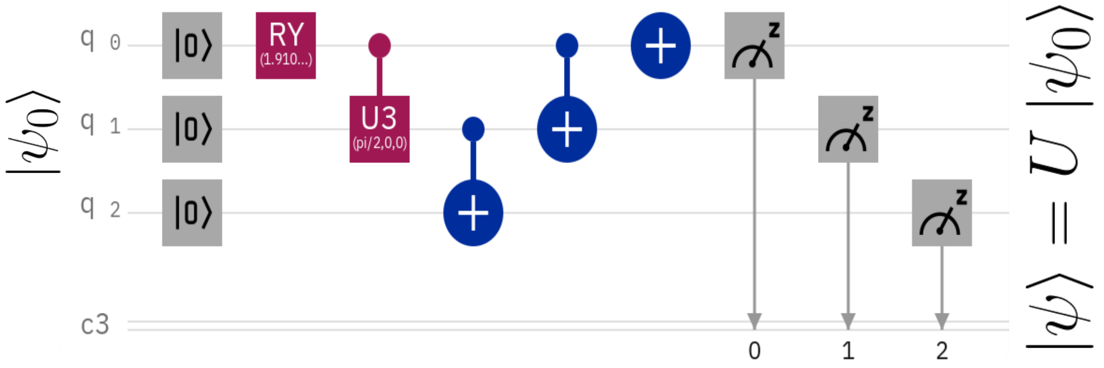


Tacchino, Francesco, et al. "Quantum computers as universal quantum Simulators: state-of-the-art and perspectives." *Advanced Quantum Technologies* 3.3 (2020): 1900052.

Quantum Gates
(Differences between QG approaches)

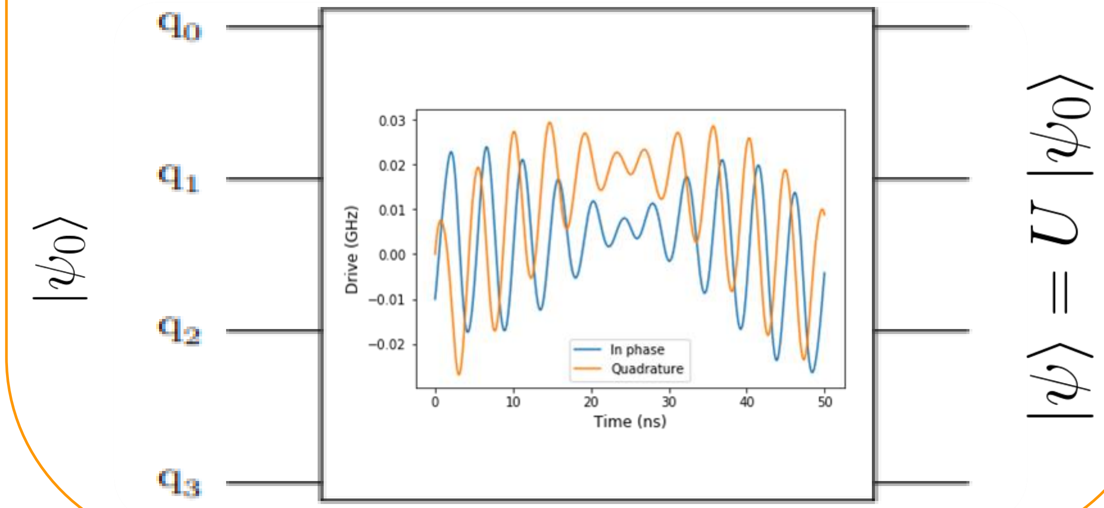
Standard (discrete gate sets)

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



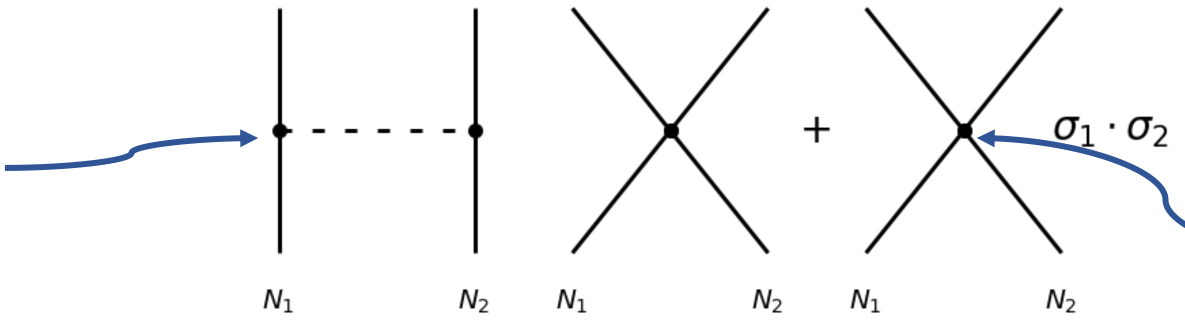
Optimal control-based

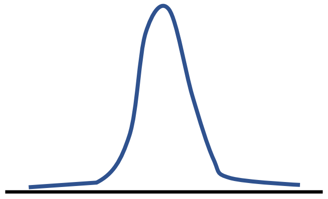
- Software reconfigurable, continuous unitary transformation (gate)
- Many-body dynamics to be simulated implemented with a single gate
- Microwave pulse to control the qubit



Example: Local chiral EFT potential at leading order

One-pion exchange (OPE)





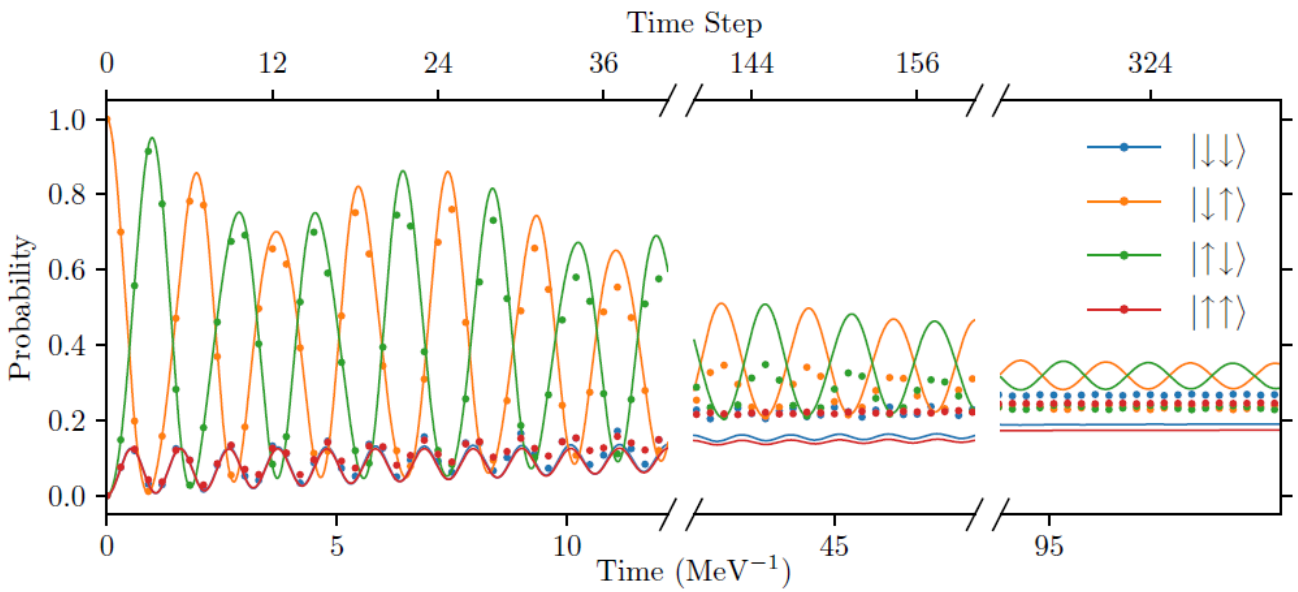
Regularized contact (cutoff in momentum)

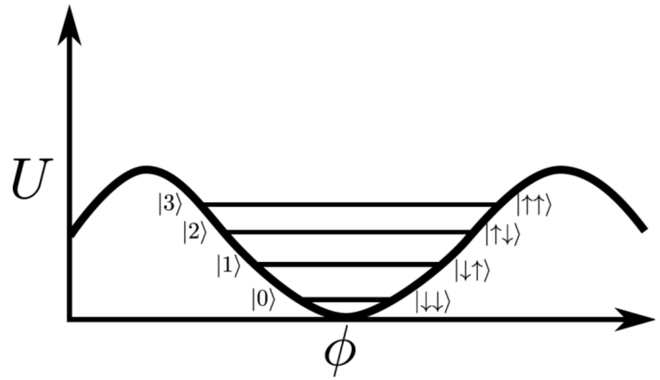
$$H_{\rm int}^{\rm LO} = V_{\rm OPE}\left[1 - \delta_{R_0}(\vec{r})\right] + \left[C_0 + C_1\, \vec{\sigma}^1 \cdot \vec{\sigma}^2\right] \delta_{R_0}(\vec{r})$$

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

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

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



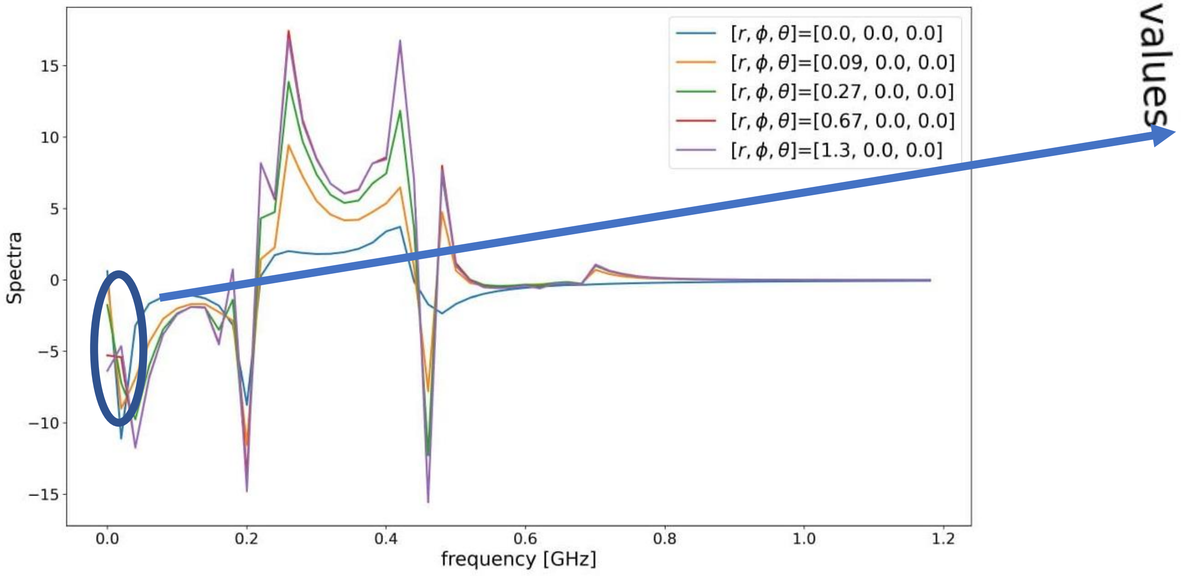


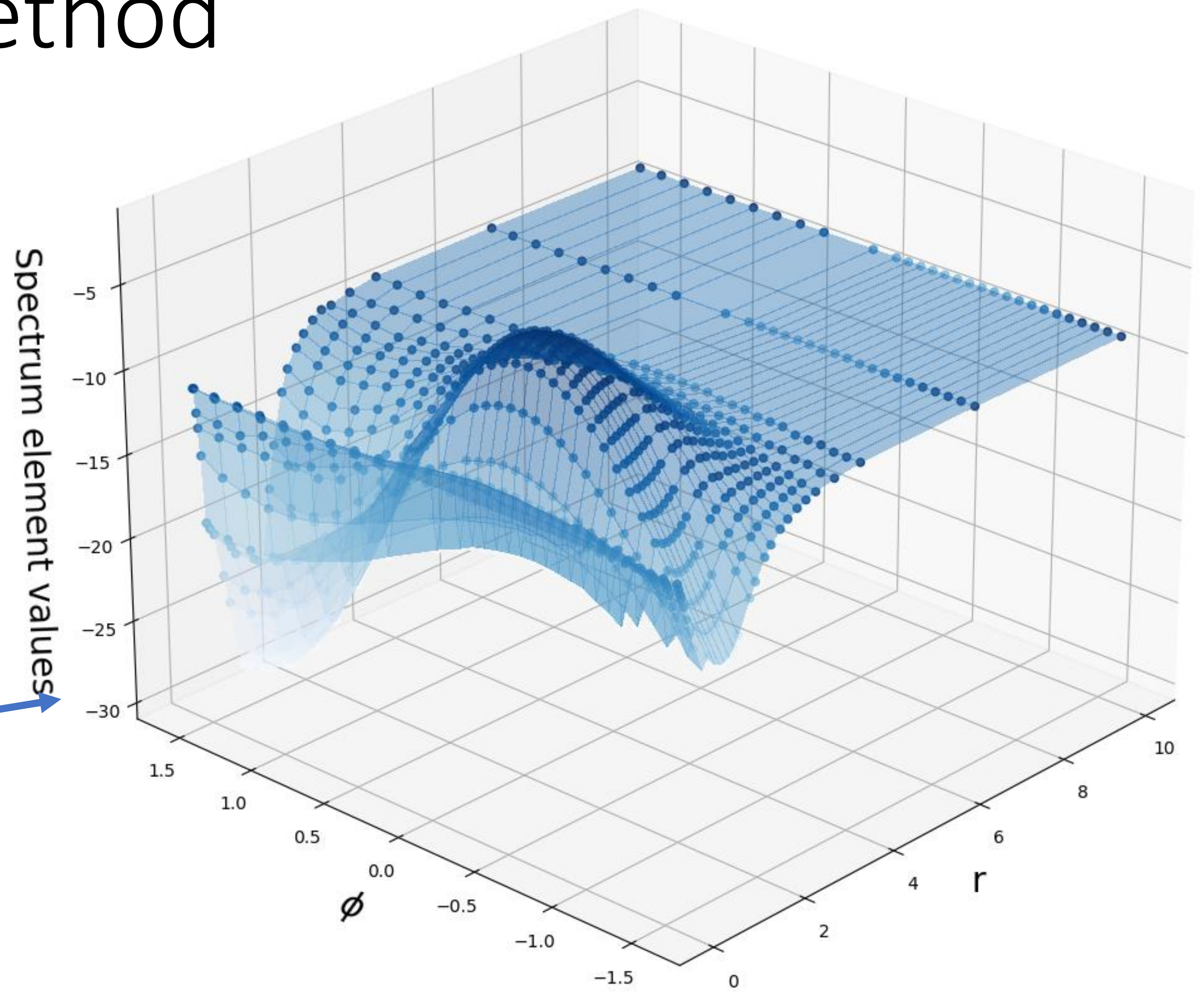
mapping

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

Fourier Transform method

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



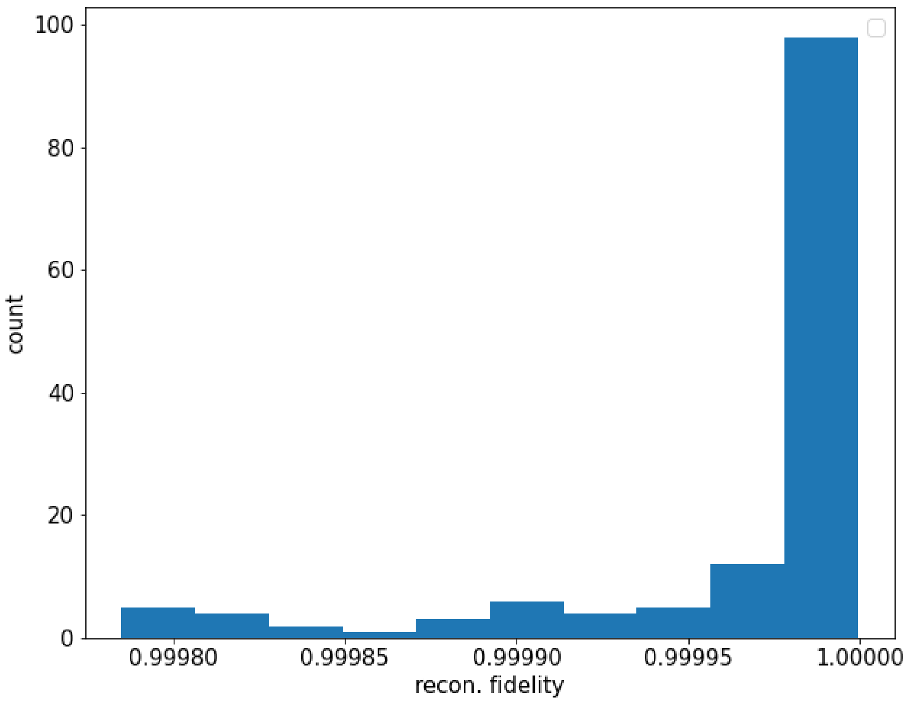


2D representation only with r and phi

Errors for Fourier transform method

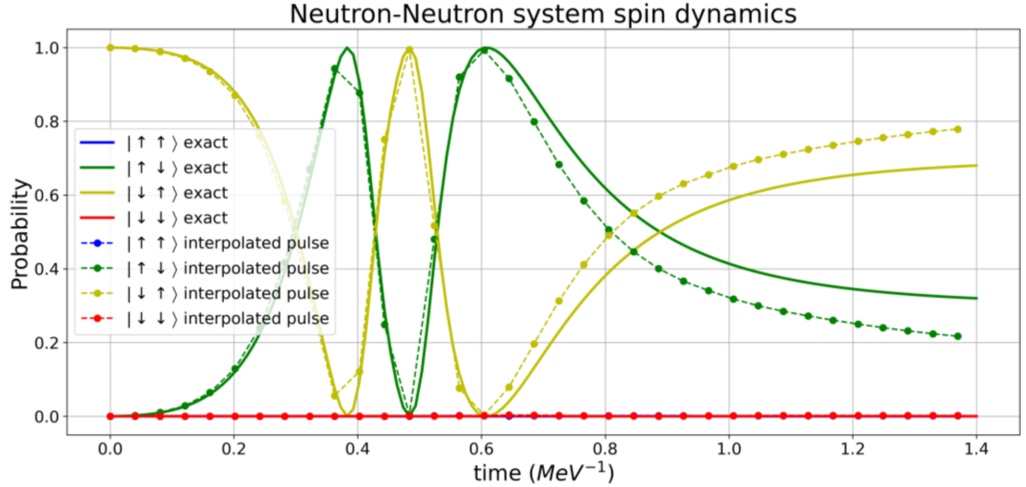
- **Fidelity** : metric to quantify the similarity between two matrices

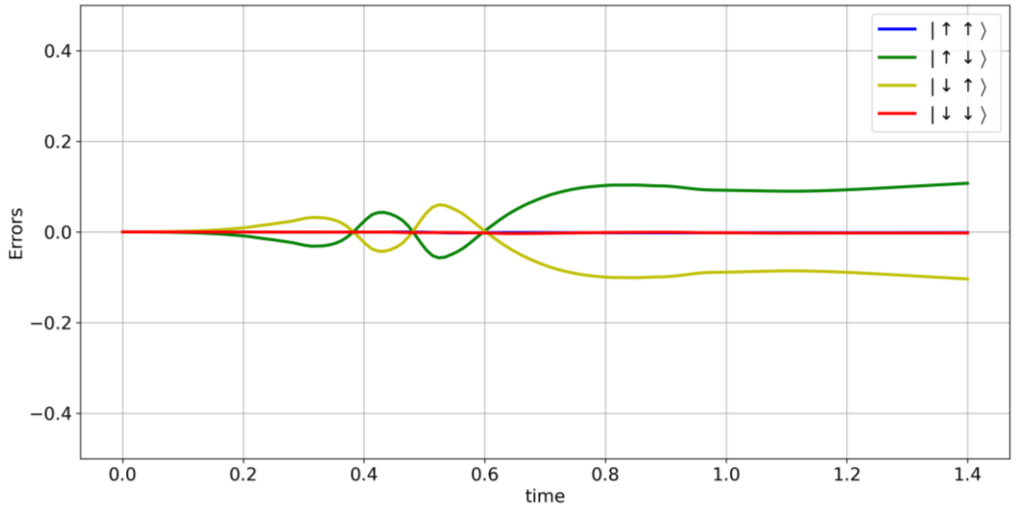
$$f(U_{recon}, U_{exact}) = \mathrm{Tr}\left(\sqrt{U_{recon}^{1/2} U_{exact} U_{recon}^{1/2}}\right)^2$$



Reconstruction fidelity

Accumulation of errors

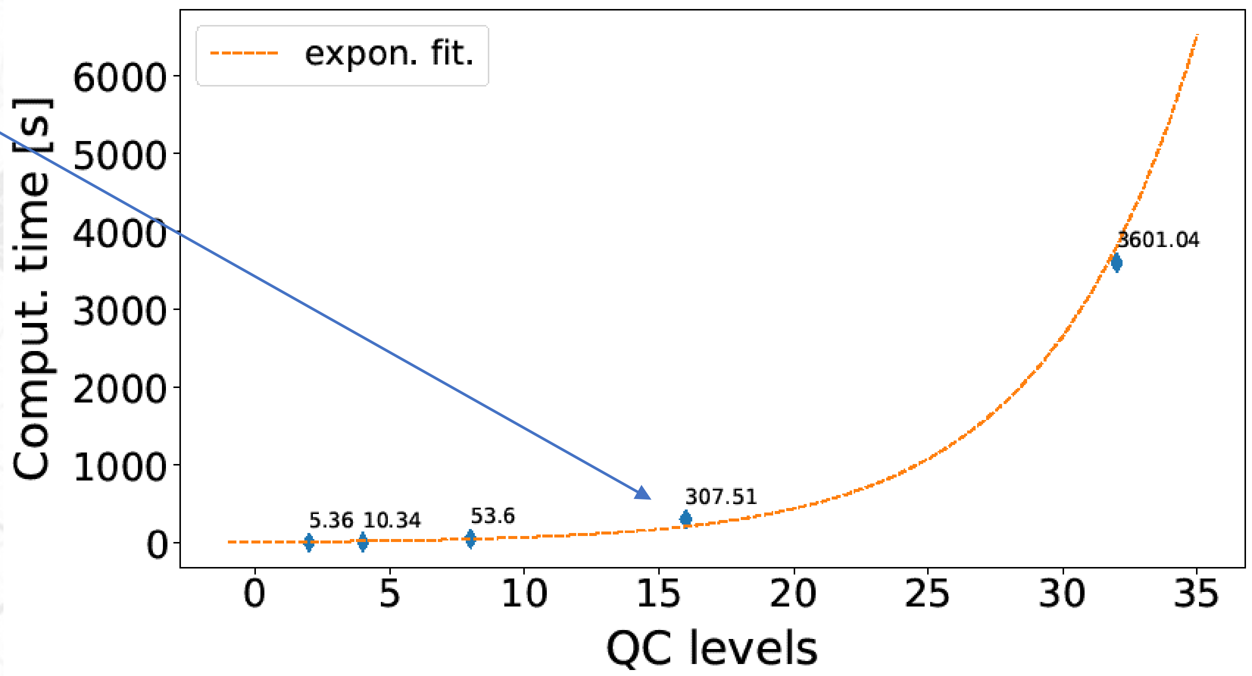




Controls Reconstructing Method

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}