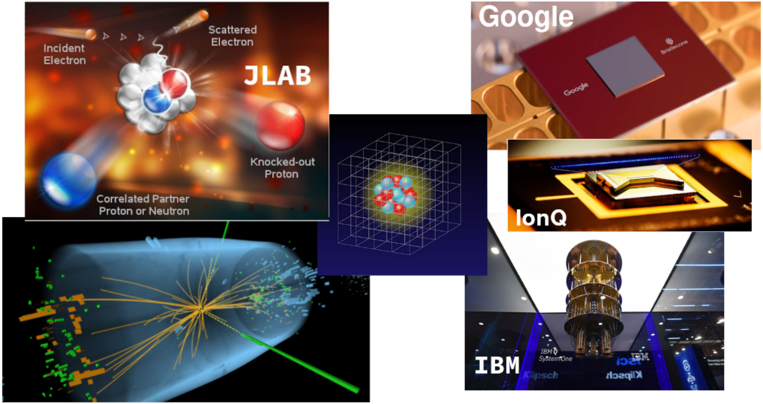
Nuclear Reactions on a Quantum Computer

Alessandro Roggero



TIFPA
Trento Institute for
Fundamental Physics
and Applications

DTP/TALENT School

ECT* – 3 July, 2025

UNIVERSITAS ATHESINA STUDIORUM

The need for ab-initio many-body dynamics in NP

- ν scattering for supernovae explosion and NS cooling
- capture reactions for crust heating and nucleosynthesis
- cross sections for dark-matter discovery and neutrino physics
- transport properties of neutron star matter for X-ray emission

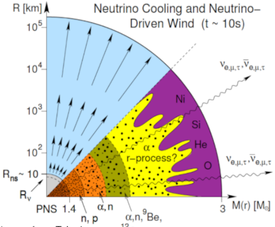
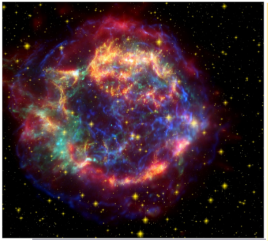


image from T.Janka



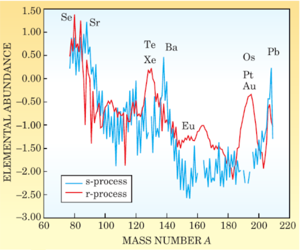
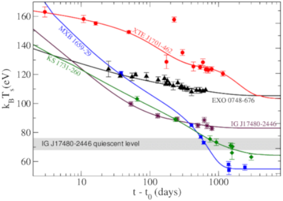


image from Cowan & Thielemann (2004)



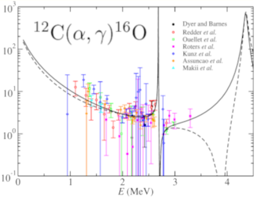
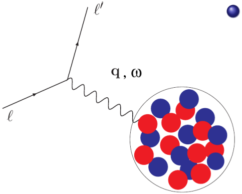


image from Brune & Davis (2015)

Inclusive cross section and the response function



- xsection completely determined by response function

$$R_O(\omega) = \sum_f \left| \langle f | \hat{O} | \Psi_0 \rangle \right|^2 \delta \left(\omega - E_f + E_0 \right)$$

  - excitation operator $\hat{O}$ specifies the vertex

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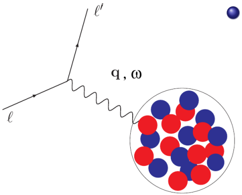

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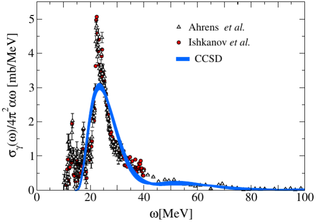
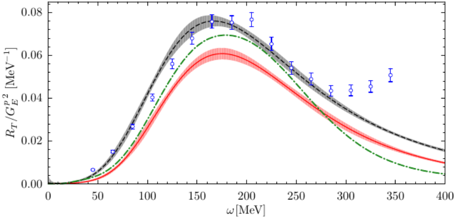
Extremely challenging classically for strongly correlated quantum systems

- dipole response of ^{16}O



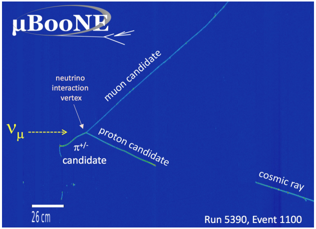
Bacca et al. (2013) LIT+CC

- quasi-elastic EM response of ^{12}C



Lovato et al. (2016) GFMC

Exclusive cross sections in neutrino oscillation experiments



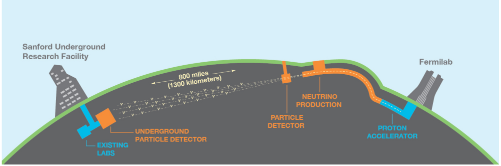
Goals for ν oscillation exp.

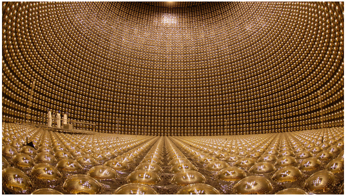
- neutrino masses
- accurate mixing angles
- CP violating phase

$$P(\nu_\alpha \to \nu_\alpha) = 1 - sin^2(2\theta) sin^2\left(\frac{\Delta m^2 L}{4E_\nu}\right)$$

- need to use measured reaction products to constrain E_ν of the event

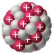
DUNE, MiniBooNE, T2K, Minerνa, NOνA,. . .





Idealized algorithm for exclusive processes at fixed q

- prepare the target ground state



Roggero & Carlson (2019)

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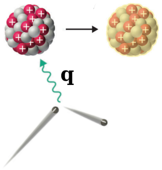
- right after scattering vertex the target is left in excited state



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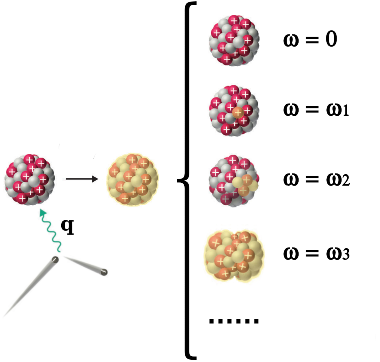

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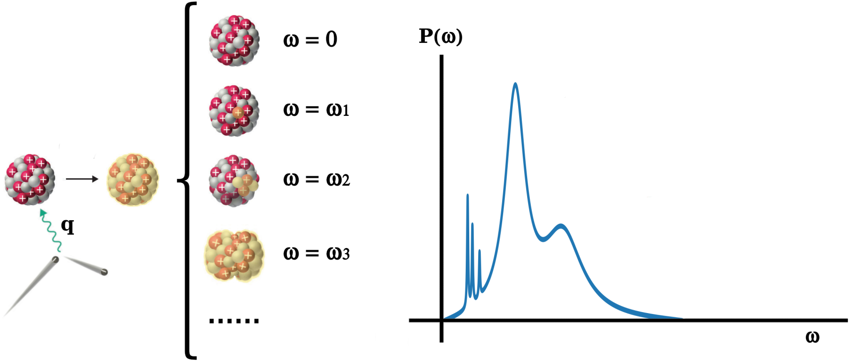

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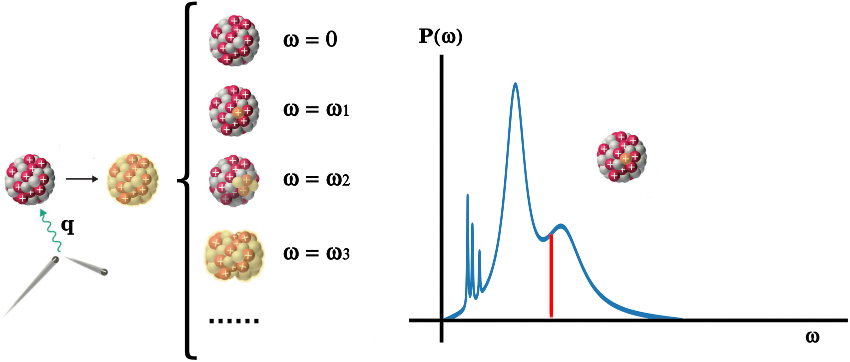

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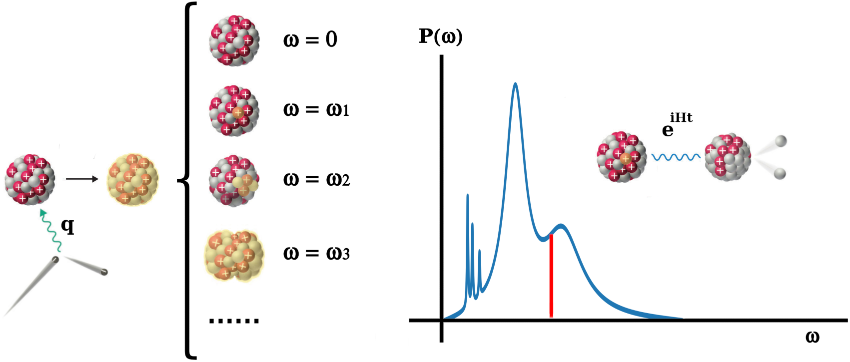

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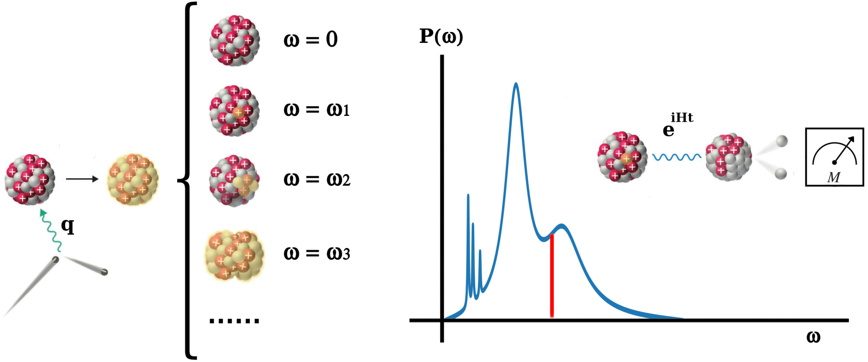

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Quantum algorithm for exclusive processes at fixed q

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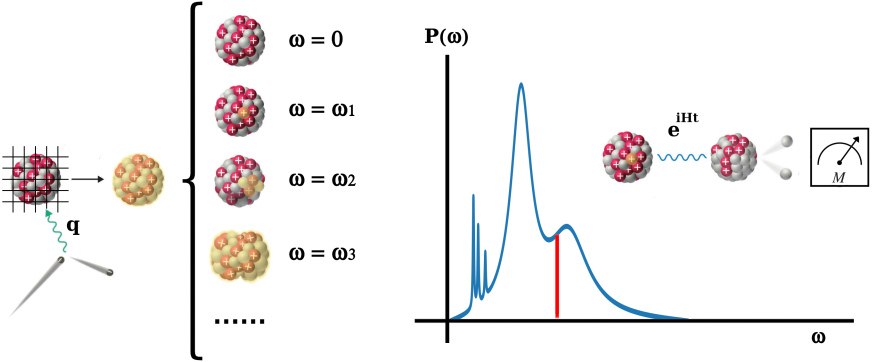

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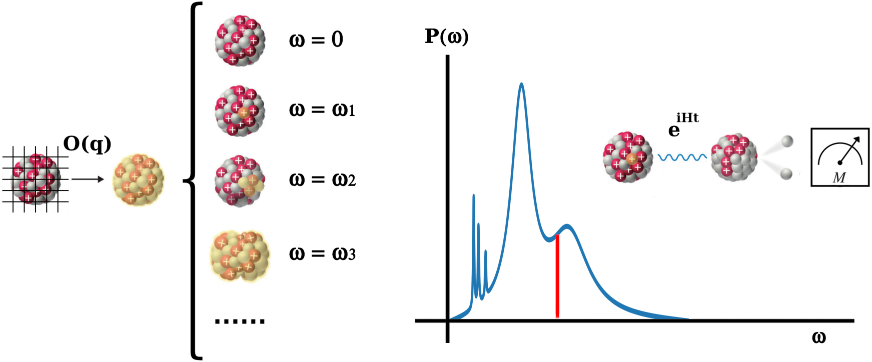
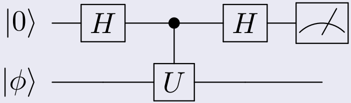


Roggero & Carlson (2019)

Can we apply a non-unitary operation?

YES, but only with some probability

- this can be useful when excitation operator is not unitary



$$\Rightarrow \quad |0\rangle \otimes \frac{\mathbb{1}+U}{2}|\phi\rangle + |1\rangle \otimes \frac{\mathbb{1}-U}{2}|\phi\rangle$$

- we will measure $|0\rangle$ with $P_0 = \frac{1}{2}\left(1 + \mathcal{R}\langle\phi|U|\phi\rangle\right) \Rightarrow |\phi_0\rangle = \dfrac{\mathbb{1}+U}{2\sqrt{P_0}}|\phi\rangle$

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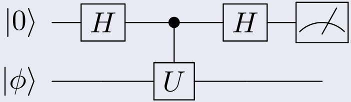

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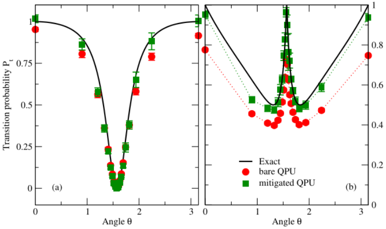
- generalization to many U possible
- tested on IBM devices for $np \to d\gamma$
  - simple $M1$ transition $^1S_0 \to ^3S_1$
  - 2 qubits for $|\phi\rangle$, 3 for controls

AR, C.Gu, A.Baroni, T.Papenbrock (2020)



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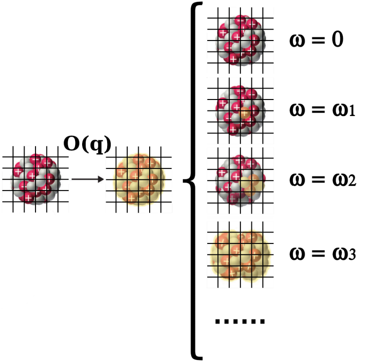

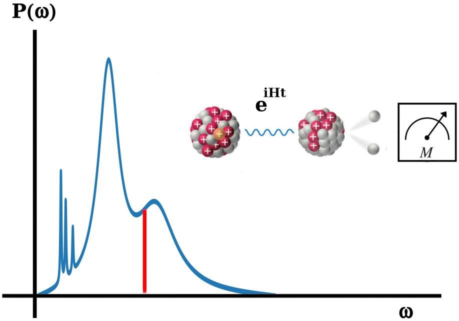

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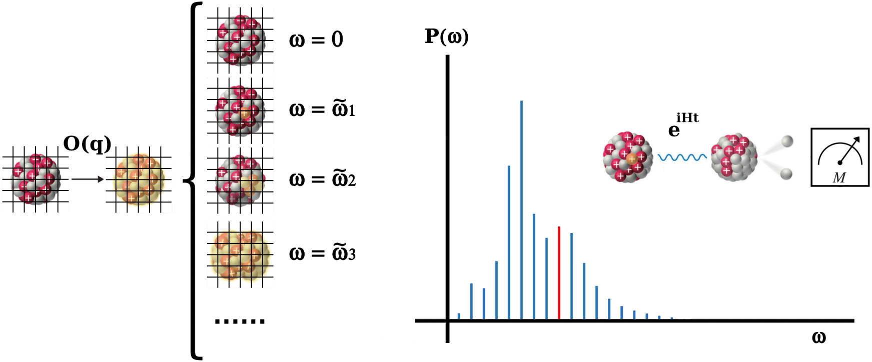
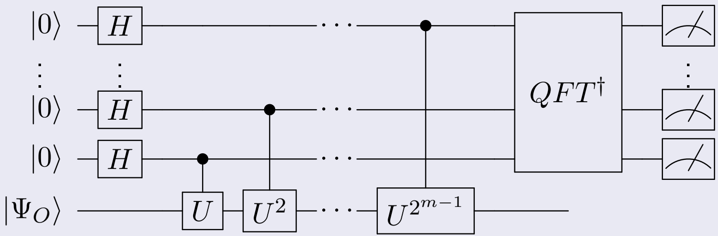


Roggero & Carlson (2019)

QPE on general states



If we start with the excited state $|\Psi_O\rangle = \sum_j c_j^O |\phi_j\rangle$ we find

$$|\Phi_3\rangle = \sum_j c_j^O \sum_{q=0}^{2^m-1} \left(\frac{1}{2^m} \sum_{k=0}^{2^m-1} \exp\left(i\frac{2\pi k}{2^m} \left(2^m \phi_j - q\right)\right)\right) |q\rangle \otimes |\phi_j\rangle$$

The new probability becomes approximately S_O with resolution $\Delta\omega \approx 1/M$

$$P(q) = \frac{1}{M^2} \sum_j \left|c_j^O\right|^2 \frac{\sin^2\left(M\pi(\phi_j - q/M)\right)}{\sin^2\left(\pi(\phi_j - q/M)\right)} \approx S_O\left(\omega = \frac{q}{M}\right)$$

Approximate response function with QPE

If we start with the excited state $|\Psi_O\rangle = \sum_j c_j^O |\phi_j\rangle$ we find,for $M = 2^m$

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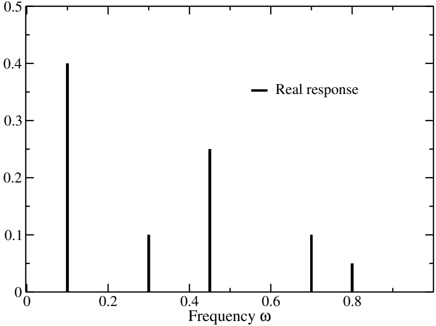
- original response recovered for $M \to \infty$: $S_O(\omega) = \sum_j \left|c_j^O\right|^2 \delta(\phi_j - \omega)$



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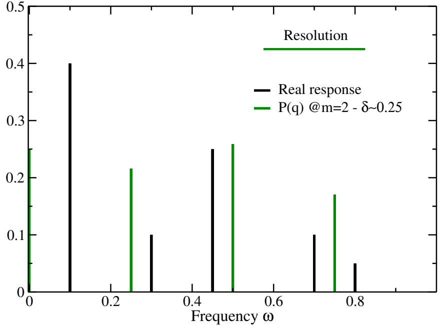

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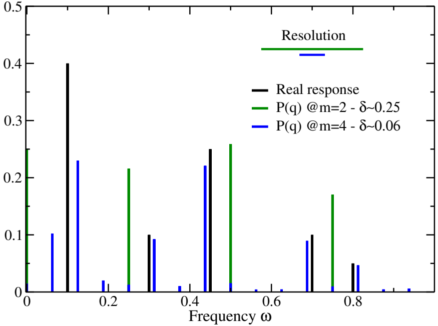

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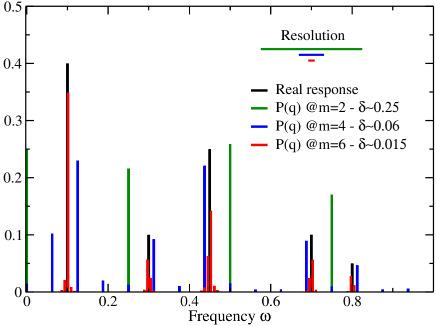
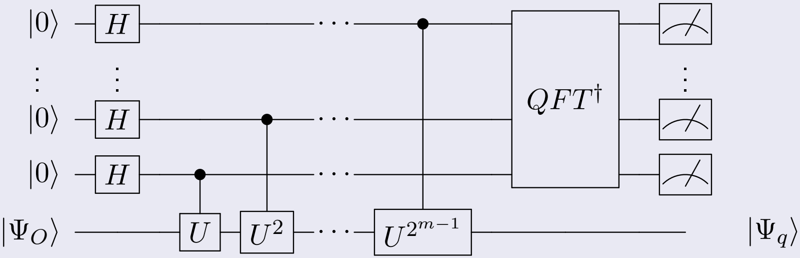


QPE as state preparation



- before the ancilla measurement we have

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- after measuring the integer value q the system qubits are left in

$$|\Psi_q\rangle = \frac{1}{M\sqrt{P(q)}} \sum_j c_j^O \frac{\sin\left(M\pi(\phi_j - \frac{q}{M})\right)}{\sin\left(\pi(\phi_j - \frac{q}{M})\right)} |\phi_j\rangle \approx \sum_{|\phi_j - \frac{q}{M}| \lesssim \frac{1}{M}} c_j^O |\phi_j\rangle$$

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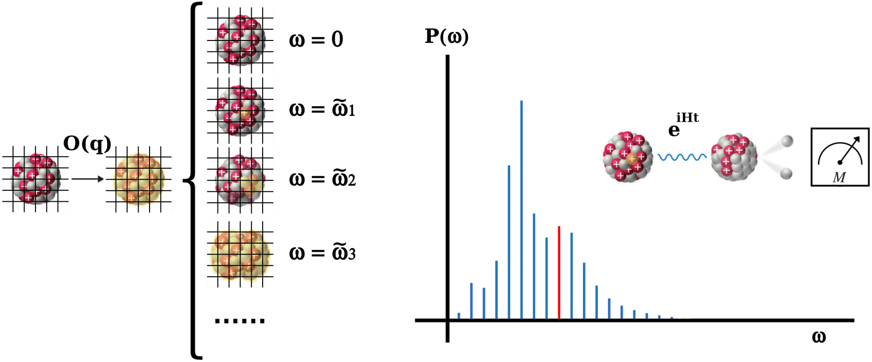

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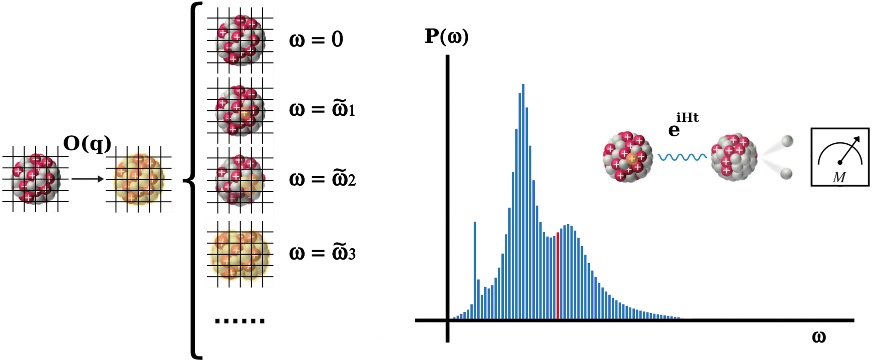

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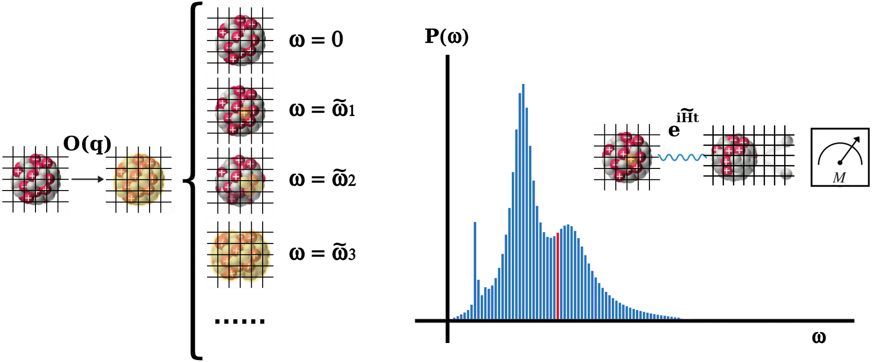

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Progress on time evolution for NP

As a starting point we can use simple nuclear interactions without pions

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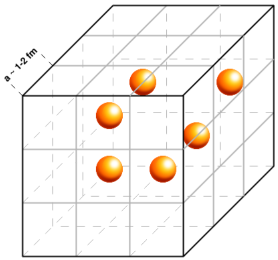
We then place nucleons on spatial lattice to regularize them



Minimal setup

- 10^3 lattice with spacing $a \approx 1 - 2fm$
- 4 spin-isospin states for each particle

  $\longrightarrow$ we need at least 4000 orbitals
- for energy resolution $\Delta\omega$ we need total evolution time $T \approx 1/\Delta\omega$

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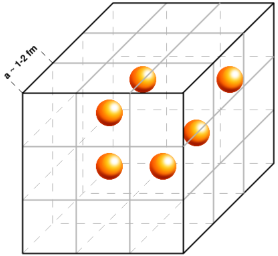

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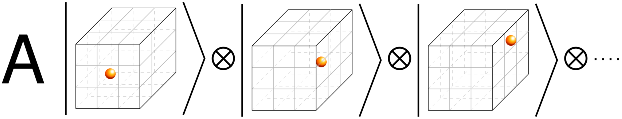
- $10^{11} - 10^{12}$ operations and ≈ 4000 qubits [Roggero et al. PRD (2020)]
- $10^9 - 10^{11}$ operations and ≈ 6000 qubits [J.Watson et al. arXiv:2312.05344]

Progress on time evolution for NP II

For nuclear reactions we want large volumes V with few particles N inside
$\rightarrow$ IDEA: why not use first quantization instead?



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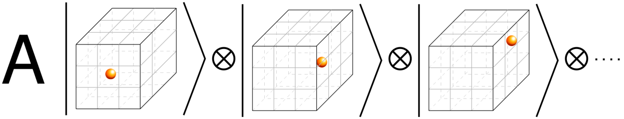

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Turns out 1st quant. can beat 2nd quant. in both memory and gates

$$C^T_{2nd} = \mathcal{O}\left(\frac{t^{3/2}}{\sqrt{\epsilon}}\sqrt{N}V\right) \qquad C^T_{1st} = \mathcal{O}\left(\frac{t^{3/2}}{\sqrt{\epsilon}}N^{7/2}\log^2(V)\right)$$

Roggero, Spagnoli, Lissoni (in prep.)

Progress on time evolution for NP III

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Can do even better using Quantum Signal Processing [Low & Chuang (2017)]

$$C^{QSP}_{1st} = \mathcal{O}\left(N\log^2(V)\left(Nt + \log\left(\frac{1}{\epsilon}\right)\right)\right)$$

Progress on time evolution for NP III

Roggero, Spagnoli, Lissoni (in prep.)

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Can do even better using Quantum Signal Processing [Low & Chuang (2017)]

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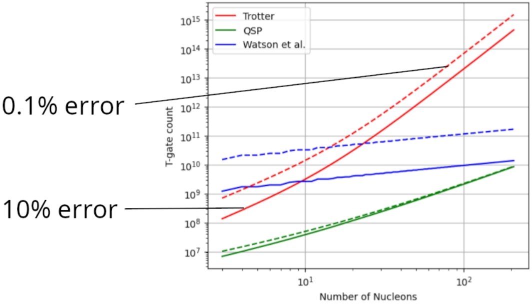

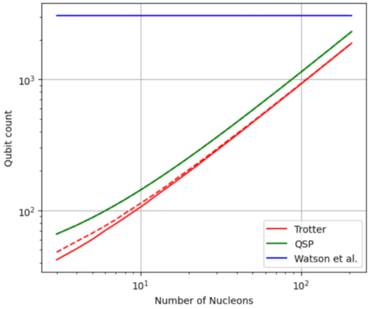

- $10^7 - 10^9$ operations and $\approx 70 - 300$ qubits [AR, Spagnoli, Lissoni (in prep.)]

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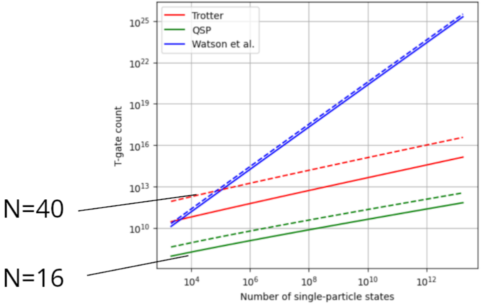

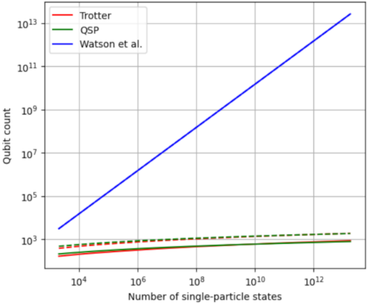

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Recap on nuclear reaction on a quantum computer

1. need to prepare the target ground state (VQE, QPE, Rodeo, QSP, ...)
2. apply the excitation operator (LCU seems reasonably good)
3. apply an energy projection with resolution $\Delta\omega$ (QPE, Rodeo, GIT, ...)
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If we only need inclusive cross section, and thus the response function $S(\omega)$, we can stop at step 3. Most (all?) energy filters do something like

$$\langle\Psi_{ex}|\delta_{\Delta\omega}(H-\omega)|\Psi_{ex}\rangle = \sum_{k=0}^{M} c_k(\omega,\Delta\omega)\langle\Psi_{ex}|P_k(H)|\Psi_{ex}\rangle$$

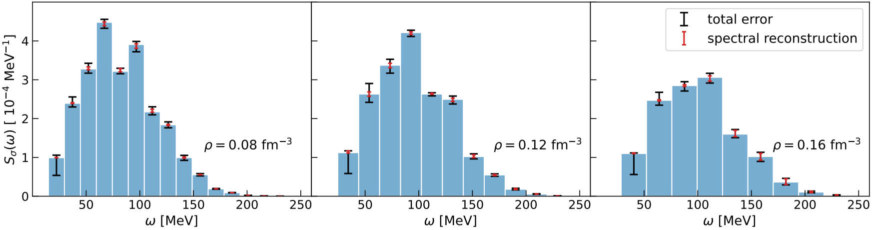
QPE and Rodeo use Fourier polynomials, GIT can also use Chebyshev

Classical simulation of reactions

Since we want Chebyshev moments, why not get them classically instead?

With EOM-CC we can get a reasonably good approximation of them in a very efficient way: 5k moments for $N = 114$ particles in ≈ 7k CPU hours

Sobczyk, Jiang, Roggero (2025)

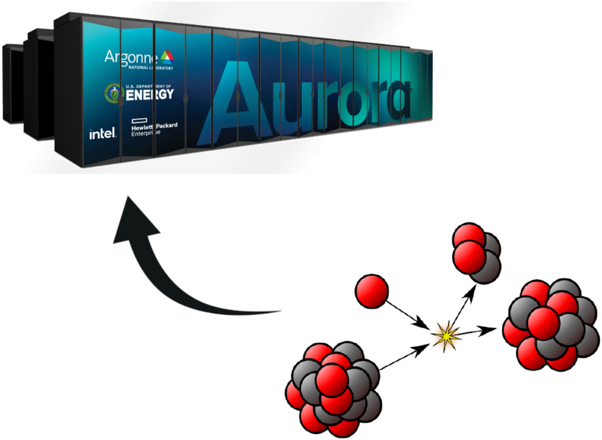


First ab-initio calculation of the frequency dependent spin response of neutron matter with controllable errors, important for ν processes

- exactly same post-processing we would use on a quantum computer

Simulations of nuclear dynamics

Classical simulations



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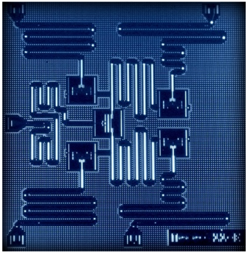
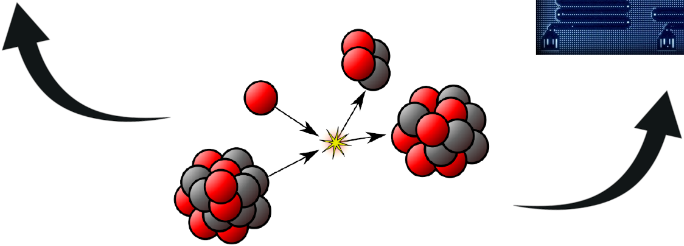


IBM



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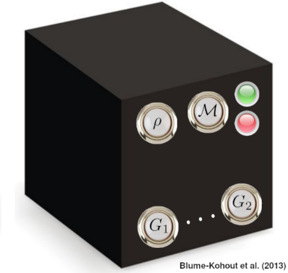

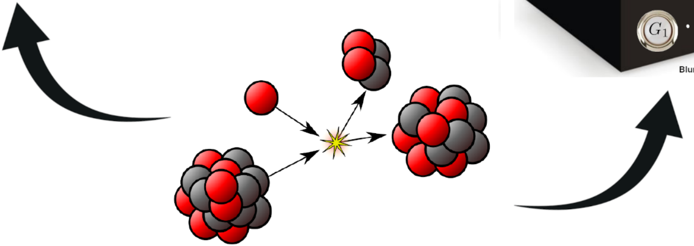

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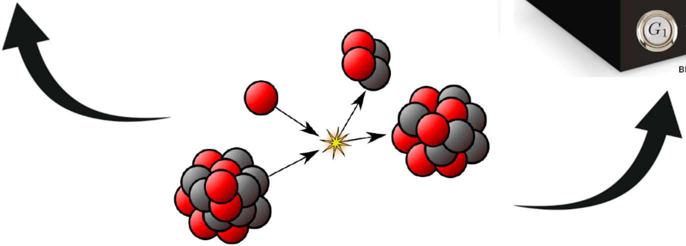
Blume-Kohout et al. (2013)



Simulations of nuclear dynamics