Nuclear structure (and reactions) with Quantum Computers - III

Alessandro Roggero

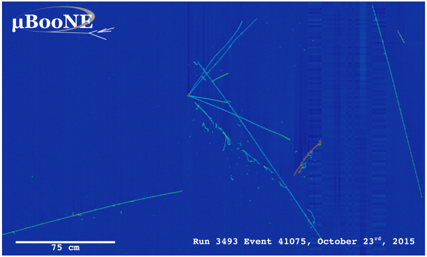


figure credit: μBooNE collab.

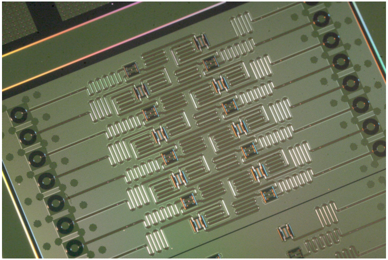


figure credit: IBM

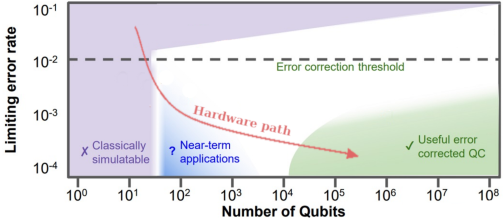
QC and QIS for NP

JLAB – 18 March, 2020

The plan for today

- nuclear dynamics, computation of scattering cross sections
  - EXAMPLE: neutrino-^{40}Ar cross section for DUNE
  - inclusive scattering and the response function
  - calculation of two-point functions
  - direct calculation of response in frequency space
- complexity of these calculations, can we actually run them on current/near-term NISQ devices?

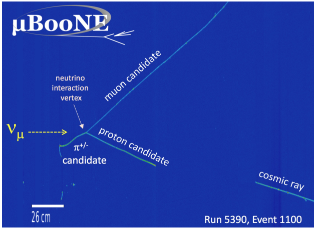
from Google AI



- advanced algorithms + one slide on error correction

- Fermionic Swap Networks
- Linear Combination of Unitaries
- Amplitude Amplification
- Qubitization

Exclusive cross sections in neutrino oscillation experiments



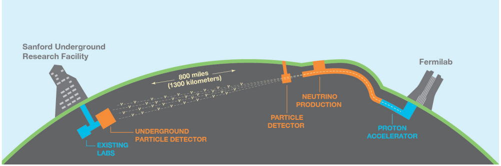
Goals for ν oscillation exp.

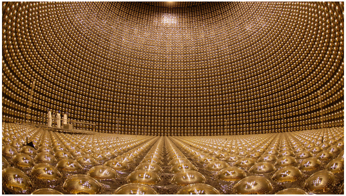
- neutrino masses
- accurate mixing angles
- CP violating phase

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

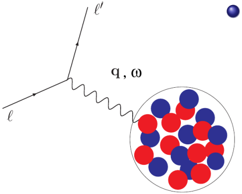
- need to use measured reaction products to constrain E_ν of the event

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





Inclusive cross section and the response function

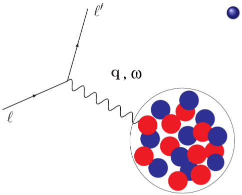


- xsection completely determined by response function

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

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

Inclusive cross section and the response function



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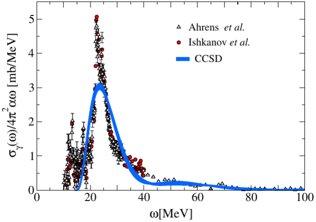
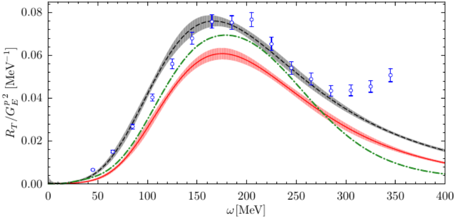
Extremely challenging classically for strongly correlated quantum systems

- dipole response of ^{16}O



Bacca et al. (2013) LIT+CC

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



Lovato et al. (2016) GFMC

Real time correlation functions

The response function $R_O(\omega)$ can be obtained from the two point function

$$C_O(t) = \langle\Psi_0|\hat{O}^\dagger(t)\hat{O}(0)|\Psi_0\rangle = FT^{-1}\left[R_O(\omega)\right]$$

using the Fourier transform. The final energy resolution is $\delta \sim \pi/t_{max}$.

- if $\hat{O}$ is unitary, $C_O(t)$ can be computed efficiently [Somma et al. (2001)]

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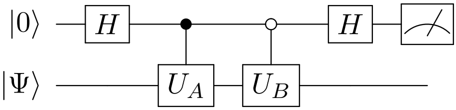
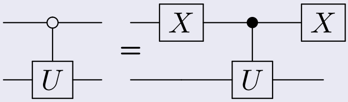


$$\Rightarrow \langle Z \rangle_a = \mathcal{R} \left[\langle \Psi | U_A^\dagger U_B | \Psi \rangle \right]$$

Anti-controlled unitary



Choose $U_B = U(t)\hat{O}$ and $U_A = \hat{O}U(t)$:

$$\langle Z \rangle_a = \mathcal{R} \left[\langle \Psi | U^\dagger(t) \hat{O}^\dagger U(t) \hat{O} | \Psi \rangle \right]$$

Real time correlation functions II

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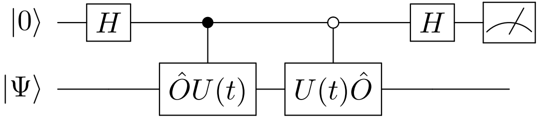

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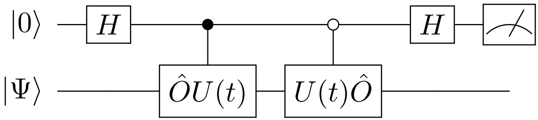

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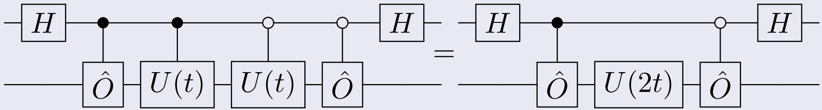
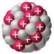


BONUS: no need for controlled time-evolution! Maximum time $\mathcal{O}(1/\delta)$

Idealized algorithm for exclusive processes at fixed q

- prepare the target ground state



Roggero & Carlson (2018)

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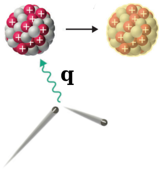

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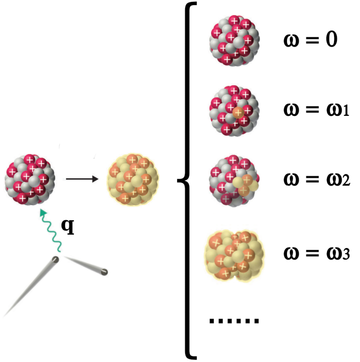

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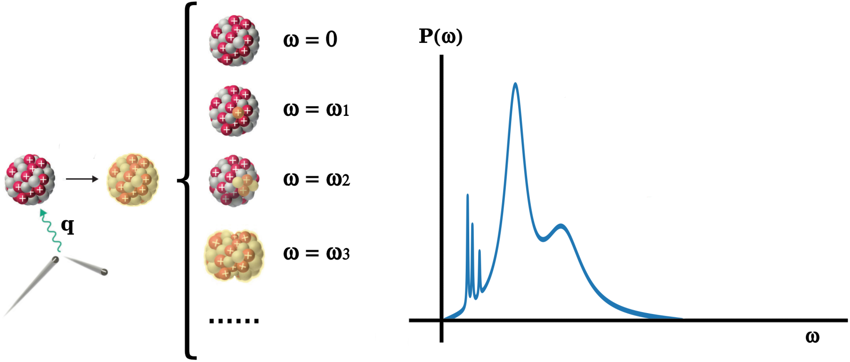

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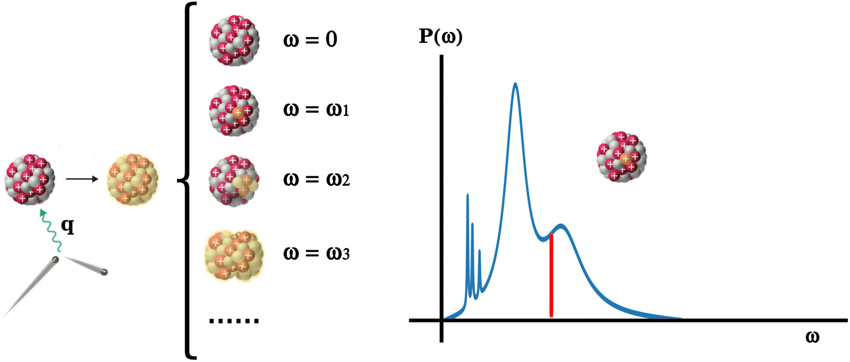

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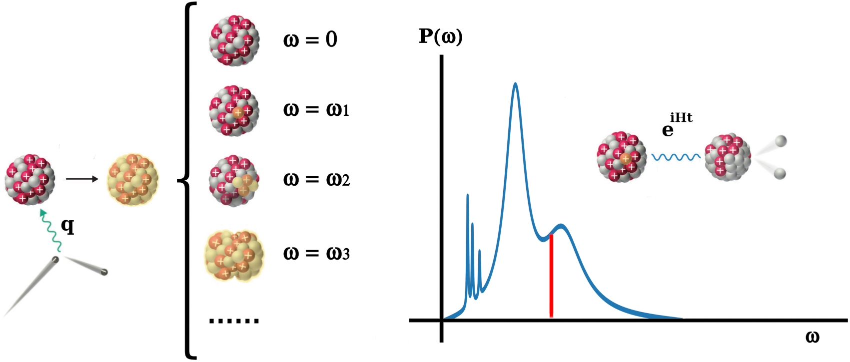

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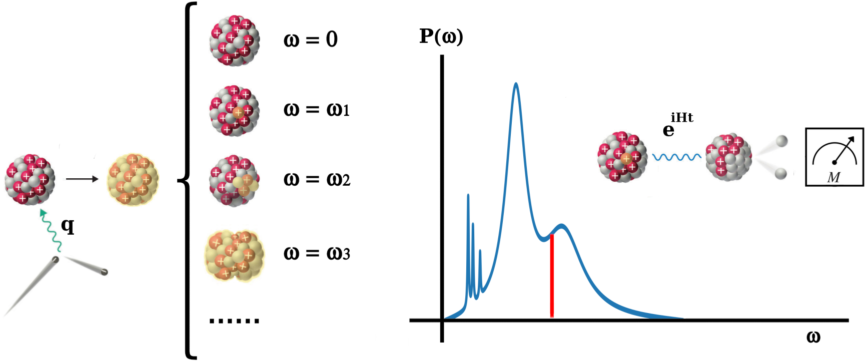

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Quantum algorithm for exclusive processes at fixed q

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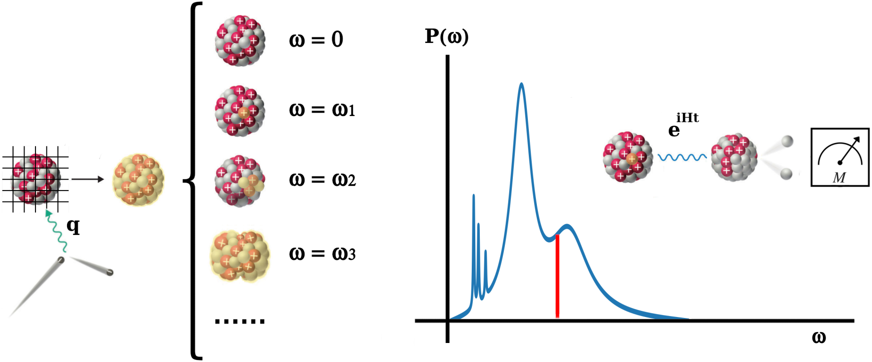

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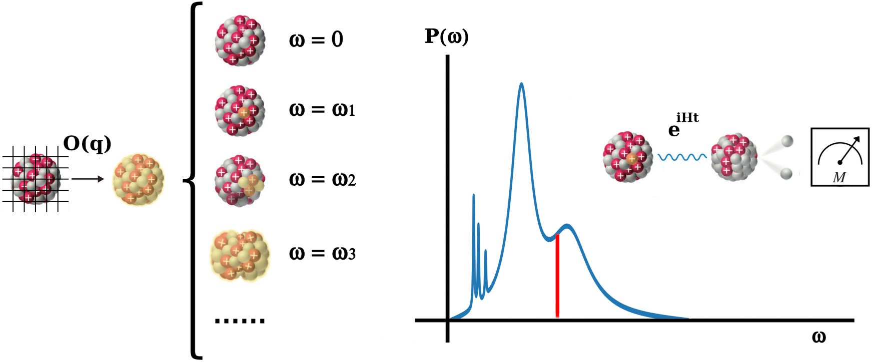
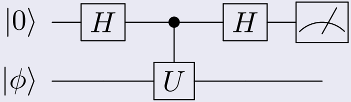


Roggero & Carlson (2018)

[from yesterday] Can we apply a non-unitary operation?

YES, but only with some probability

- this can be useful for example if the transition matrix element we considered before is genereated by a non unitary operator



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

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

Concrete example: projection operators

If we take U to be the reflection around $|\psi\rangle$, like $U = (2|\psi\rangle\langle\psi| - \mathbb{1})$, we find

$$P_0 = |\langle\phi|\psi\rangle|^2 \quad \Rightarrow \quad |\phi_0\rangle = \frac{|\psi\rangle\langle\psi|}{\sqrt{P_0}}|\phi\rangle = |\psi\rangle$$

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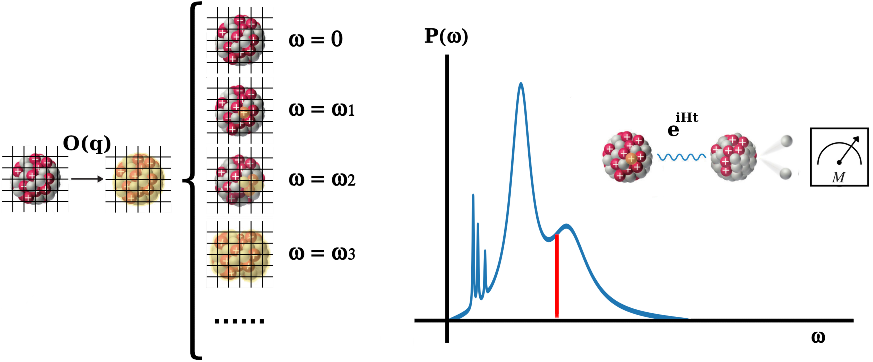

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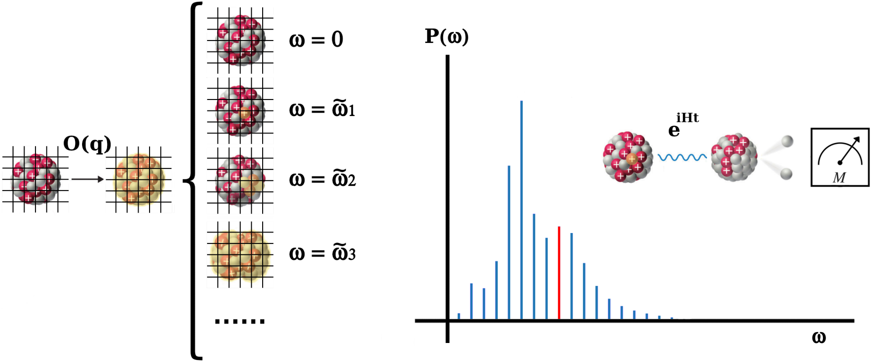

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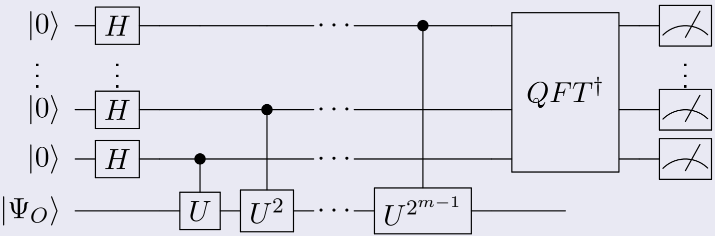
QPE on general states



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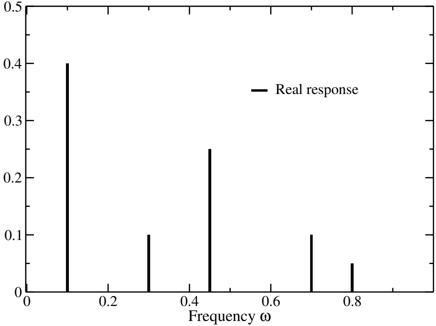
- original response recovered for $M \to \infty$: $S_O(\omega) = \sum_j \left|c_j^O\right|^2 \delta(\phi_j - \omega)$



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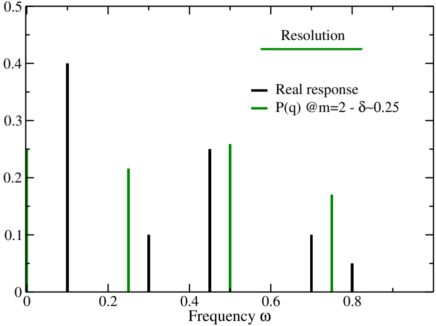

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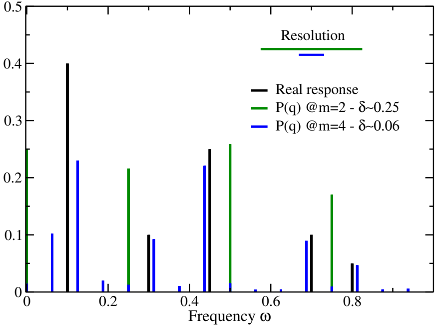

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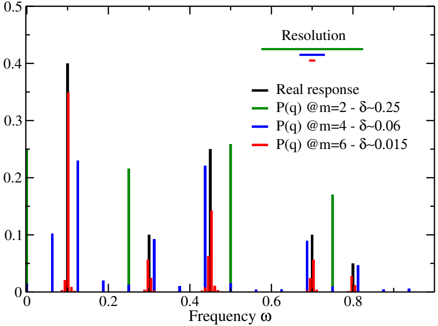
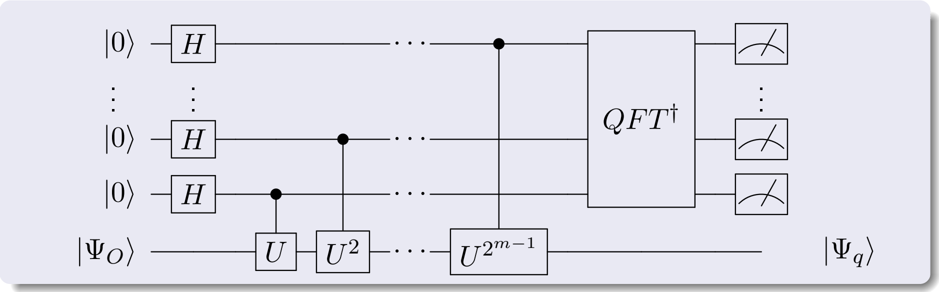


QPE as state preparation



- before the ancilla measurement we have

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

- 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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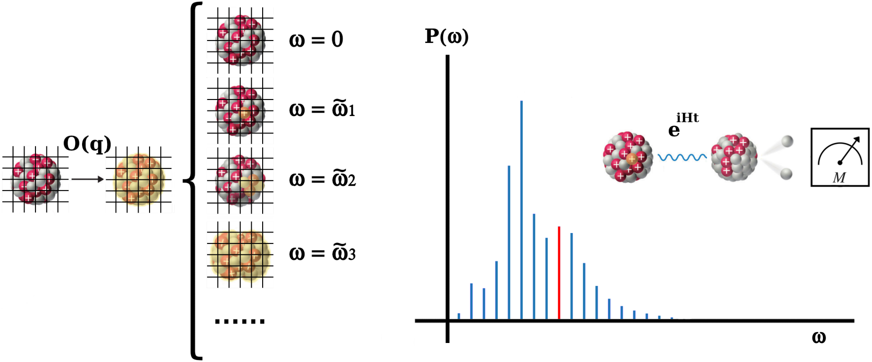

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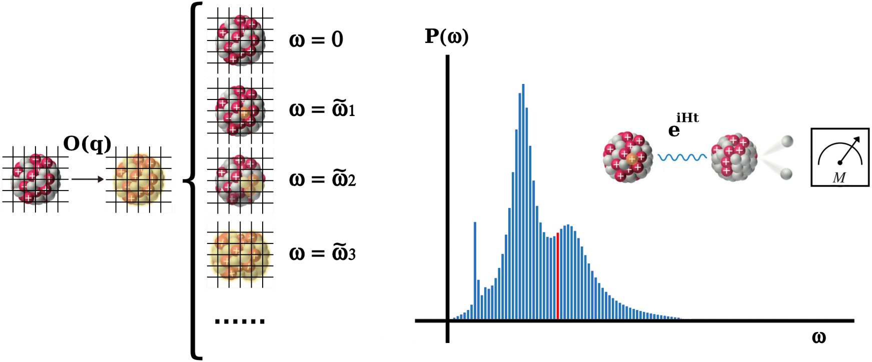

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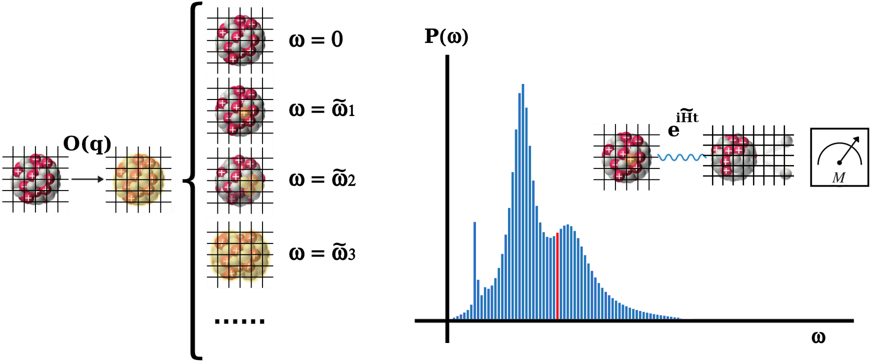

Roggero & Carlson (2018)

How practical is all this?Can we make it in time for DUNE?

- pionless EFT on a 10^3 lattice of size 20 fm [$a = 2.0$ fm]

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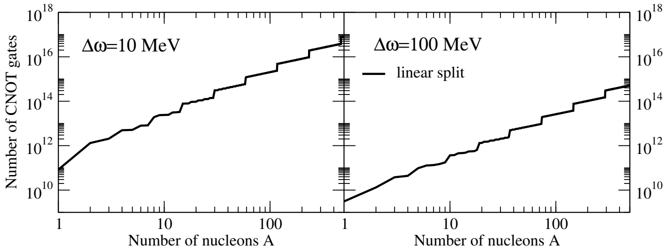

For ^{40}Ar we need $\approx 10^{12} - 10^{14}$ CNOT gates to run the QPE part

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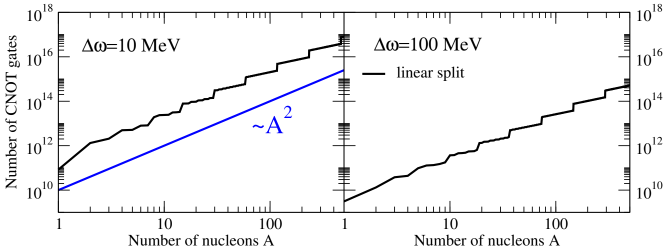

For ^{40}Ar we need $\approx 10^{12} - 10^{14}$ CNOT gates to run the QPE part

How practical is all this?Can we make it in time for DUNE?

- pionless EFT on a 10^3 lattice of size 20 fm [$a = 2.0$ fm]

we need a quantum device with ≈ 4000 qubits (currently we have < 100)

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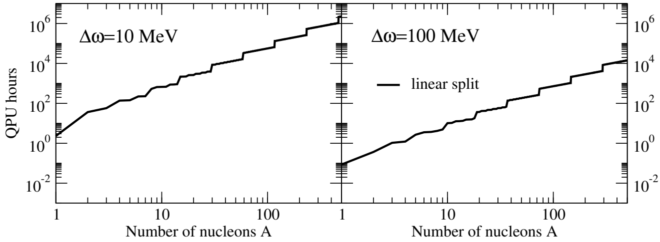

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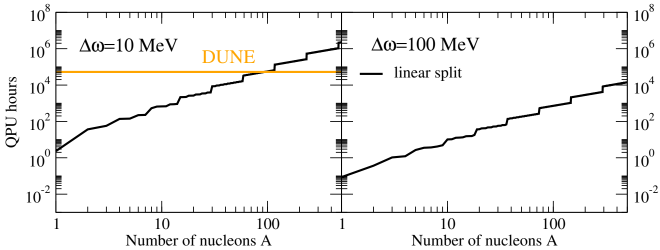

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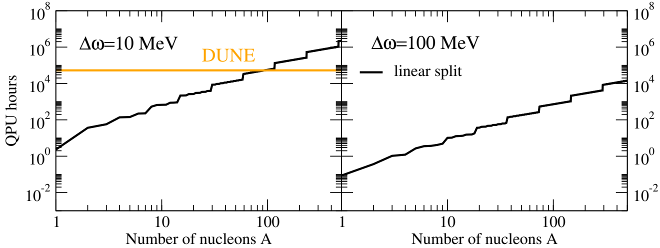

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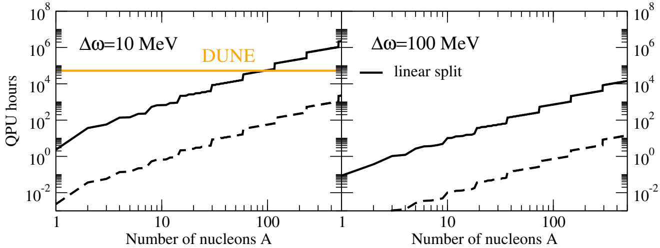

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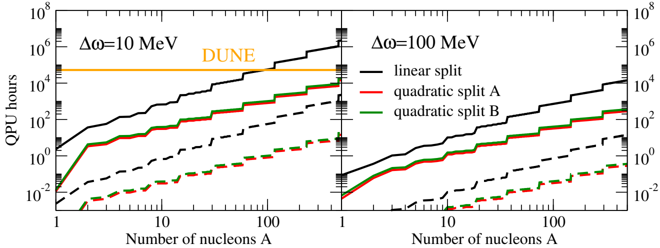

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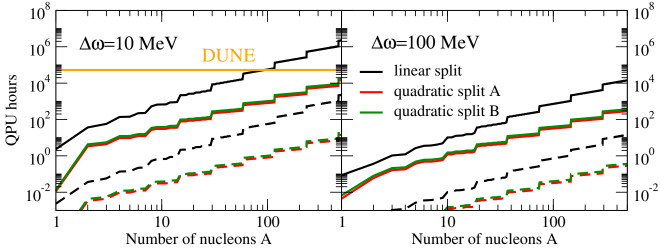

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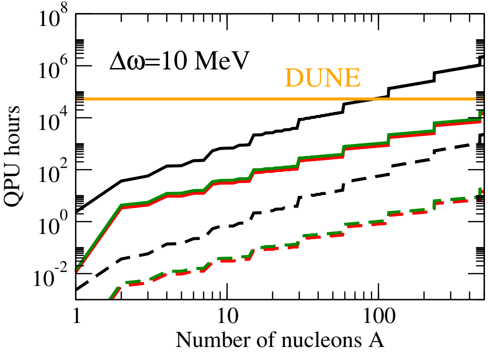

coherence time for ^{40}Ar	
simple	≈ 15 months
optimized	≈ 15 minutes

- algorithm efficiency is critical
- there is still a long way to go
- find new algorithms and/or approximations for near term

A.R., A.Li, J.Carlson, R.Gupta, G.Perdue (2019)

Summary: quantum algorithms for the nuclear response

$$S_O(\omega) = \int dt e^{i\omega t} C_O(t) \quad \text{with} \quad C_O(t) = \langle \Psi_0 | O(t) O(0) | \Psi_0 \rangle$$

- strategy A [Ortiz, Somma et al (2001-2003)]
  - compute $C_O(t)$ on quantum computer for different times
  - perform Fourier transform classically using $t_{max} = \mathcal{O}(1/\Delta)$
  - the total cost is $\mathcal{O}(1/\Delta)$ gates and $\mathcal{O}\left(\frac{1}{\Delta\epsilon^2}\right)$ repetitions
- strategy B [Roggero & Carlson (2018)]
  - sample directly final states from approximate response function

$$|\Phi_B\rangle \approx \sum_\omega \sqrt{S_O(\omega)} \, |\omega\rangle \otimes |\Psi_\omega\rangle$$

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- both algorithms have a gate cost of $\mathcal{O}\left(\text{poly}(A)/\Delta\right)$ for A nucleons and target energy resolution Δ!
- both algorithms are (probably) too expensive for a realistic description of final states in neutrino ^{40}Ar scattering with NISQ devices

Quantum Error Correction and the Threshold Theorem(s)

check out lecture notes from: S.Aaronson, D.Bacon, A.Childs & J.Preskill

- effect of environment can be described using quantum channels

$$\rho = |\Psi\rangle\langle\Psi| \quad \rightarrow \quad \Lambda(\rho) = \sum_k O_k^\dagger \rho O_k \quad \text{with} \quad \sum_k O_k^\dagger O_k = \mathbb{1}$$

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Threshold Theorem(s) Ben-Or, Aharonov, Kitaev, Knill, Gottesman,...

If $p < p_{th} = 1/c$ we can extend τ_{coh}^{eff} with $\mathcal{O}\left(\text{polylog}\left(\tau_{coh}^{eff}/c\right)\right)$ effort