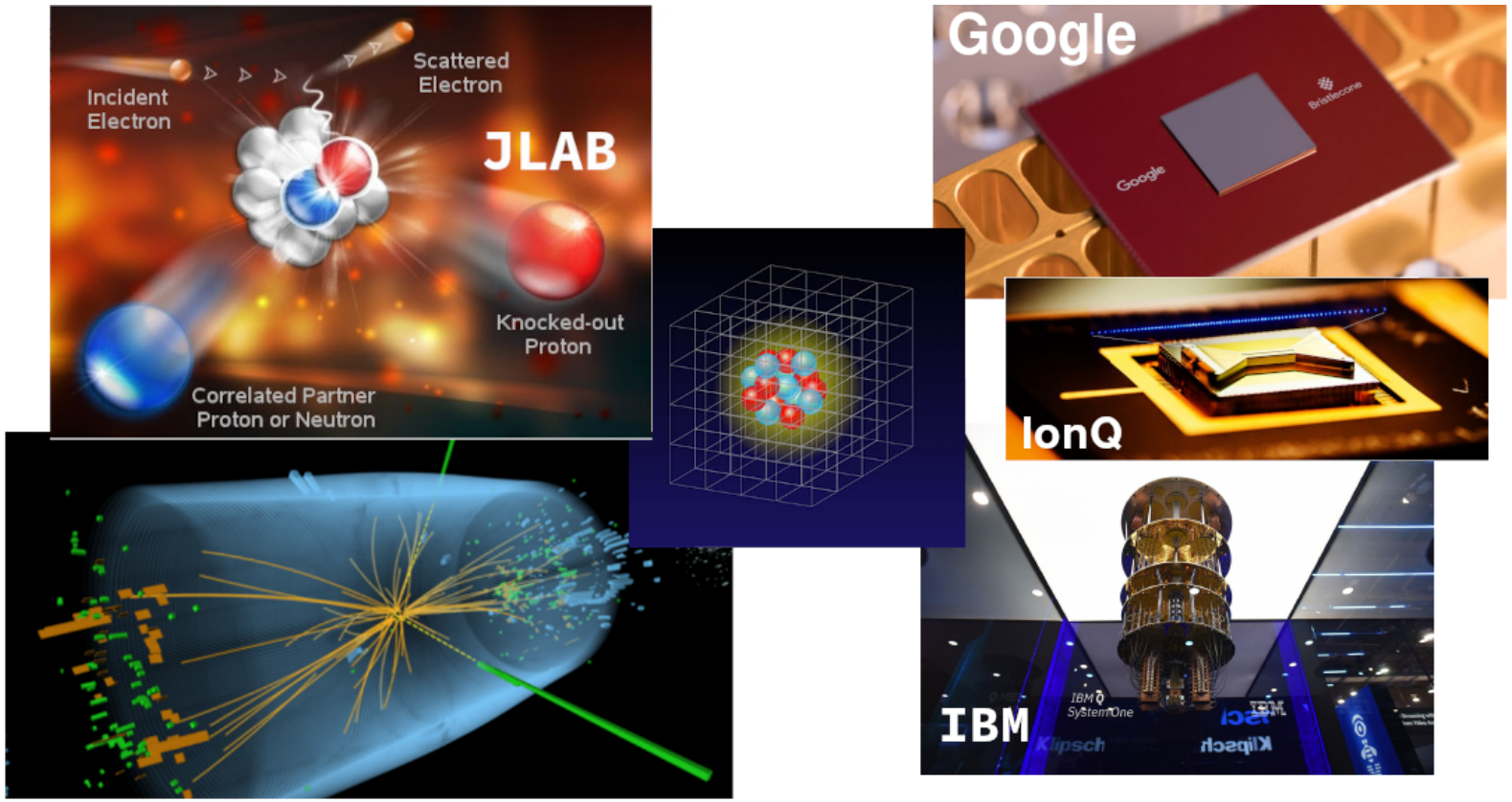
Quantum Simulations - II

Alessandro Roggero



TIFPA
Trento Institute for Fundamental Physics and Applications

NNP Summer School

MIT – 19 July, 2022

UNIVERSITAS ATHESINA STUDIORUM

Qubit mapping for nuclear Hamiltonians

PROBLEM: Nuclear Physics is not a spin model! What about fermions?

$$\hat{H} = \sum_i \frac{\hat{p}_i^2}{2m} + \frac{1}{2}\sum_{i,j} \hat{V}_{ij} + \frac{1}{6}\sum_{i,j,k} \hat{W}_{ijk} + \cdots$$

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- first discretize the problem by describing it using a set of M orbitals and build many-body states in occupation number basis (Fock space)

$$\hat{H} = \sum_{ij} K_{ij}\hat{a}_i^\dagger\hat{a}_j + \sum_{ijkl} V_{ijkl}\hat{a}_i^\dagger\hat{a}_j^\dagger\hat{a}_k\hat{a}_l + \sum_{ijklmn} W_{ijklmn}\hat{a}_i^\dagger\hat{a}_j^\dagger\hat{a}_k^\dagger\hat{a}_l\hat{a}_m\hat{a}_n + \cdots$$

with $\{\hat{a}_i, \hat{a}_j^\dagger\} = \delta_{ij}$ and $\{\hat{a}_i^\dagger, \hat{a}_j^\dagger\} = \{\hat{a}_i, \hat{a}_j\} = 0$.

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- the Hilbert space has dimension 2^M and could be fitted into M qubits
- need a correct map for the creation/annihilation operators there

Fermion to spin mapping: Jordan Wigner transformation

The fermionic Fock space with M modes can be mapped into the Hilbert space of M spins using the following identification

$$\left.\begin{aligned} a_k &= \left(\prod_{j=0}^{k-1} -Z_j\right) \frac{X_k + iY_k}{2} \\ a_k^\dagger &= \left(\prod_{j=0}^{k-1} -Z_j\right) \frac{X_k - iY_k}{2} \end{aligned}\right\} \quad \Rightarrow \quad \{a_j, a_k^\dagger\} = \delta_{j,k}$$

- occupation encoded into value of spin projection, $\sigma_k^\pm = \frac{X_k \pm iY_k}{2}$

$$|vac\rangle = |\uparrow\uparrow\uparrow\uparrow\rangle \quad a_2^\dagger |vac\rangle = |\uparrow\uparrow\downarrow\uparrow\rangle \quad a_2^\dagger |\uparrow\uparrow\downarrow\uparrow\rangle = 0$$

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- fermionic phase encoded into the string of Pauli Z operators

$$\begin{aligned} a_2^\dagger a_1^\dagger |vac\rangle &= \left(Z_0 Z_1 \sigma_2^-\right)\left(-Z_0 \sigma_1^-\right)|vac\rangle \\ &= -\sigma_2^- Z_1 \sigma_1^- |vac\rangle \\ &= \sigma_2^- \sigma_1^- Z_1 |vac\rangle = \sigma_1^- Z_1 \sigma_2^- |vac\rangle = -a_1^\dagger a_2^\dagger |vac\rangle \end{aligned}$$

since $\{\sigma_k^\pm, Z_k\} = 0$ and operators commute when acting on $i \neq k$.

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- works great for 1D local models, otherwise many Z terms

$$a_8^\dagger a_1 = -\sigma_8^- Z_7 Z_6 Z_5 Z_4 Z_3 Z_2 Z_1 \sigma_1^+$$

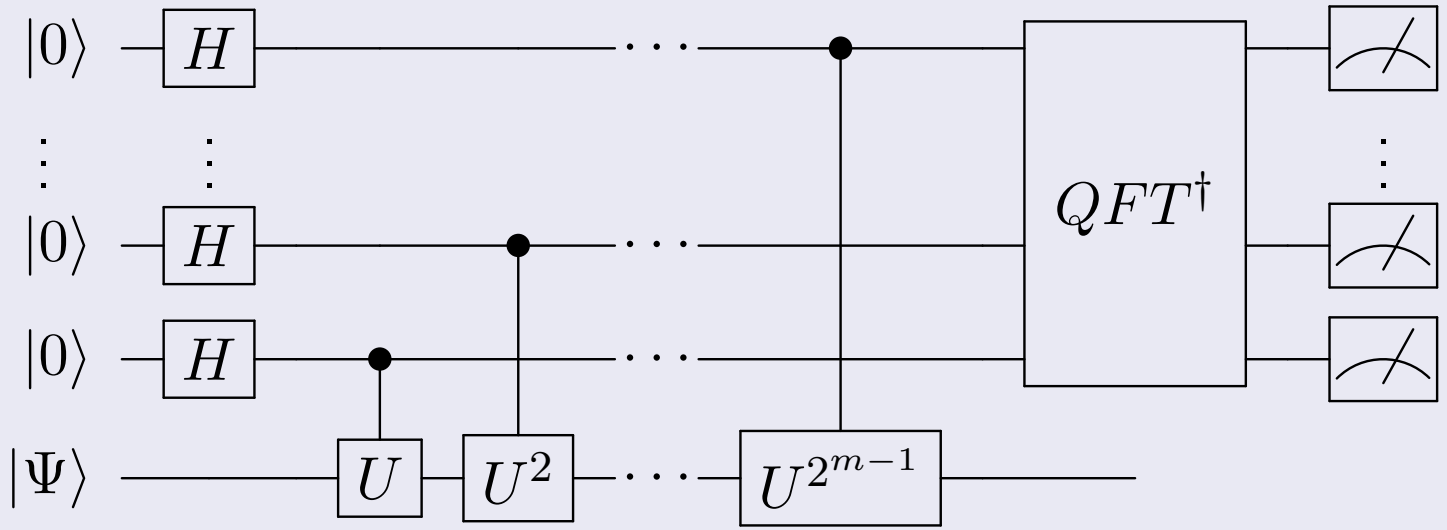
- even if Hamiltonian has local NN and $3N$ forces the corresponding spin model can have terms acting on all spins at the same time

Many other mappings available

- Bravy-Kitaev
- auxiliary fermions
- BK-Superfast
- LDPC codes

Bravyi & Kitaev (2000) , Verstraete & Cirac (2005), Havlicek et al. (2017), Steudtner & Wehner (2017)

QPE on general states



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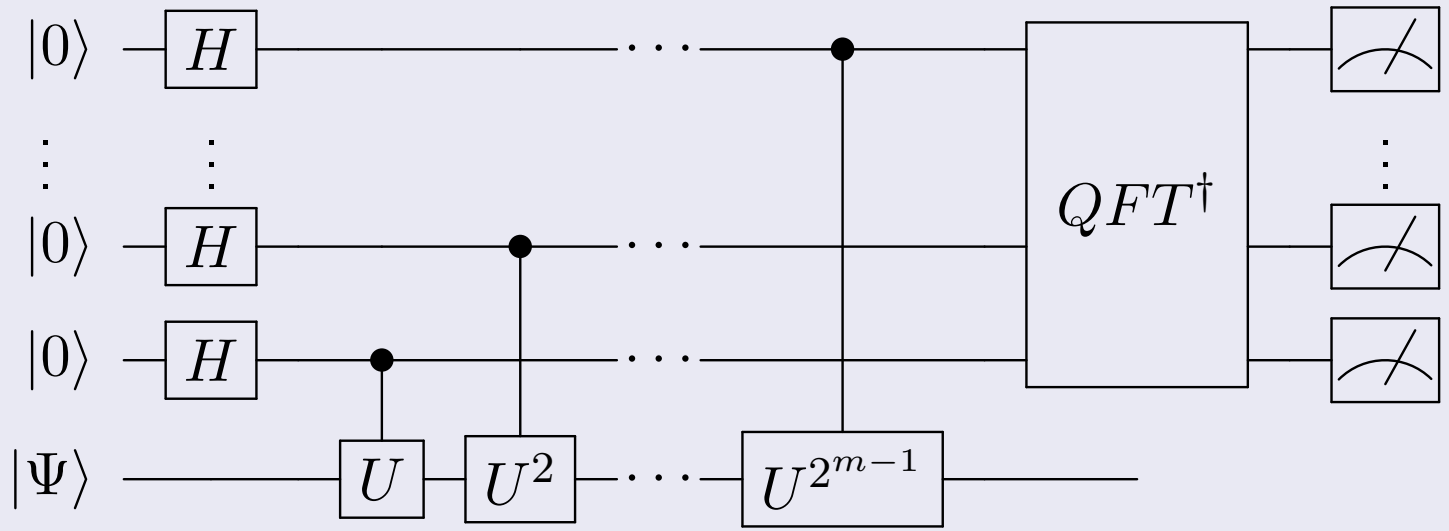


If we start with a generic state $|\Psi\rangle = \sum_j c_j |\phi_j\rangle$ we find

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

The new probability becomes

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

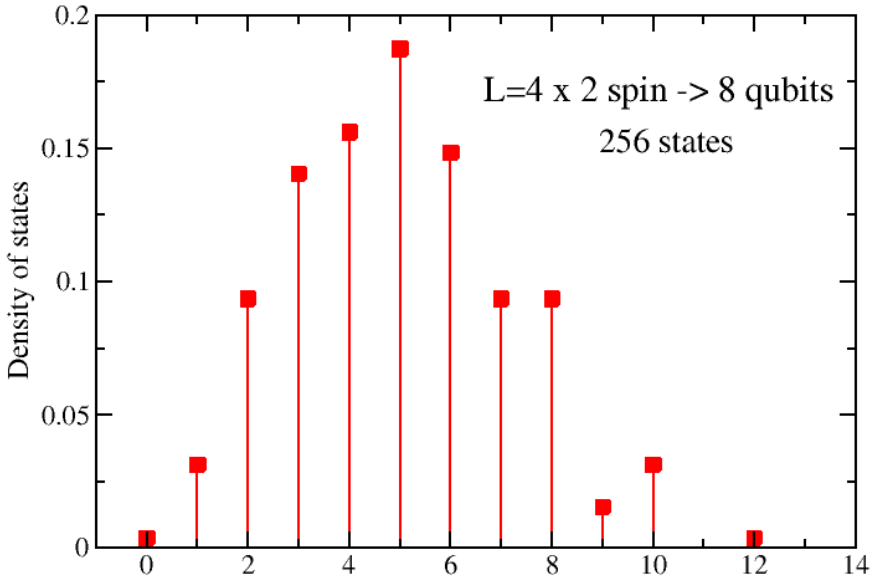
EXAMPLE: Spectrum of 1D Hubbard model

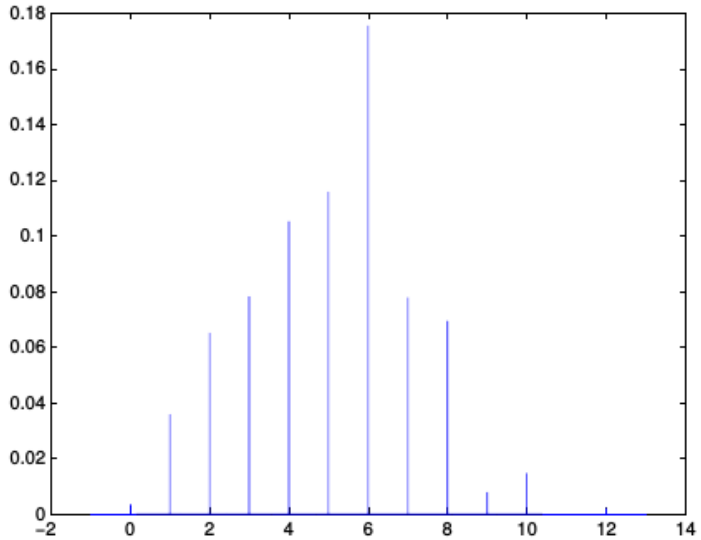
example taken from Ovrum & Horth-Jensen (2007)

$$H_H = \sum_{i}^{L} \sum_{\sigma=\uparrow,\downarrow} \left[\epsilon a^\dagger_{i,\sigma} a_{i,\sigma} - t \left(a^\dagger_{i+1,\sigma} a_{i,\sigma} + a^\dagger_{i,\sigma} a_{i+1,\sigma} \right) \right] + U \sum_{i}^{L} n_{i,\uparrow} n_{i,\downarrow}$$

- we can estimate the spectrum using QPE with random initial states
- consider simple case with $t = 0$, $\epsilon = U = 1$ Ovrum&Horth-Jensen (2007)

$m = 16$ ancilla qubits





Time evolution for Hubbard model

$$H'_H = \sum_i^L \sum_{\sigma=\uparrow,\downarrow} n_{i,\sigma} + \sum_i^L n_{i,\uparrow} n_{i,\downarrow} \qquad n_{i,\sigma} = a^\dagger_{i,\sigma} a_{i,\sigma}$$

- using Jordan-Wigner transformation we can map this into $2L$ qubits

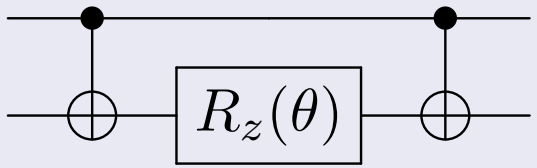
$$n_{i,\uparrow} = \frac{\mathbb{1} + Z_{2i-1}}{2} \qquad n_{i,\downarrow} = \frac{\mathbb{1} + Z_{2i}}{2}$$

$$H_{JW} = h_0 + h_1 \sum_{j=1}^{2L} Z_j + h_2 \sum_{j<k=1}^{2L} Z_j Z_k$$

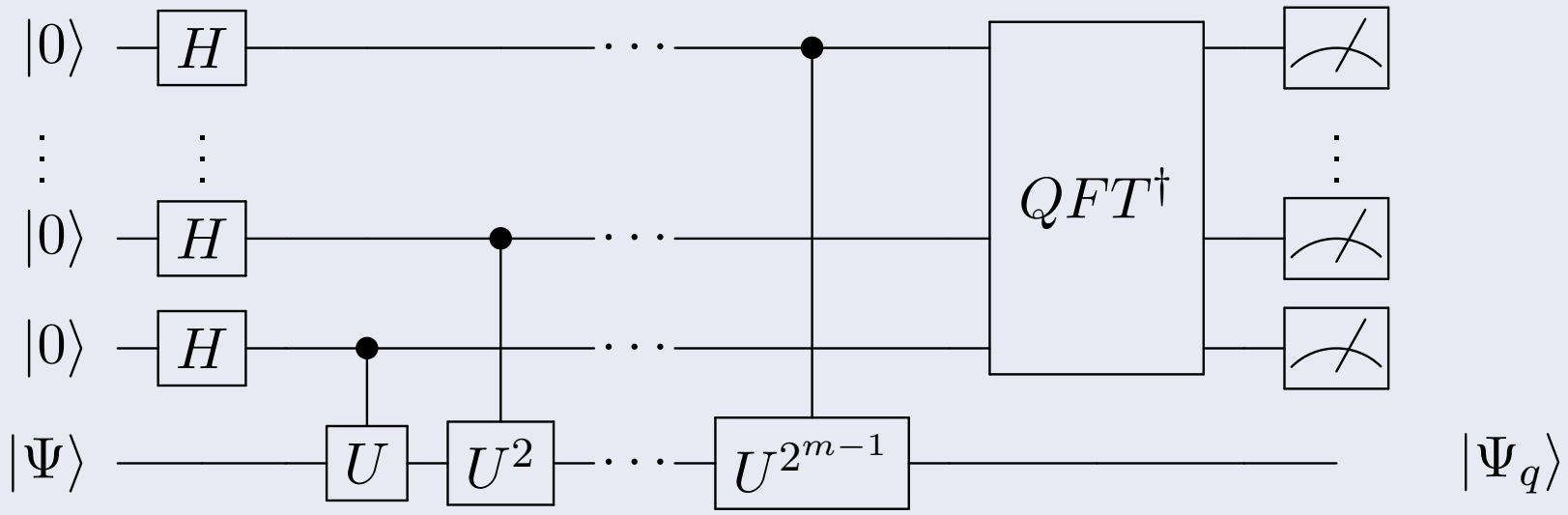
- propagator $U(\tau)$ can be obtained using one and two-qubit Z rotatations

EXERCISE

Show that $U_2 = e^{-i\frac{\theta}{2} Z_1 Z_2}$ is



QPE as state preparation



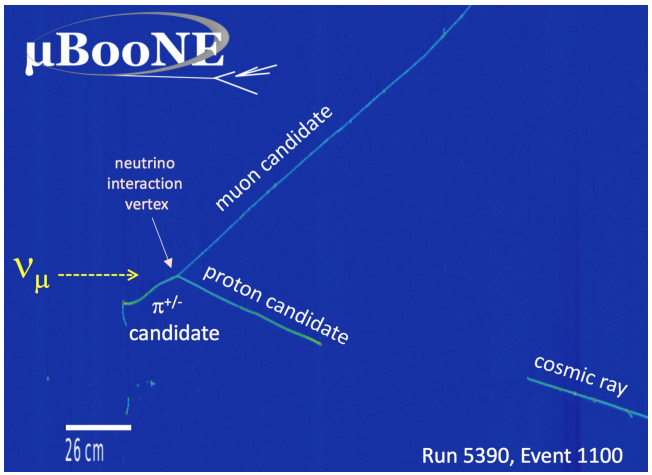
- before the ancilla measurement we have

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

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

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

Exclusive cross sections in neutrino oscillation experiments



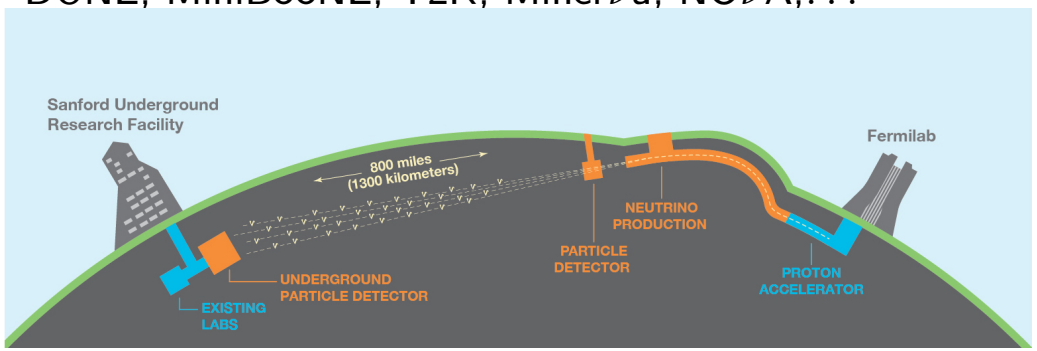
Goals for ν oscillation exp.

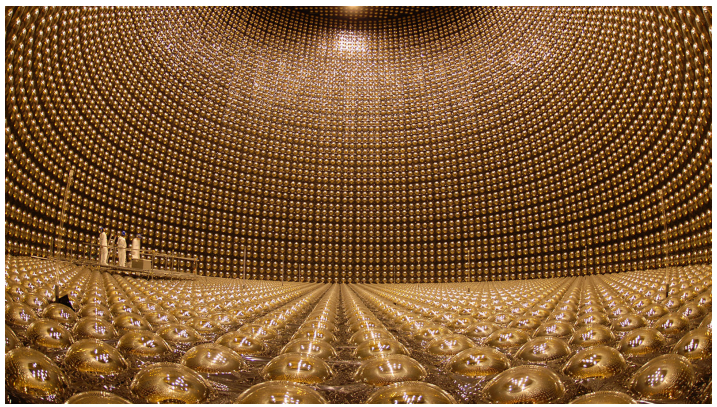
- neutrino masses
- accurate mixing angles
- CP violating phase

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

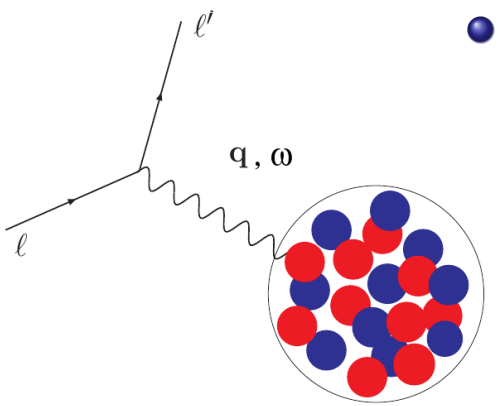
- need to use measured reaction products to constrain E_ν of the event

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





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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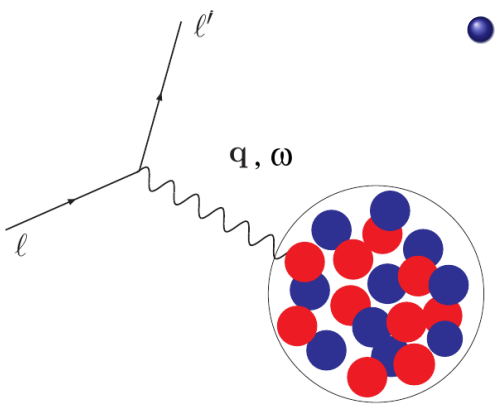

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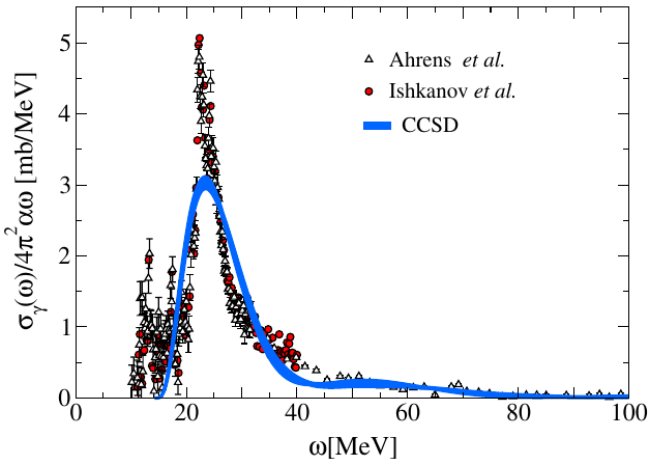
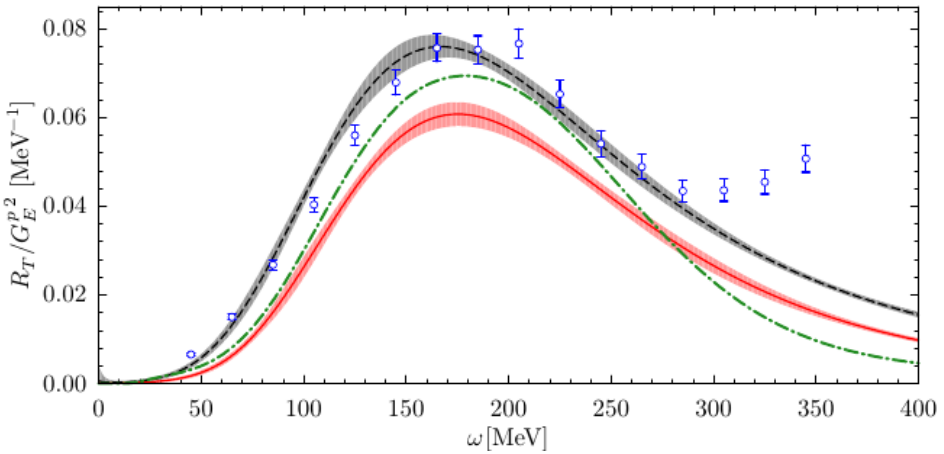
Extremely challenging classically for strongly correlated quantum systems

- dipole response of ^{16}O



Bacca et al. (2013) LIT+CC

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



Lovato et al. (2016) GFMC

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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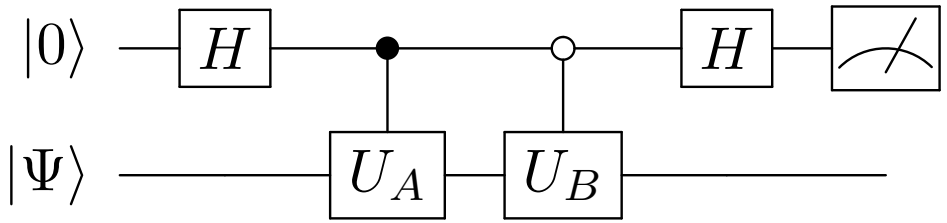
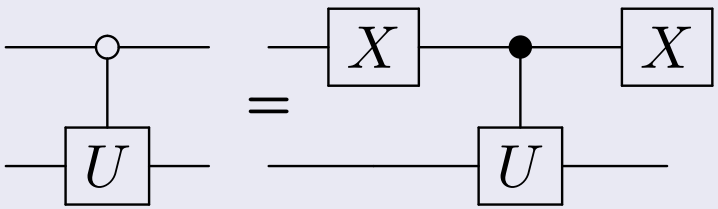


$$\Rightarrow \langle Z \rangle_a = \mathcal{R} \left[\langle \Psi | U_A^\dagger U_B | \Psi \rangle \right]$$

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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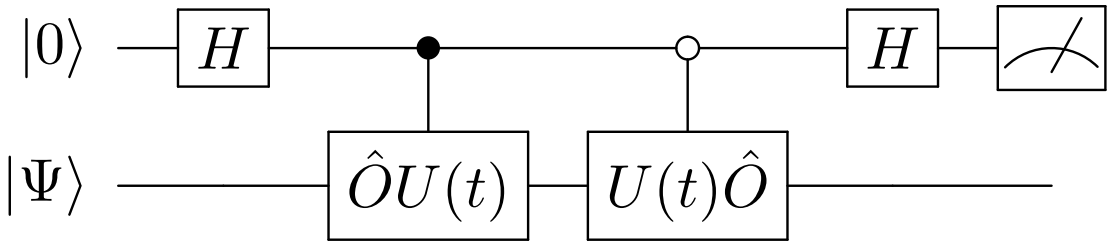

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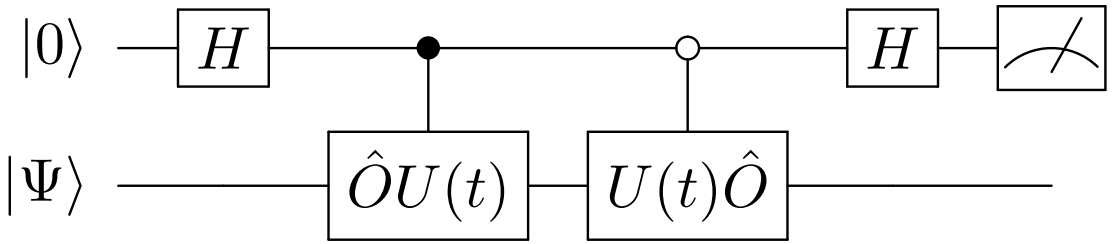

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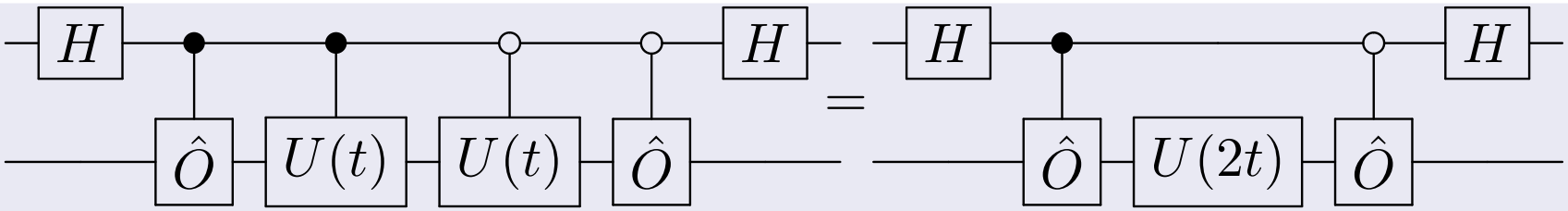
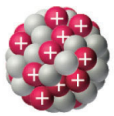


BONUS: no need for controlled time-evolution! Maximum time $\mathcal{O}(1/\delta)$

Idealized algorithm for exclusive processes at fixed q

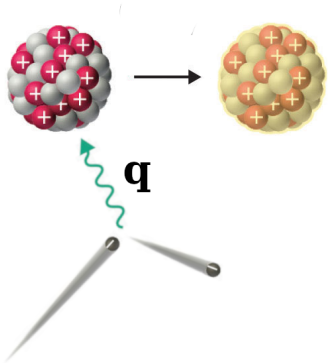
- prepare the target ground state



Roggero & Carlson (2019)

Idealized algorithm for exclusive processes at fixed q

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



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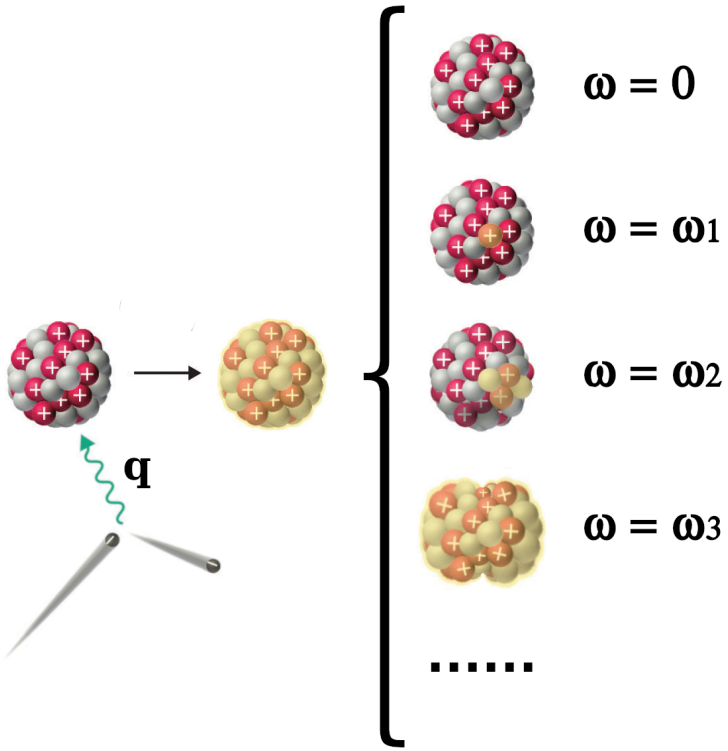

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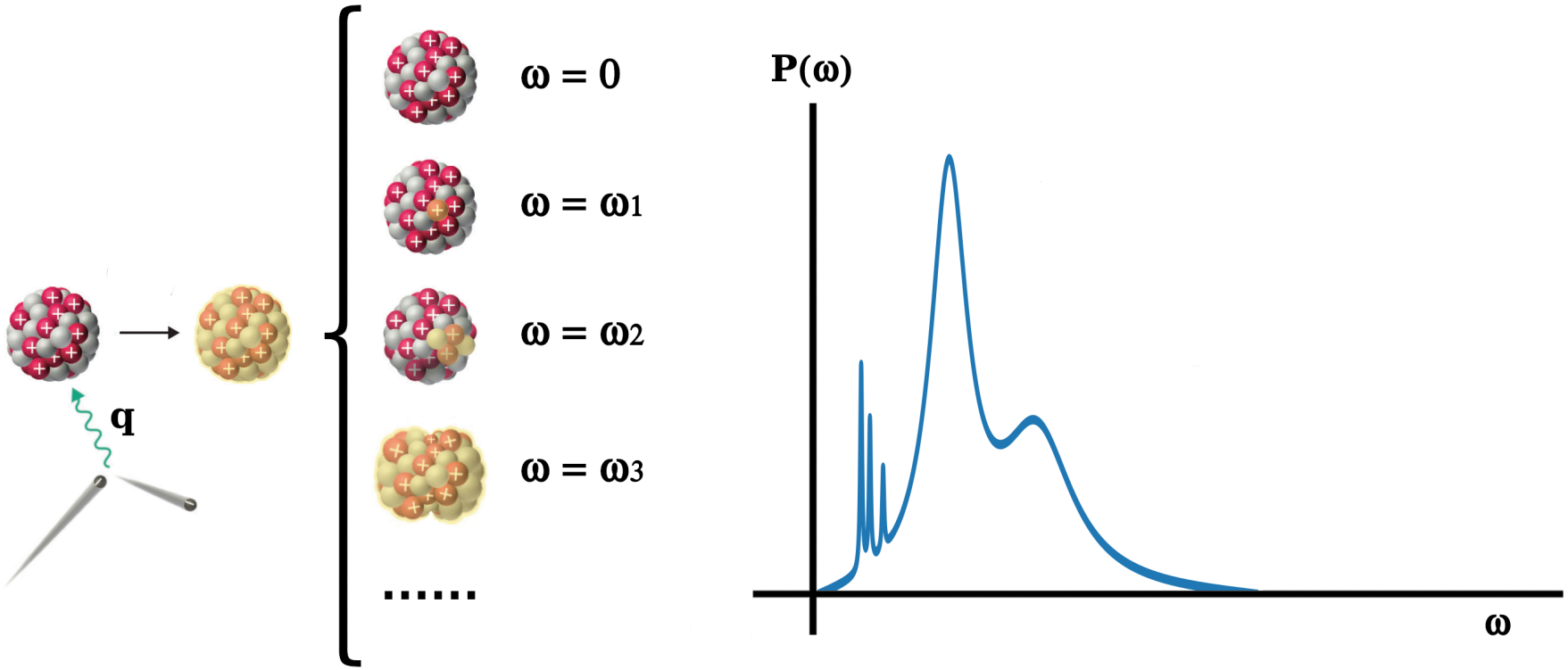

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Idealized algorithm for exclusive processes at fixed q

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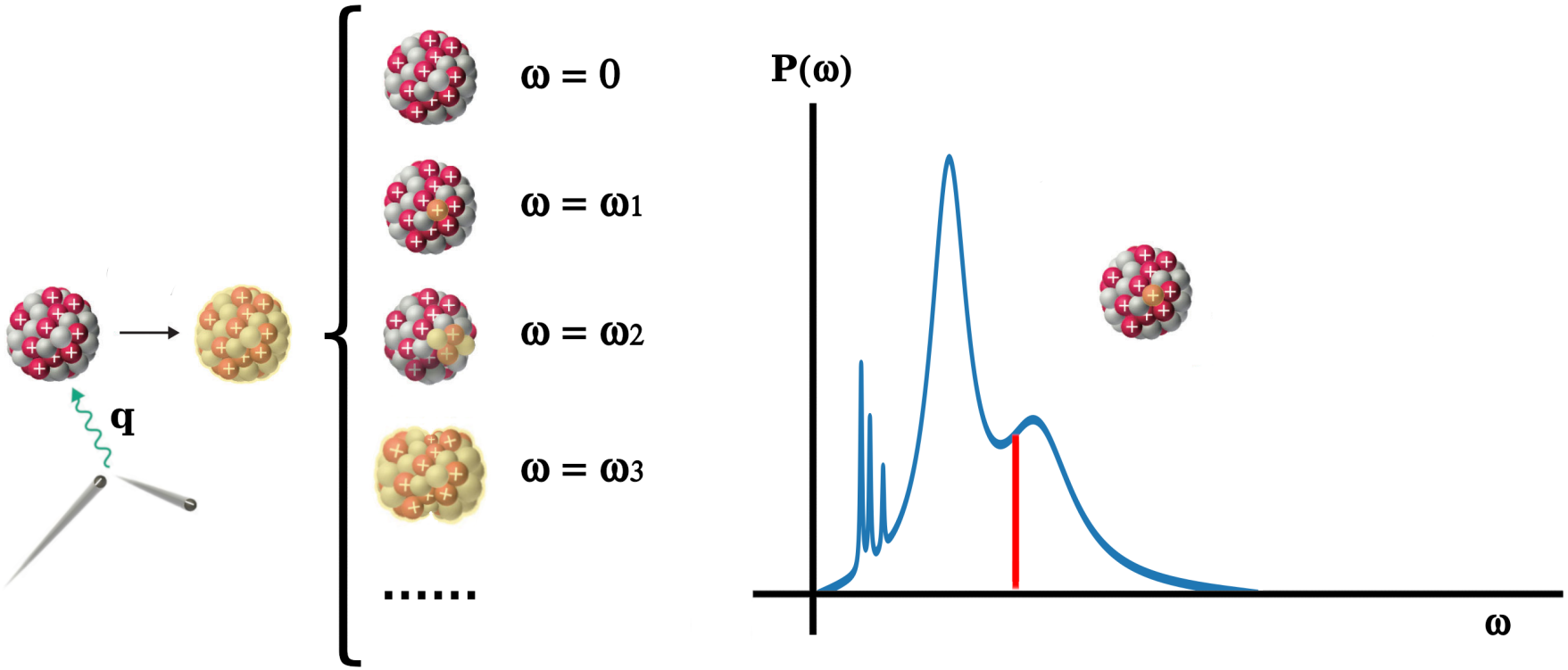
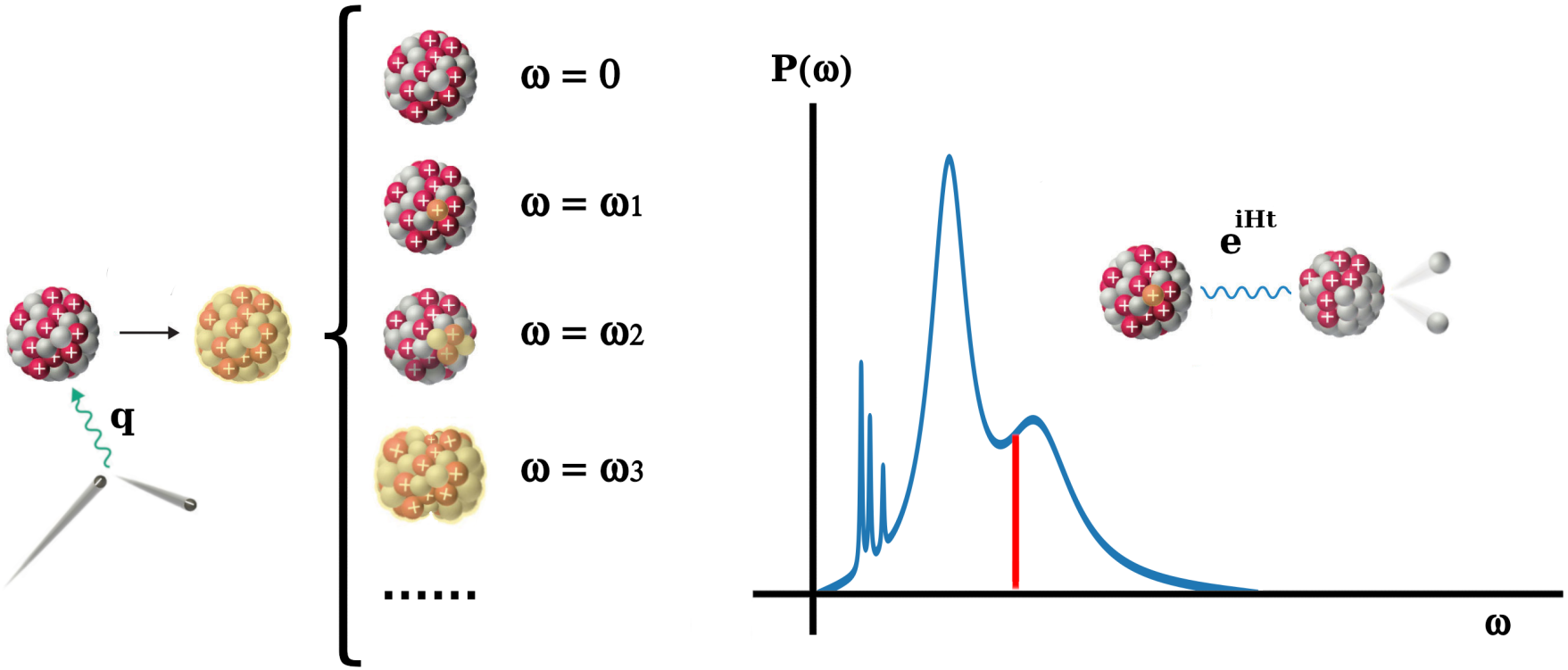
- right after scattering vertex the target is left in excited state
- energy measurement selects subset of final nuclear states



Roggero & Carlson (2019)

Idealized algorithm for exclusive processes at fixed q

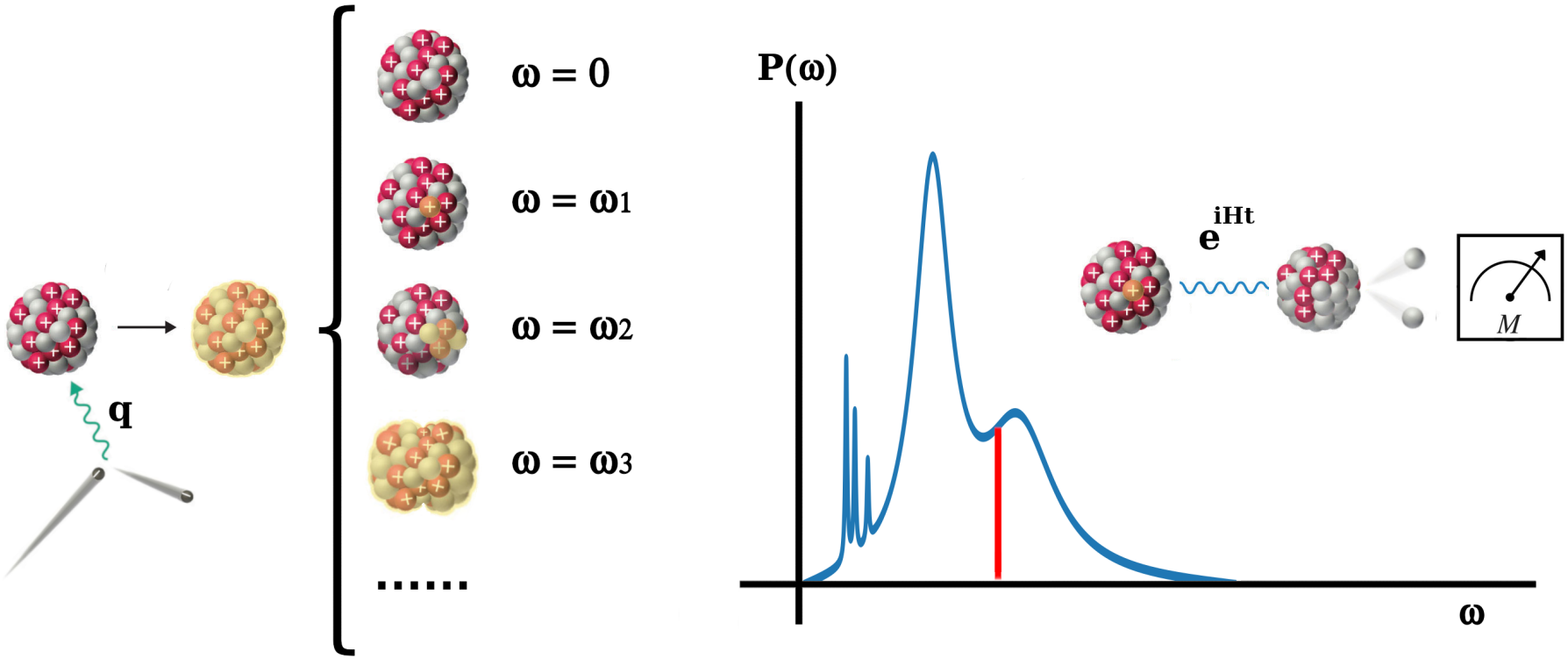
- prepare the target ground state
- right after scattering vertex the target is left in excited state
- energy measurement selects subset of final nuclear states
- further time evolution to let system decay



Roggero & Carlson (2019)

Idealized algorithm for exclusive processes at fixed q

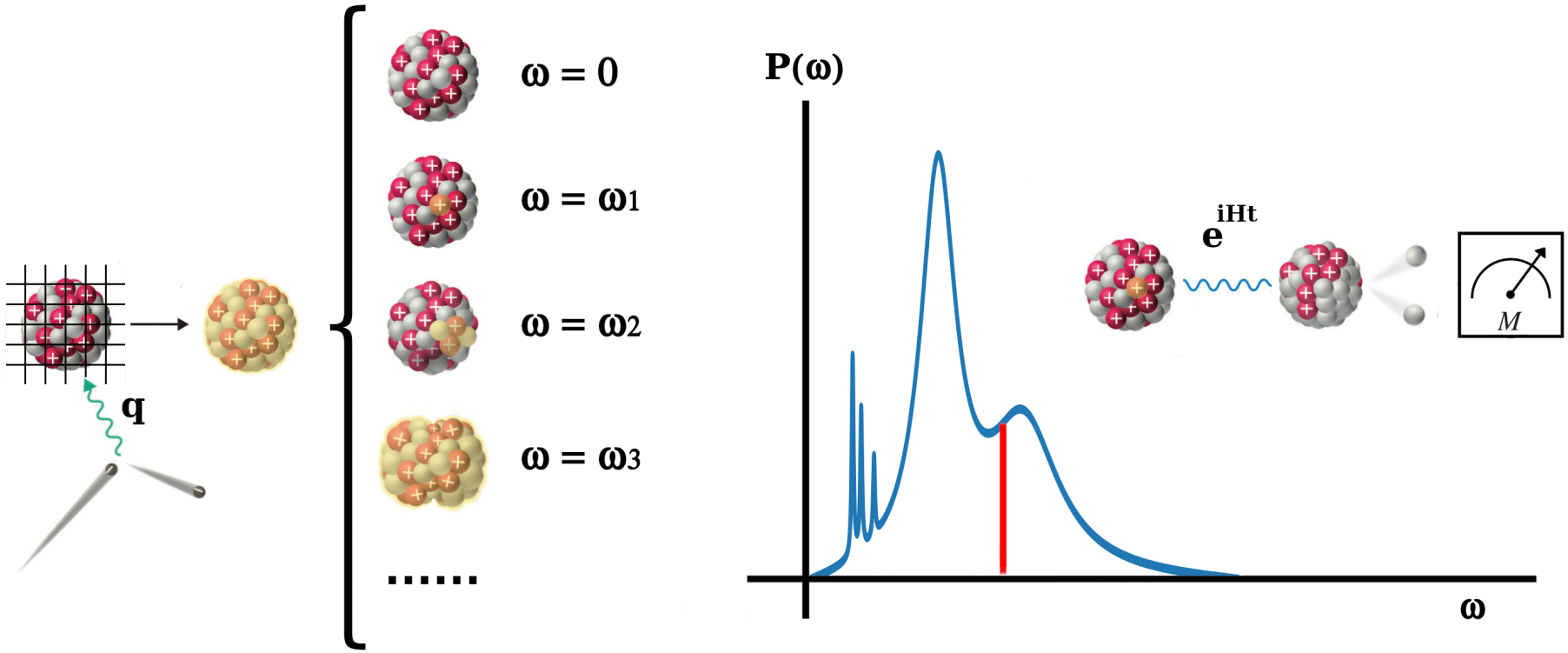
- prepare the target ground state
- right after scattering vertex the target is left in excited state
- energy measurement selects subset of final nuclear states
- further time evolution to let system decay
- measure asymptotic state in detector



Roggero & Carlson (2019)

Quantum algorithm for exclusive processes at fixed q

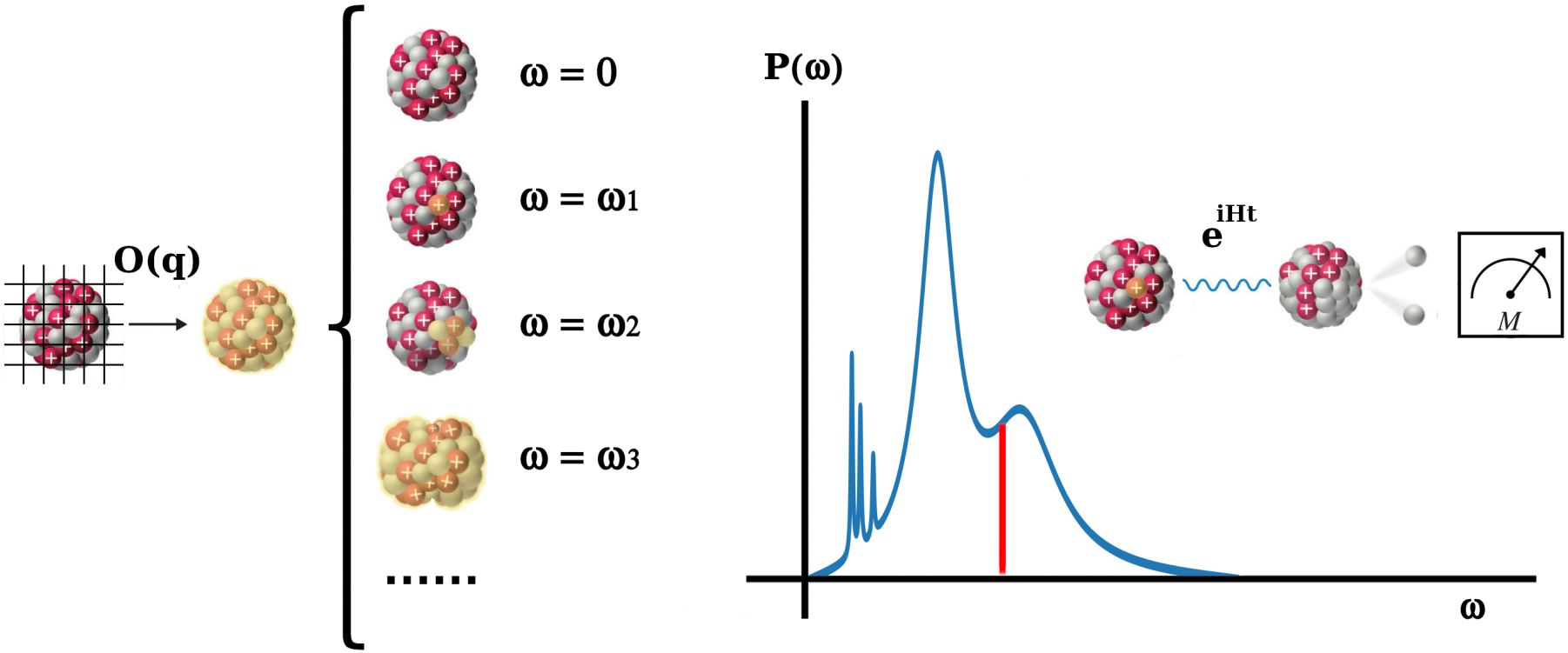
- prepare the target ground state on a finite qubit basis
- right after scattering vertex the target is left in excited state
- energy measurement selects subset of final nuclear states
- further time evolution to let system decay
- measure asymptotic state in detector



Roggero & Carlson (2019)

Quantum algorithm for exclusive processes at fixed q

- prepare the target ground state on a finite qubit basis
- apply vertex operator $O(q)$ to ground state probabilistically
- energy measurement selects subset of final nuclear states
- further time evolution to let system decay
- measure asymptotic state in detector

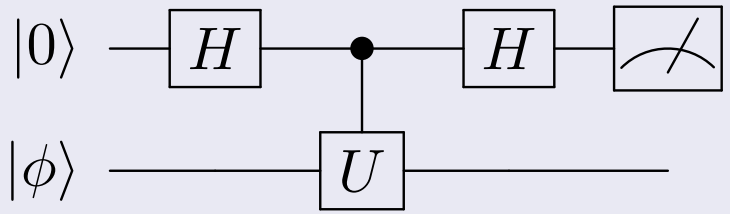


Roggero & Carlson (2019)

Can we apply a non-unitary operation?

YES, but only with some probability

- this can be useful when excitation operator is not unitary



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

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

Can we apply a non-unitary operation?

YES, but only with some probability

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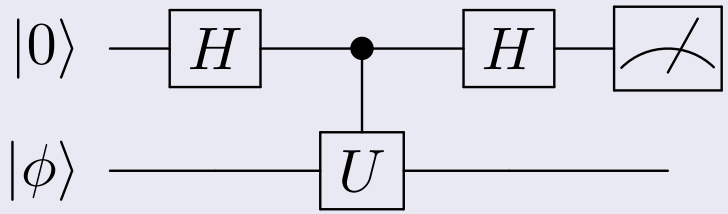

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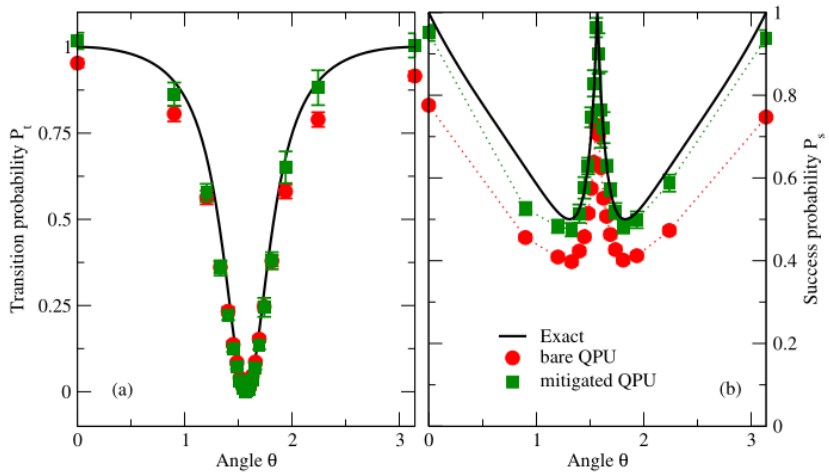
- generalization to many U possible
- tested on IBM devices for $np \to d\gamma$
  - simple $M1$ transition ${}^1S_0 \to {}^3S_1$
  - 2 qubits for $|\phi\rangle$, 3 for controls



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

Quantum algorithm for exclusive processes at fixed q

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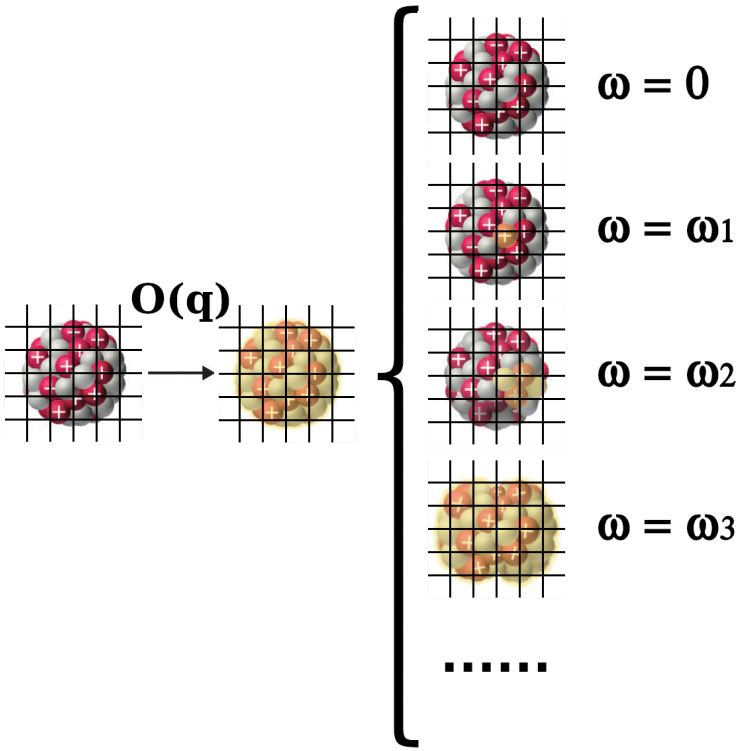

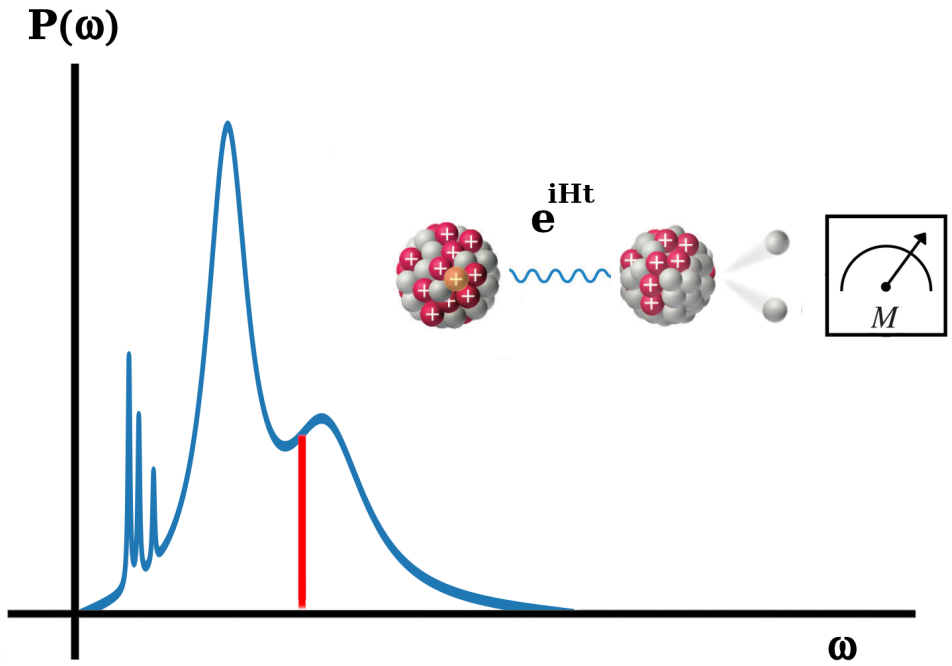

Roggero & Carlson (2019)

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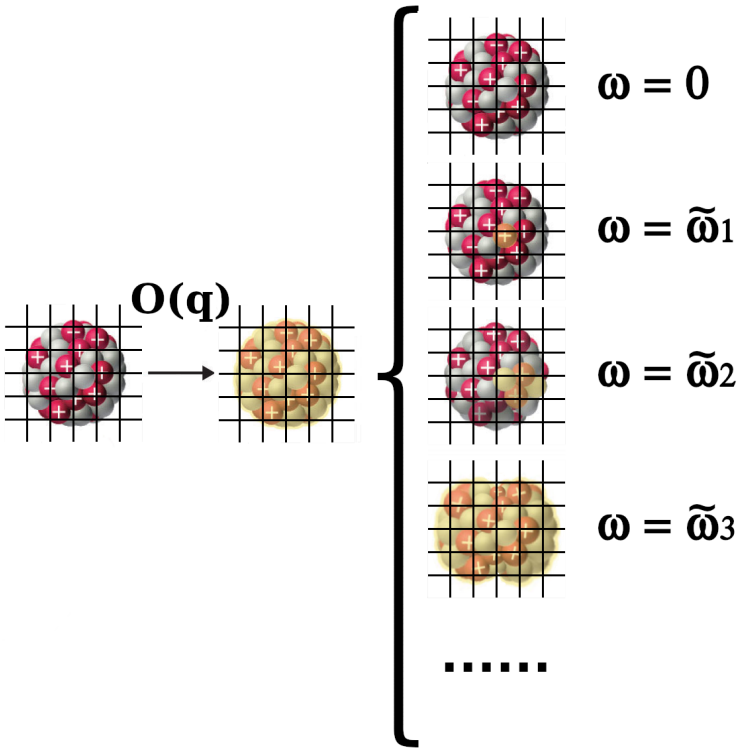
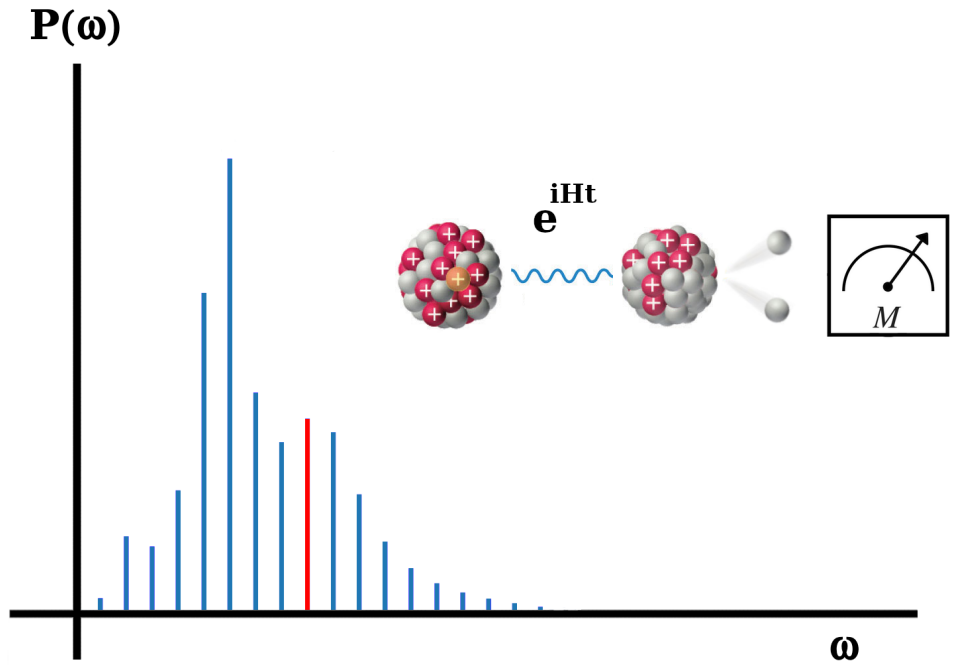
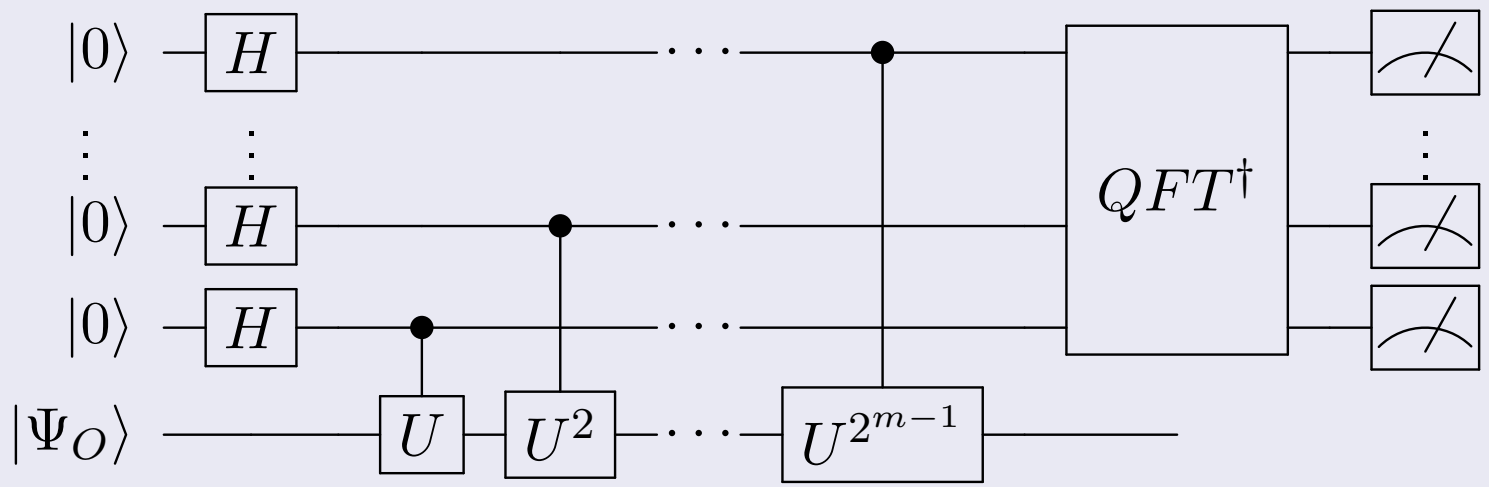




Roggero & Carlson (2019)

QPE on general states



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

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

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

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

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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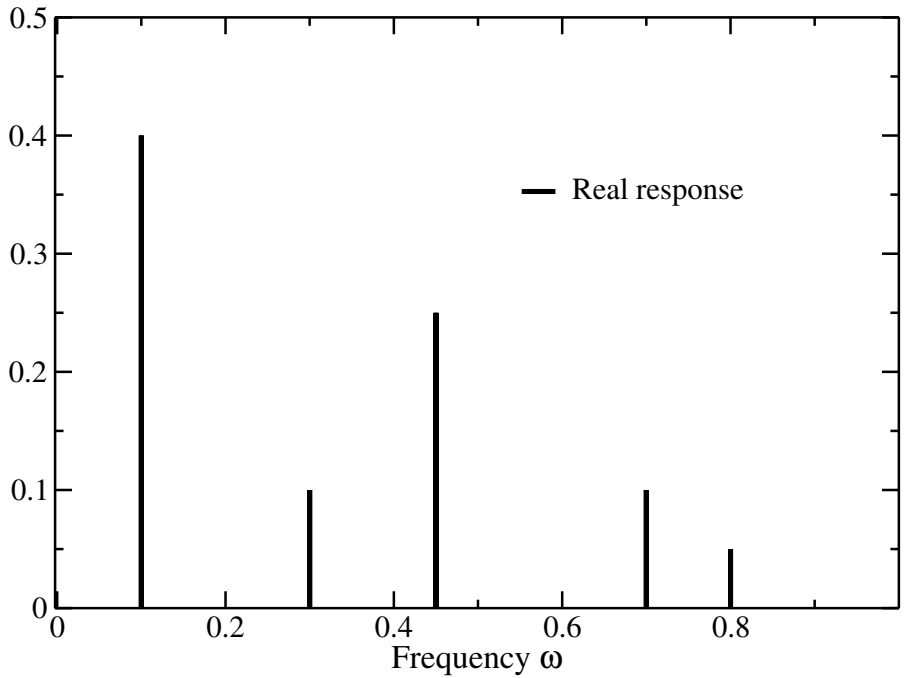

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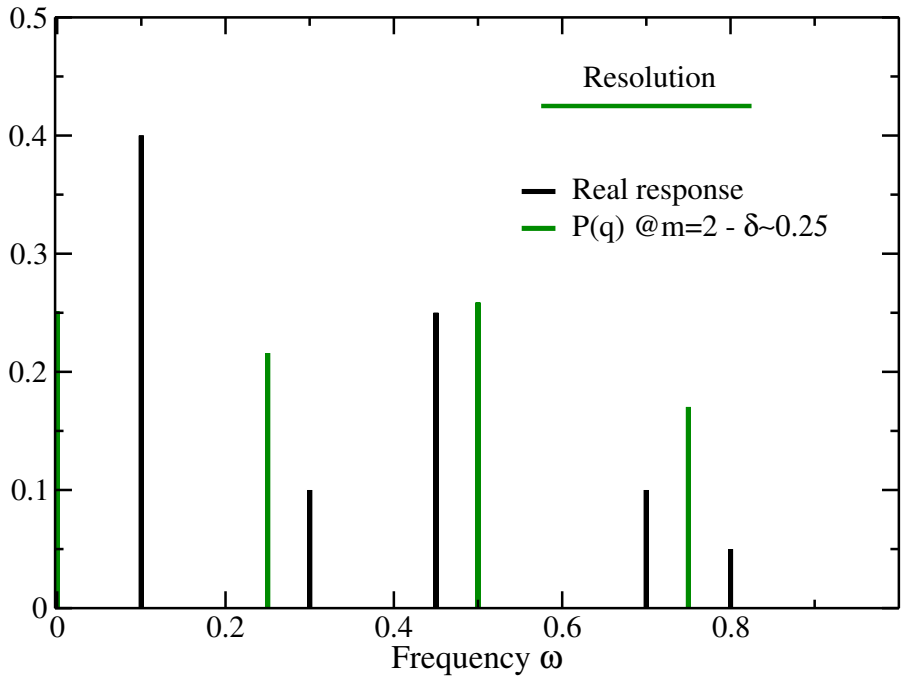

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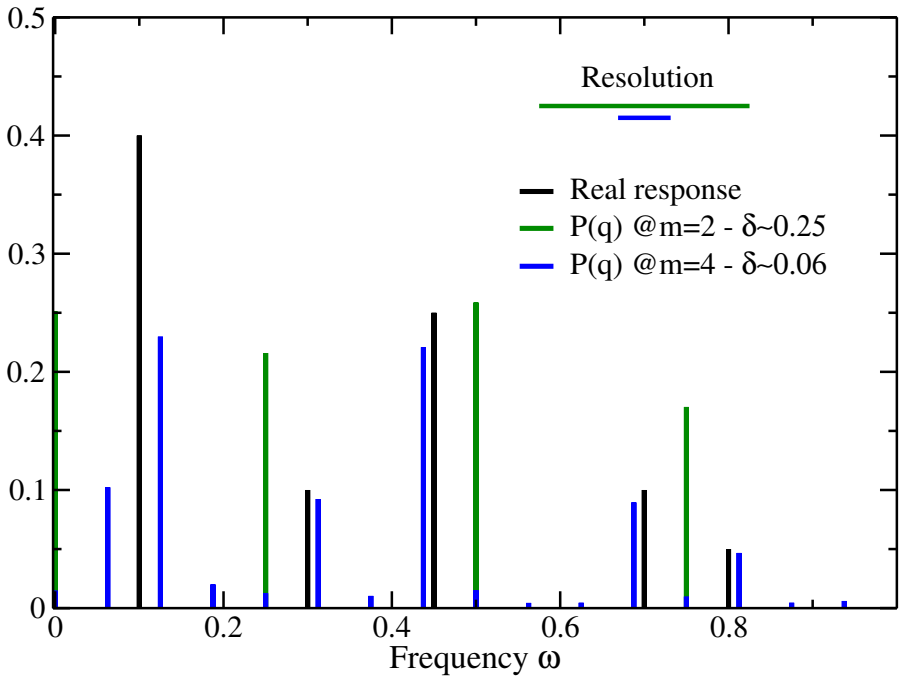

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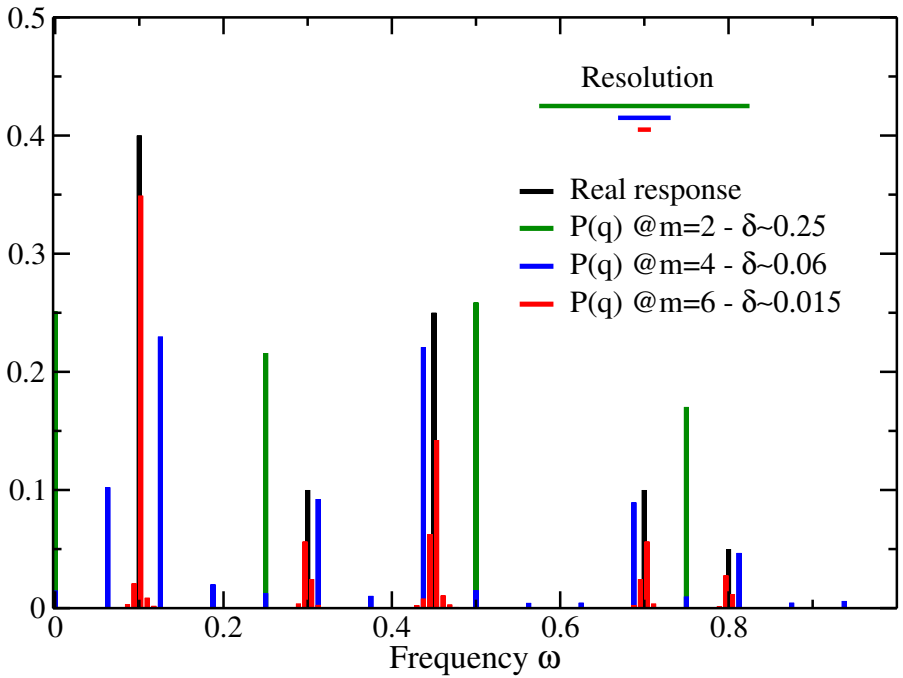
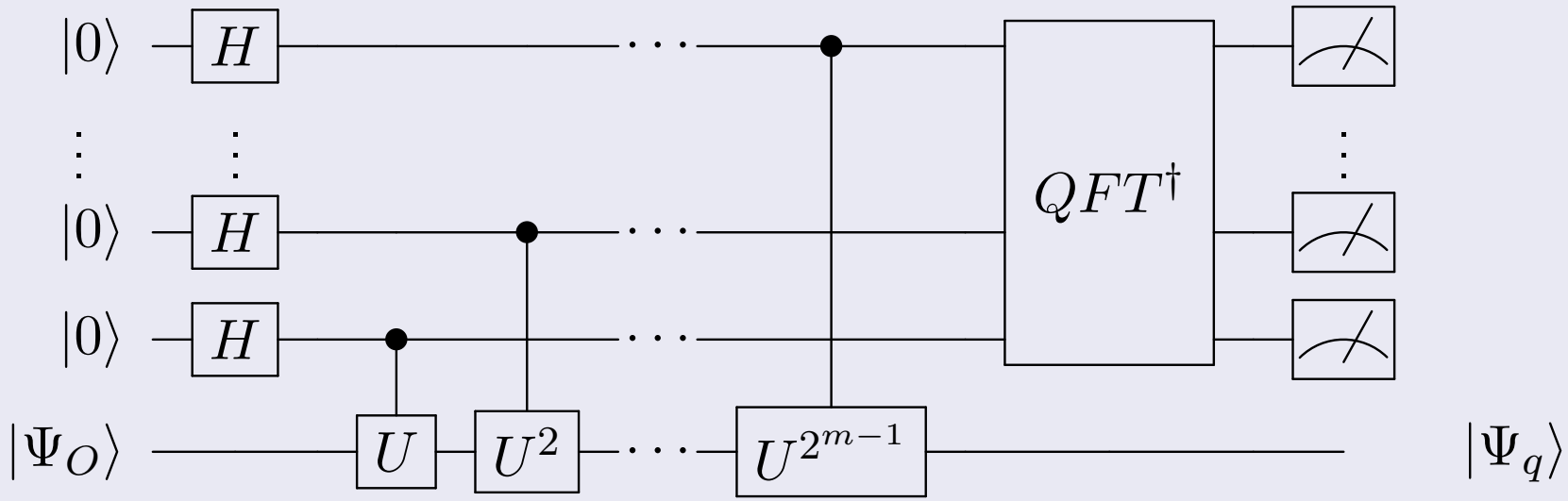


QPE as state preparation



- 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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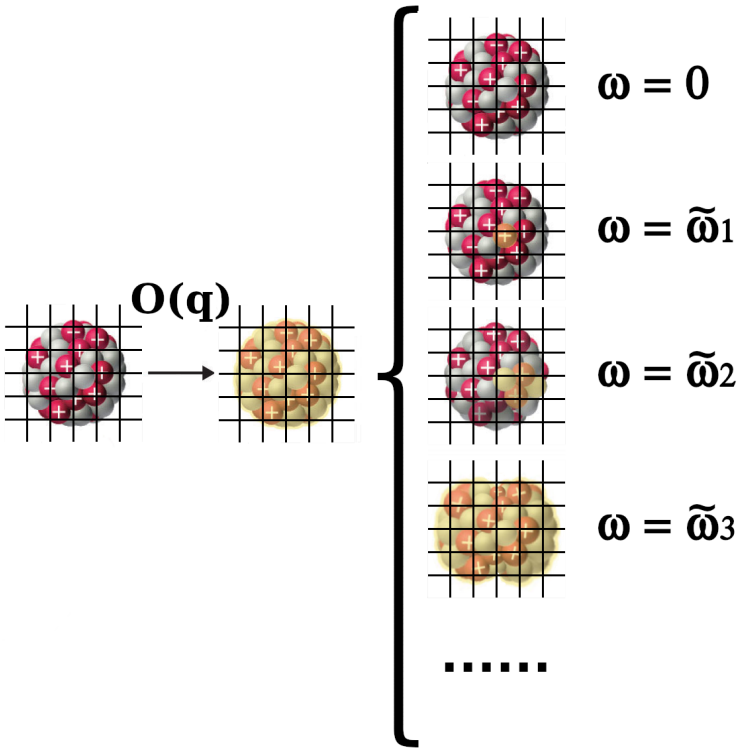

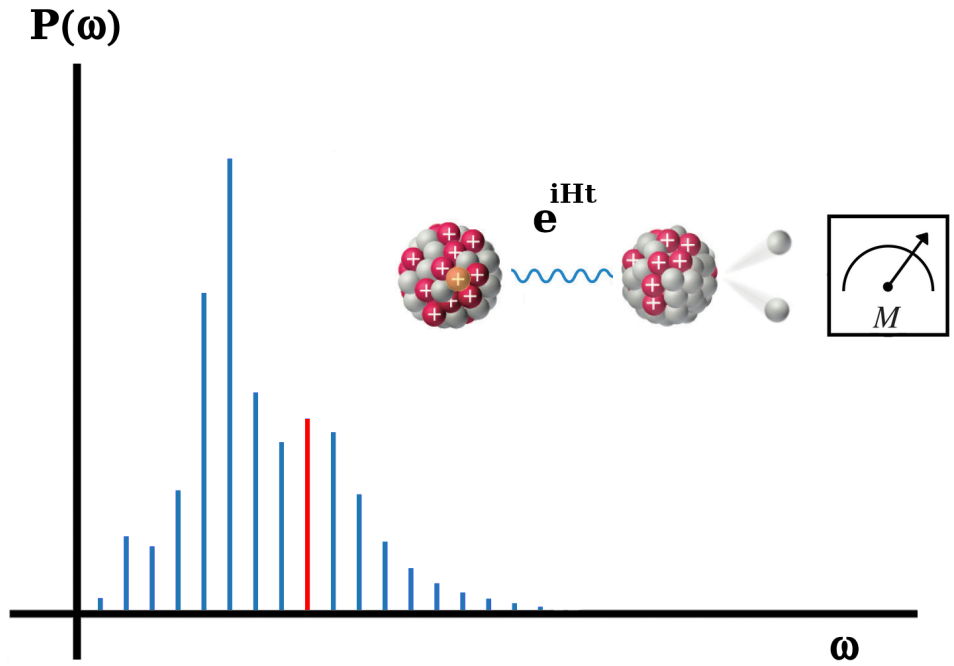

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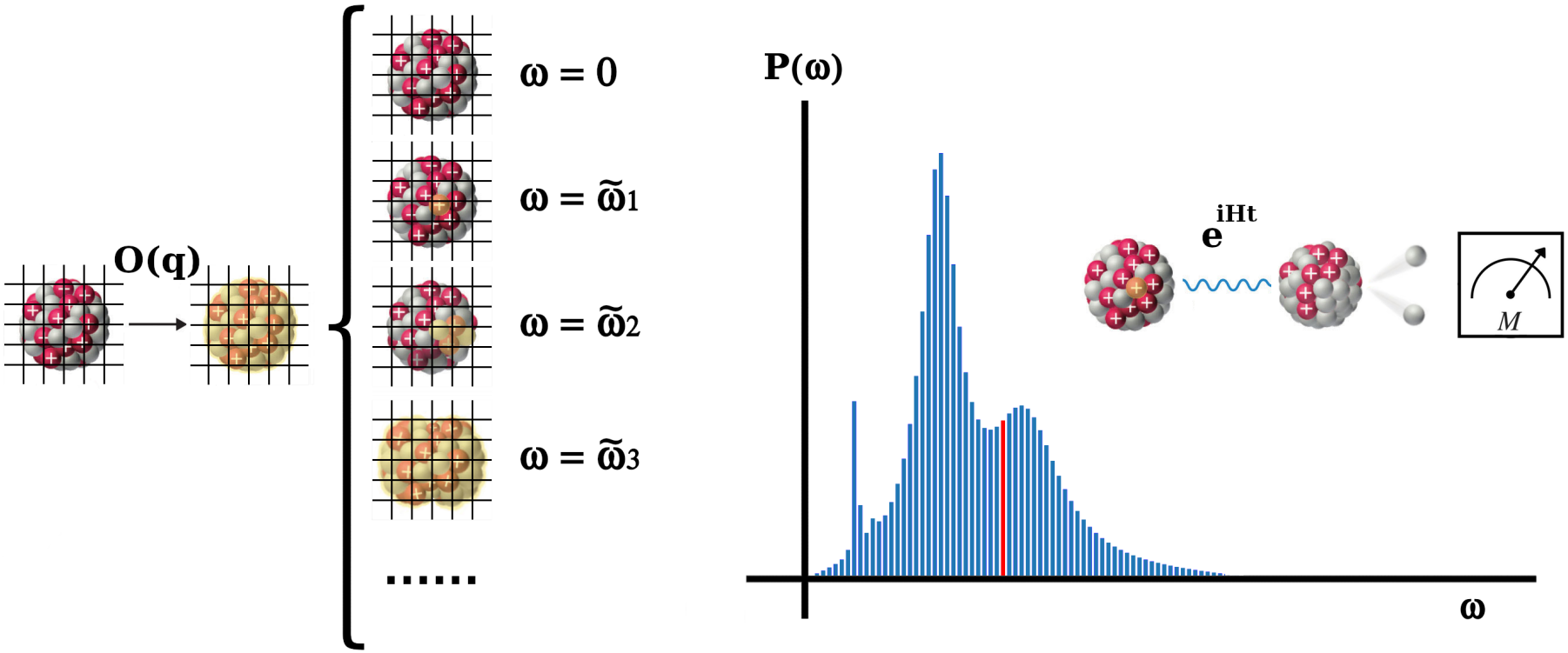

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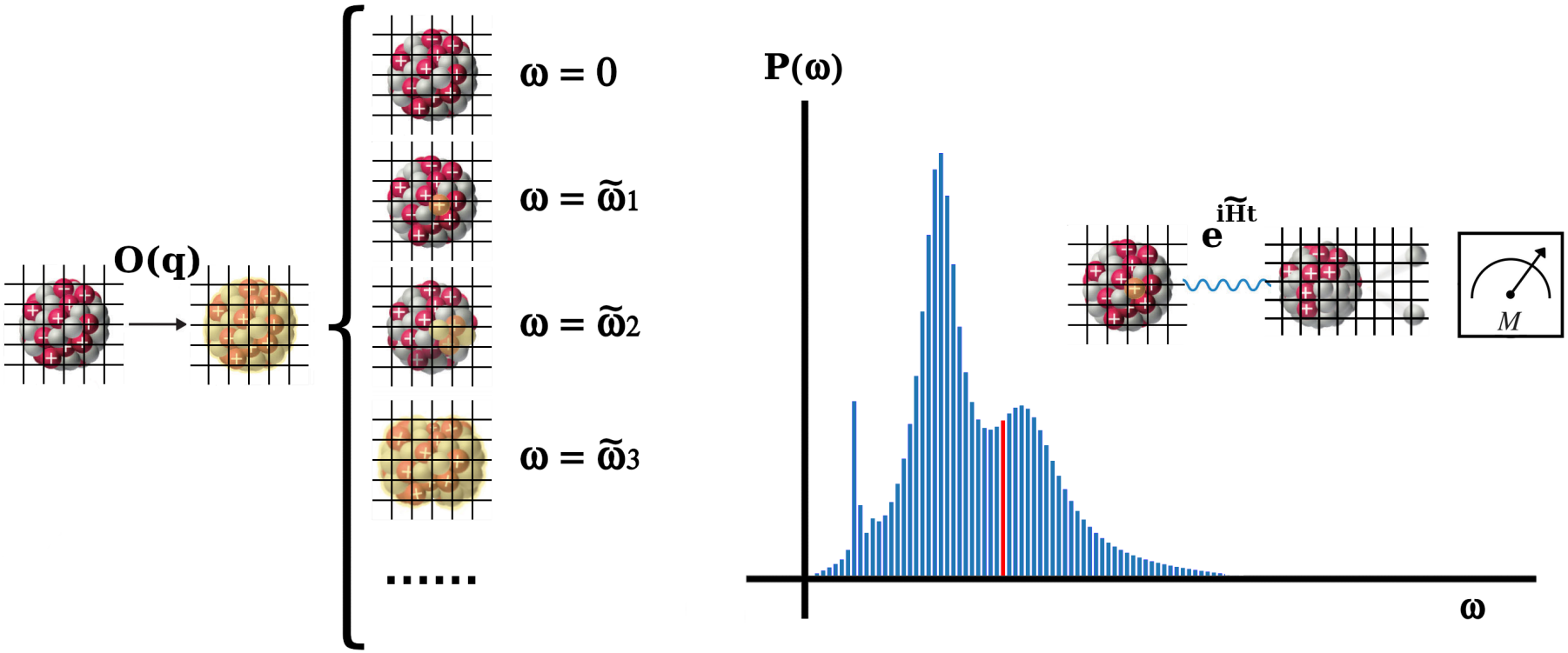

Roggero & Carlson (2019)

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

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

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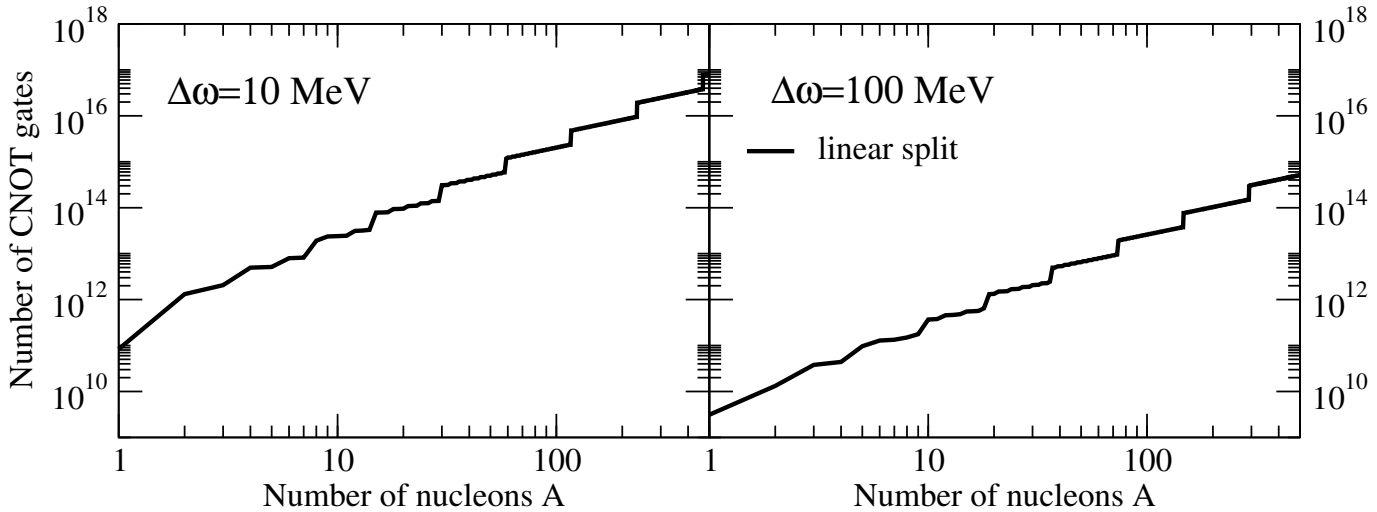

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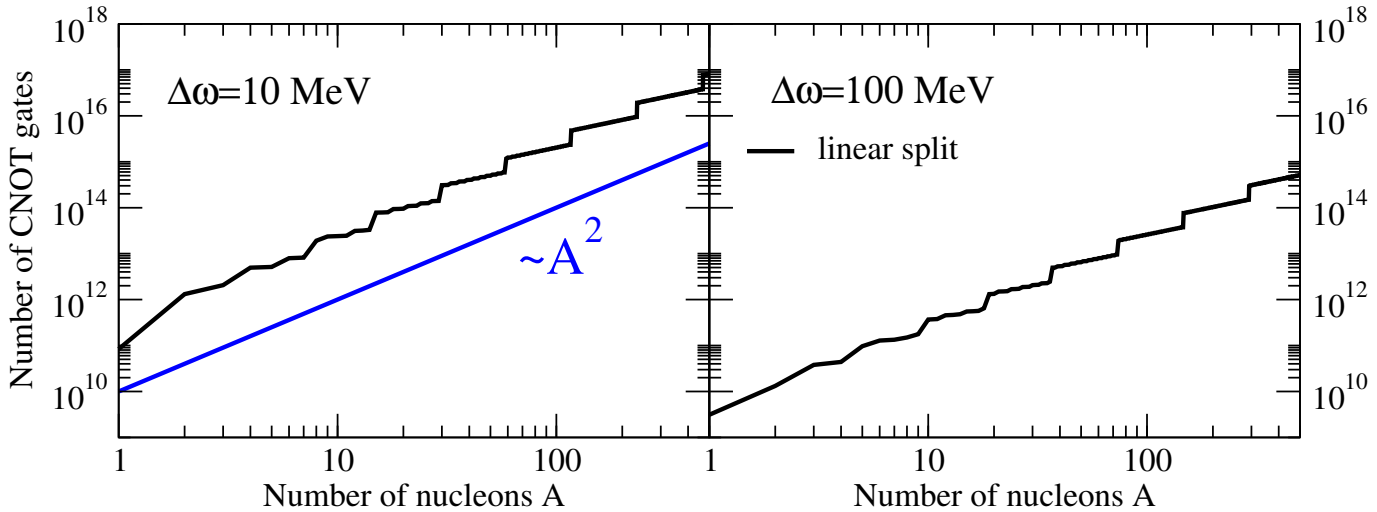

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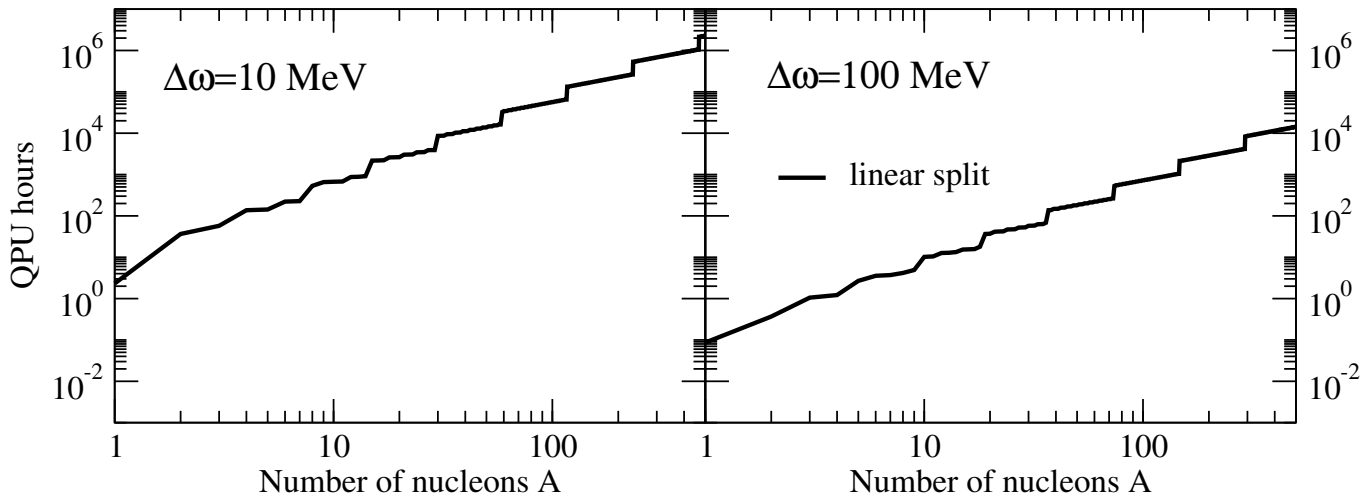

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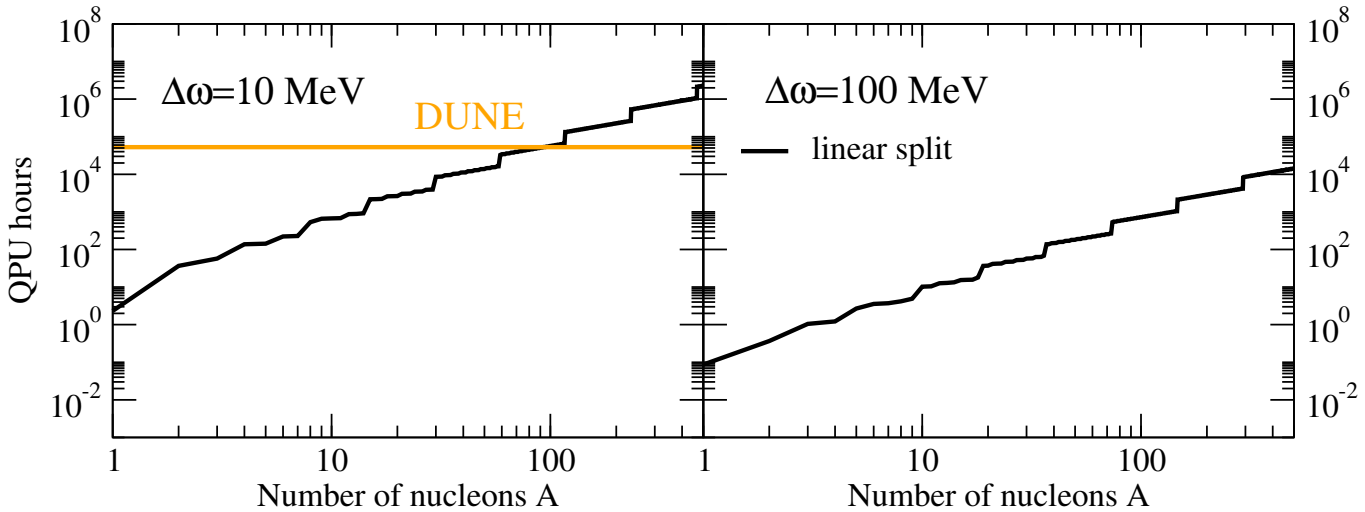

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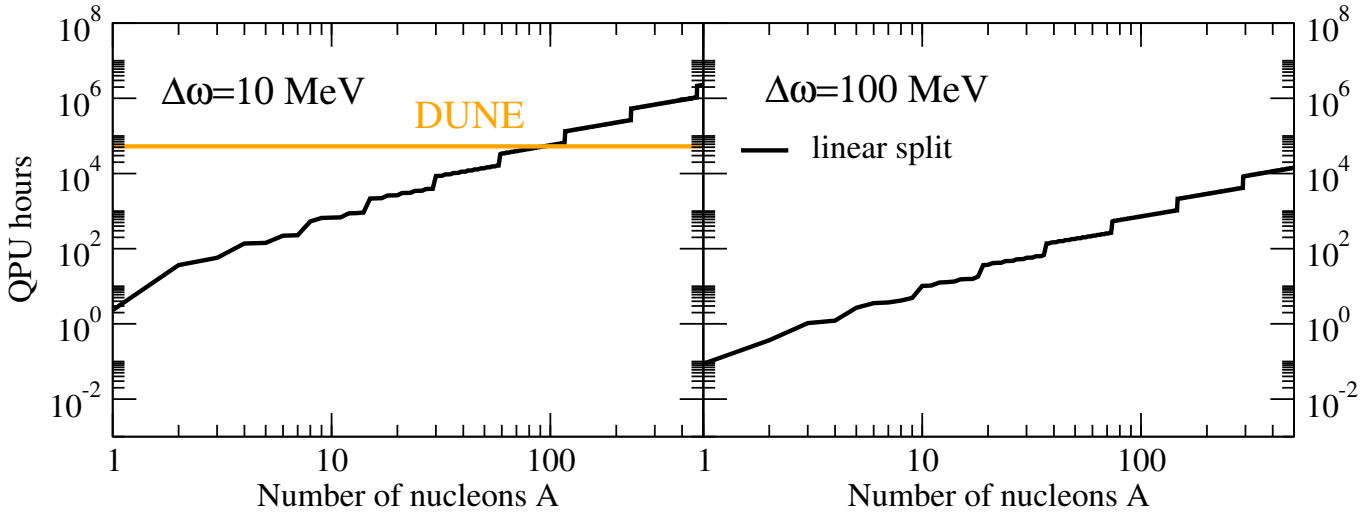

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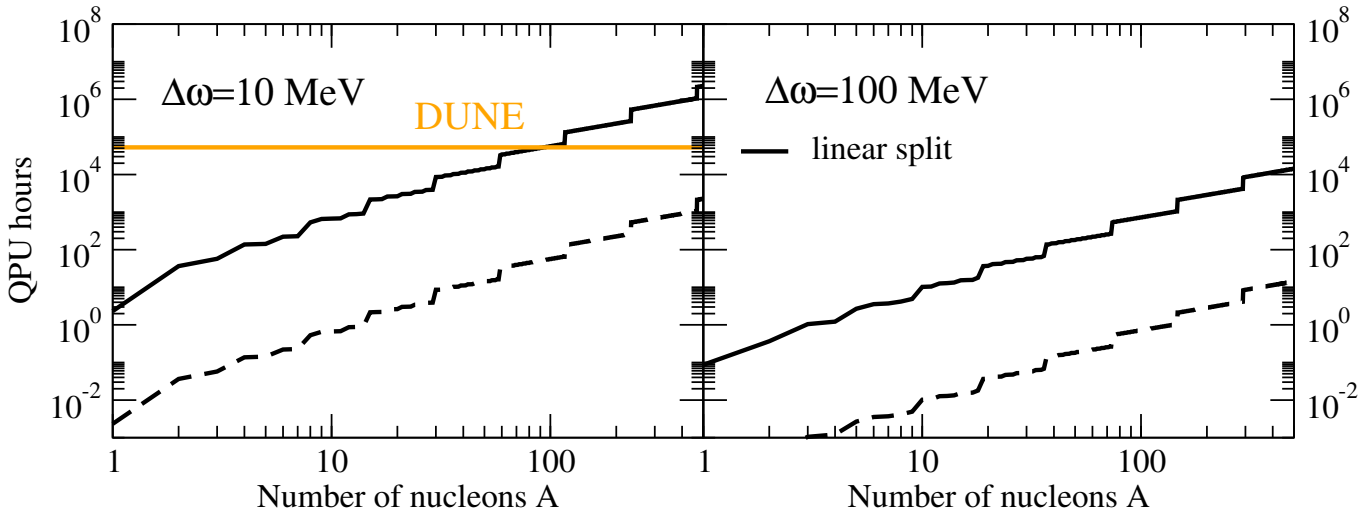

- simple scheme: we need to keep coherence for ≈ 15 months (6 days)
- parallel scheme: we need to keep coherence for ≈ 11 hours (9 minutes)

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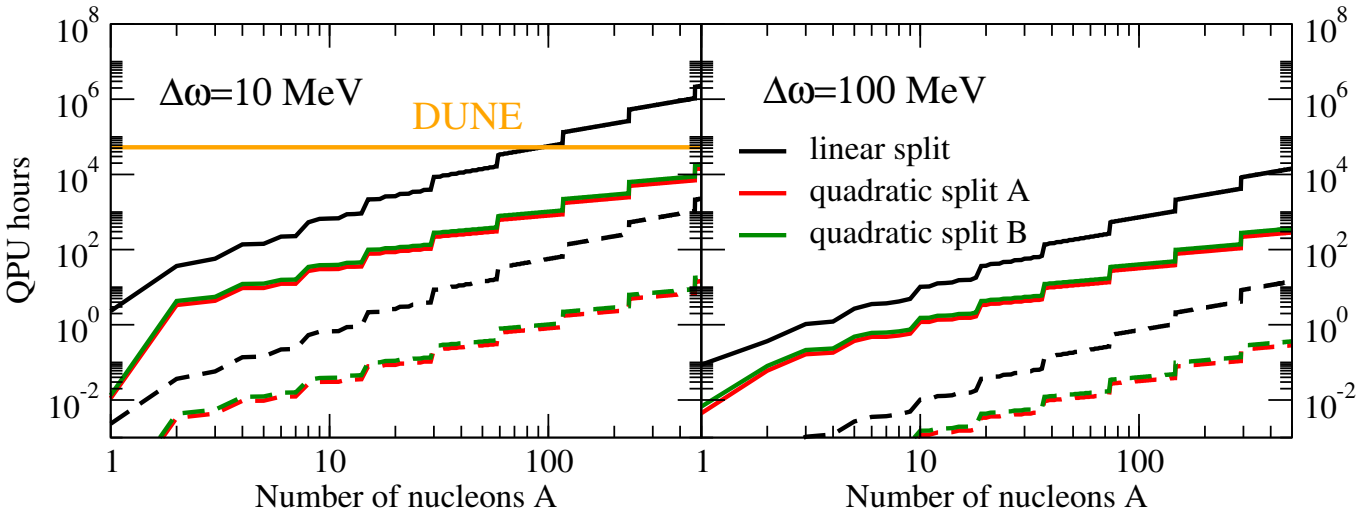

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- parallel scheme: we need to keep coherence for ≈ 11 hours (9 minutes)
- faster schemes: we need to keep coherence for ≈ 15 minutes (36 sec.)

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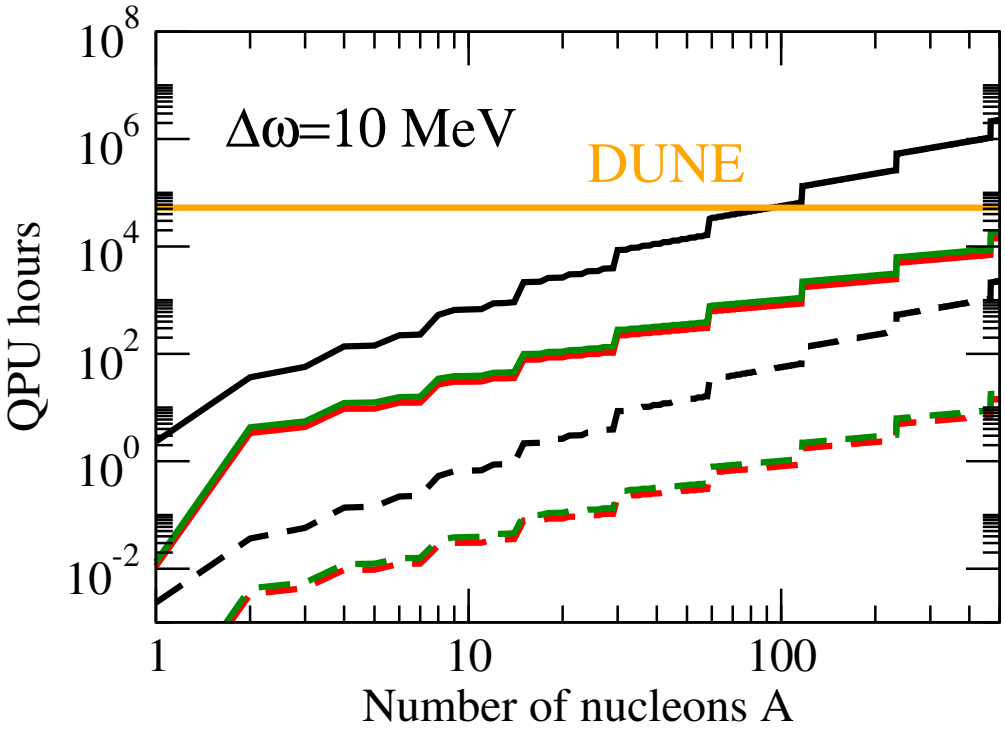

coherence time for ^{40}Ar

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 (2020)

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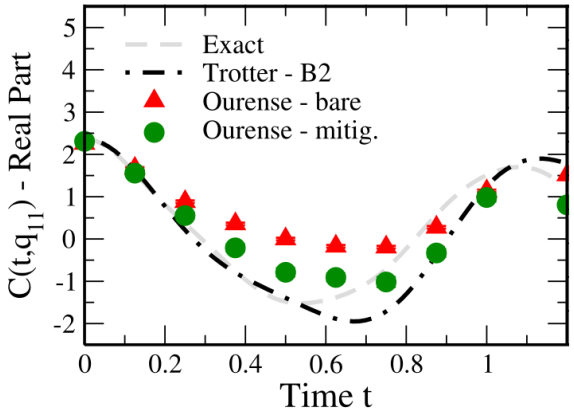
- both algorithms have a gate cost of $\mathcal{O}\left(\text{poly}(A)/\Delta\right)$ for A nucleons and target energy resolution Δ!
- both algorithms are (probably) too expensive for a realistic description of neutrino scattering off of ^{40}Ar with NISQ devices

Future perspectives on quantum simulations



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- gate fidelity still not at ideal level

A.Baroni, J.Carlson, R.Gupta, A.Li, G.Perdue, A.R. (2022)

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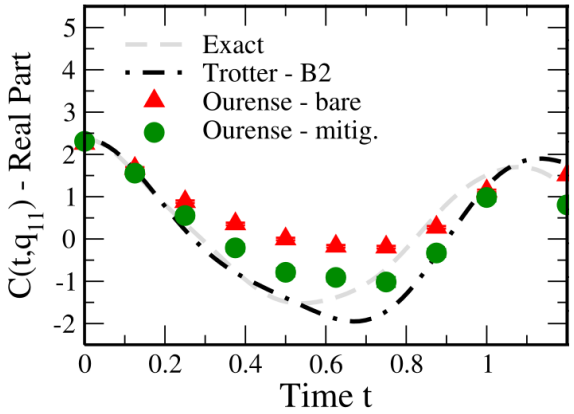

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- we can measure time-dependent entanglement evolution
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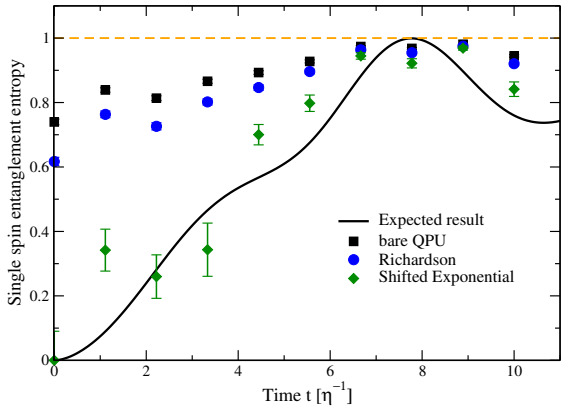
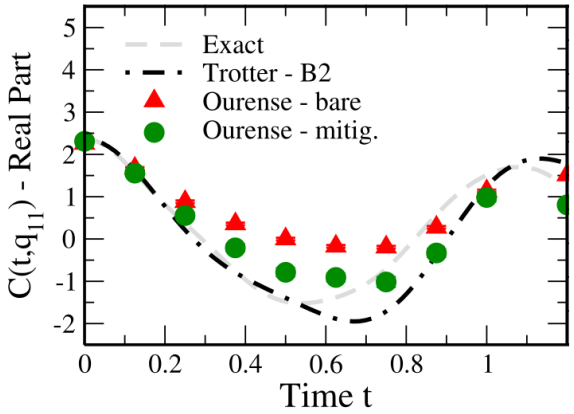


Future perspectives on quantum simulations



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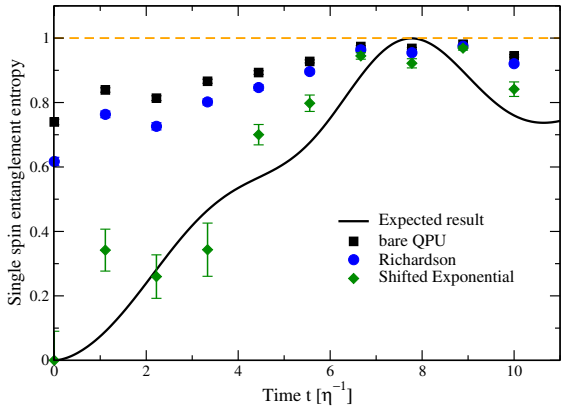
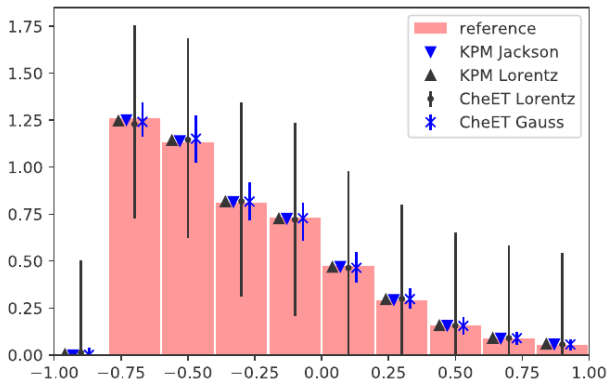




- quantum devices are not quite where we would like them to be
- can we port quantum algorithms to classical simulations?

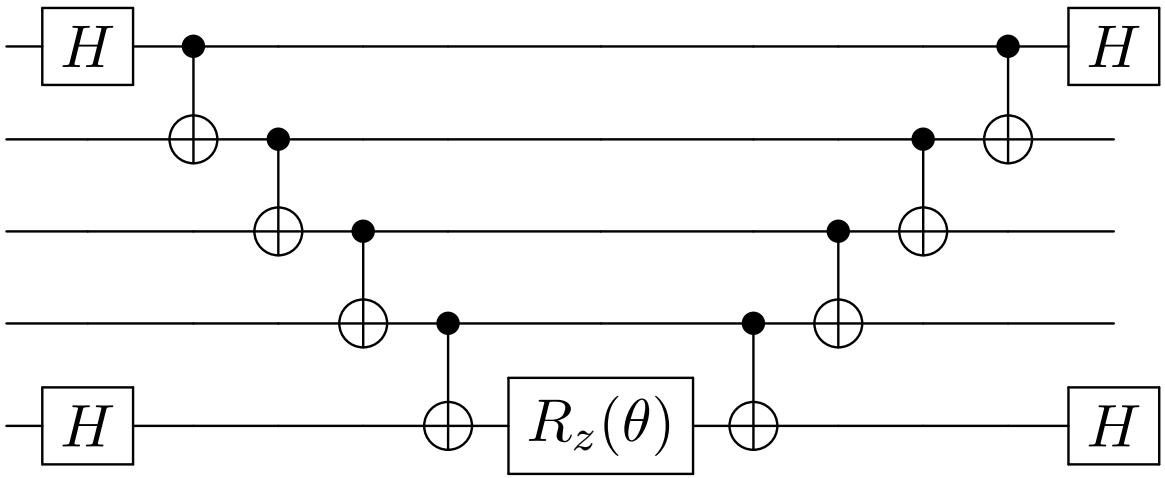
J.Sobczyk & A.R. (2022)

Problem of non-locality of Jordan-Wigner mapping

The Jordan-Wigner mapping stores the information about the fermionic parity into strings of Z operators between fermionic modes:

$$a_p^\dagger a_q = \frac{X_p X_q + Y_p Y_q}{2} \left(Z_{p+1} \cdots Z_{q-1}\right)$$

This leads to large CNOT circuits to compute the parity, for instance



$$= \exp\left(i\frac{\theta}{2} X_1 X_5 Z_2 Z_3 Z_4\right)$$

When executing the full propagator many phases cancel [Hastings et al. (2014)]

$$U_1(\tau) = \prod_{p,q} \exp(i\tau h_{p,q} a_p^\dagger a_q)$$

Problem of non-locality of Jordan-Wigner mapping II

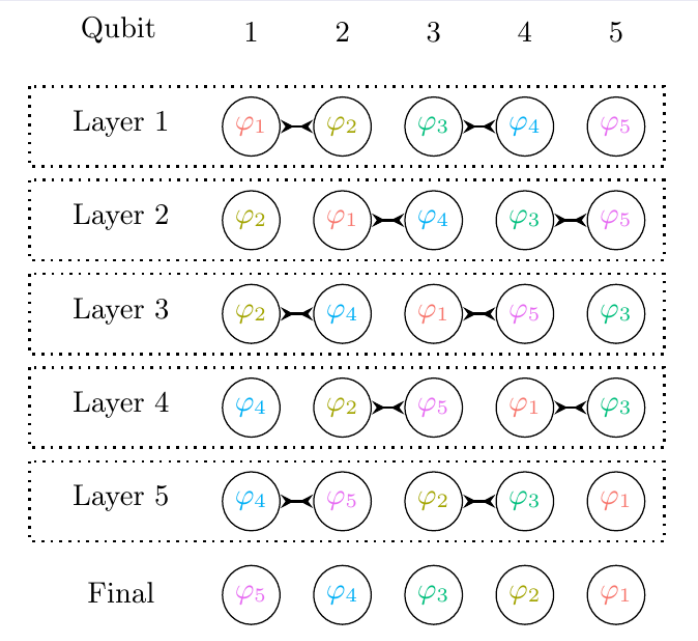
When executing the full propagator many phases cancel [Hastings et al. (2014)]

$$U_1(\tau) = \prod_{p,q}^{n} \exp(i\tau h_{p,q} a_p^\dagger a_q) = \prod_{p,q}^{n} u_{p,q}(\tau)$$

Fermionic Swap Network

Babbush et al. (2017), Kivlichan et al. (2018)

We can implement $U_1(\tau)$ exactly using only $3\binom{n}{2}$ two qubit gates



- n layers of $\frac{n-1}{2}$ two qubit gates

$$W_{i,i+1} = u_{i,i+1}(\tau) f_{SWAP}$$

$$f_{SWAP} = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & -1 \end{pmatrix}$$

- final qubit order is reversed

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

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

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Bit-Flip error

$$\Lambda_X(\rho) = (1-p)\rho + pX\rho X$$

$$|1\rangle \xrightarrow{\Lambda_x} \begin{cases} |1\rangle & \text{with prob} \quad (1-p) \\ |0\rangle & \text{with prob} \quad p \end{cases}$$

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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