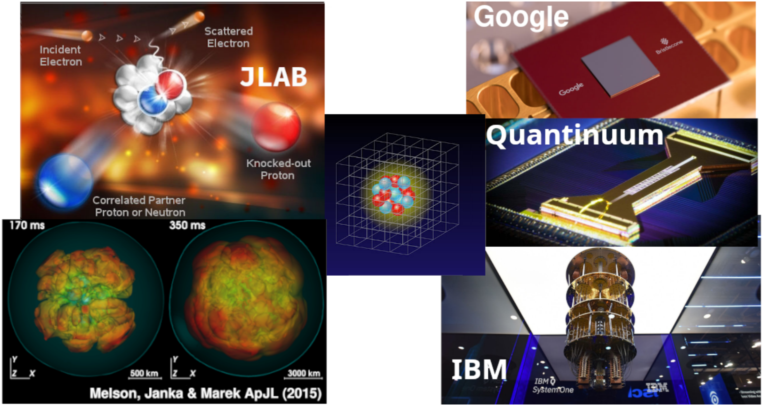
Quantum Computing for Nuclear Physics

Alessandro Roggero



TIFPA INFN

RPMBT22 - Tsukuba

23 Sep, 2024

MOdeling
Nuclear
STructure and
REactions

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

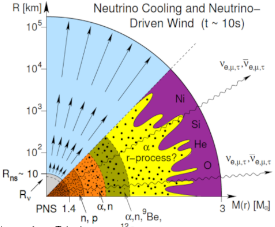
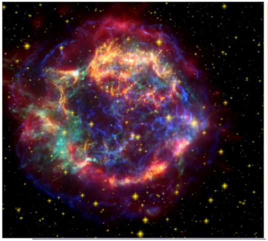


image from T.Janka



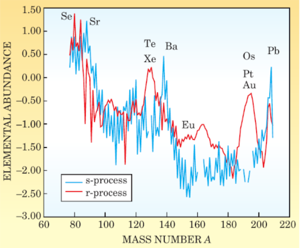
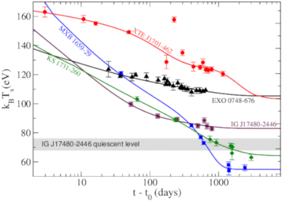


image from Cowan & Thielemann (2004)



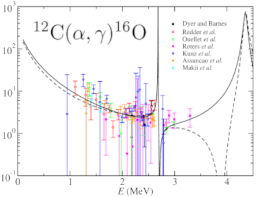
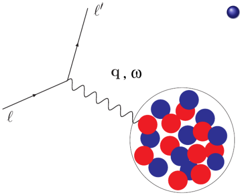


image from Brune & Davis (2015)

Inclusive cross section and the response function



- cross section determined by the 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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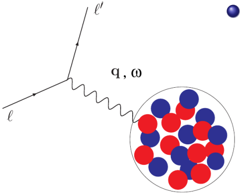

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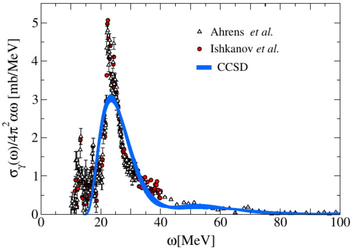
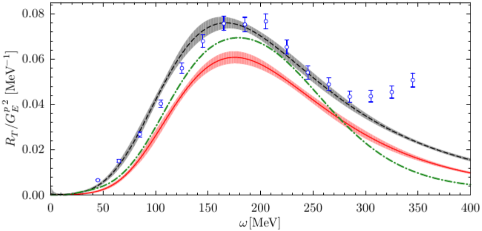
Extremely challenging classically for strongly correlated quantum systems

- dipole response of ^{16}O



Bacca et al. PRL(2013) **LIT+CC**

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



Lovato et al. PRL(2016) **GFMC+Laplace**

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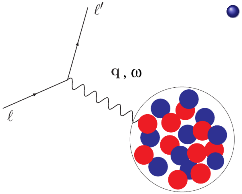

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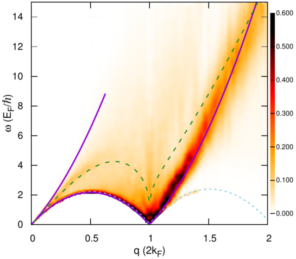
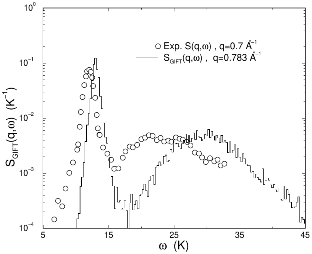
Same structure not only in NP but also condensed matter, chemistry,. . .

- density excitations in 1D-rods



Motta et al. PRA(2016) **QMC+Laplace**

- neutron scattering of liquid ^{4}He



Vitali et al. PRB(2010) **QMC+Laplace**

Many body dynamics with Integral Transforms

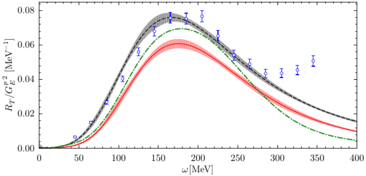
A possible way out with integral transform techniques

Efros (1989), Carlson & Schiavilla (1992), Efros, Leidemann & Orlandini (1994)

$$T(\sigma) = \int d\omega K(\sigma,\omega) R_O(\omega) = \langle 0|\hat{O}^\dagger K\left(\sigma, \hat{H} - E_0\right)\hat{O}|0\rangle$$

Laplace

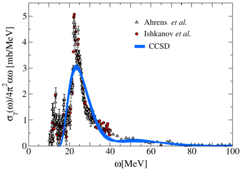
$$K(\sigma,\omega) = e^{-\sigma\omega}$$



Lovato et al. PRL(2016) **GFMC**

Lorentz

$$K(\sigma,\omega;\Gamma) = \frac{\Gamma}{\Gamma^2 + (\sigma-\omega)^2}$$



Bacca et al. PRL(2013) **LIT+CC**

PROBLEM: the inversion procedure is often ill-posed, difficult to assign error bars on the reconstructed response function

Many body dynamics with Integral Transforms II

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Fourier

$$K(\sigma,\omega) = e^{-i\sigma\omega}$$

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The transformation is **unitary** so the inversion is “easy”

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ADVANTAGE: if we did, we could do more than linear response!

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Quantum Computing and Quantum Simulations

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Quantum System we have control over

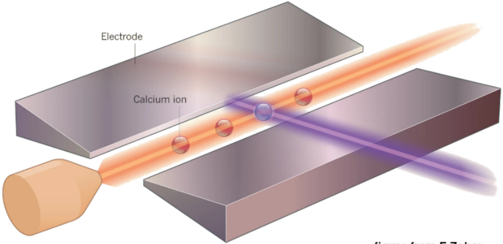

figure from E.Zohar

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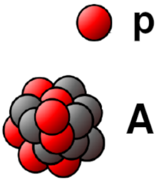

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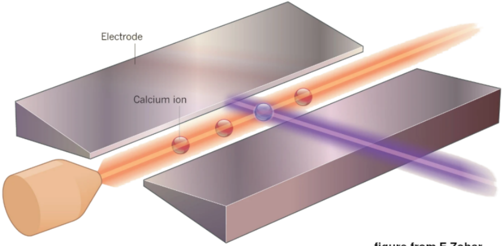

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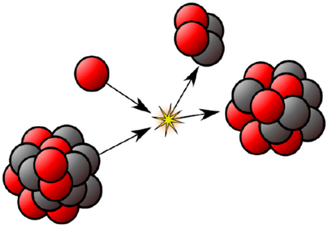

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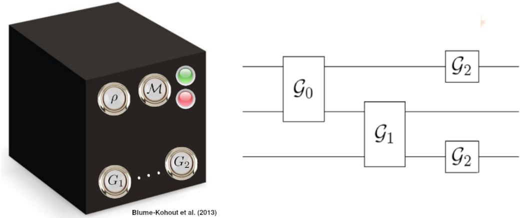

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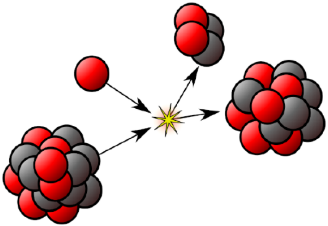
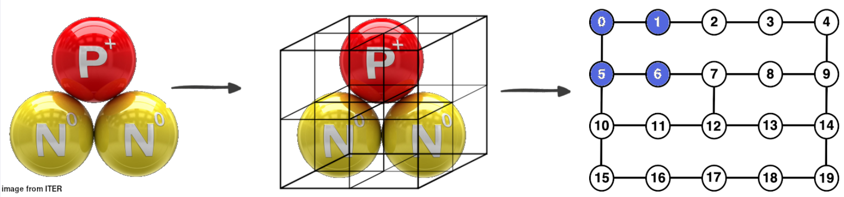


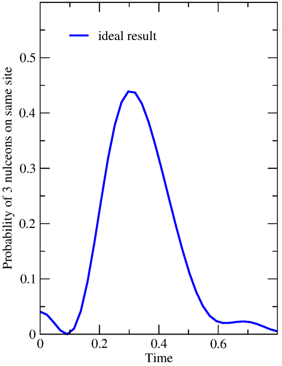
First programmable quantum devices are here

some figures from M.Savage

Real time dynamics on current generation devices

AR, Li, Carlson, Gupta, Perdue PRD(2020)





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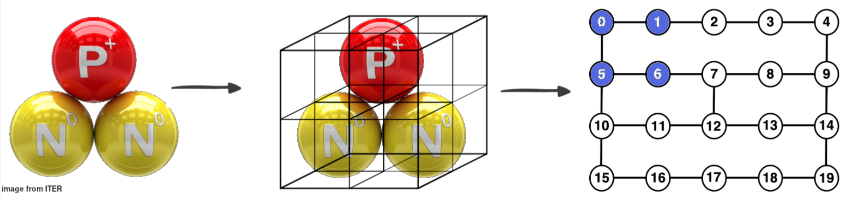
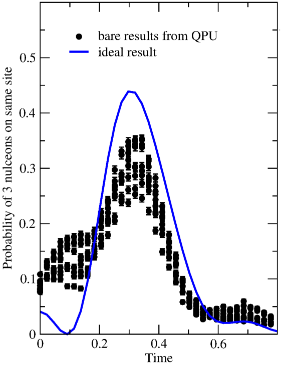
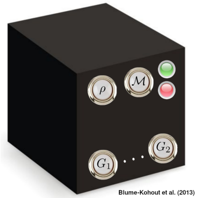




Error sources

- decoherence (environment)
- imperfect calibration



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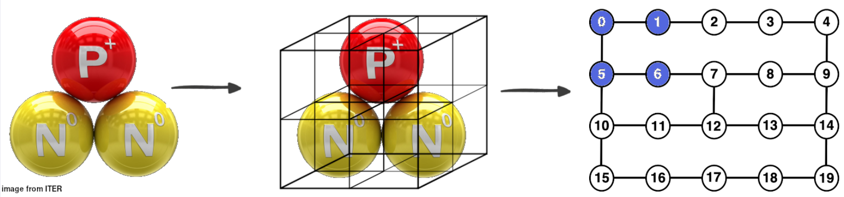
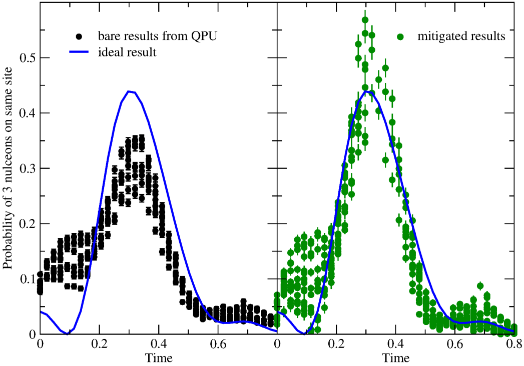
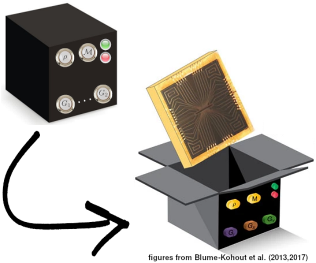




- Error mitigation is crucial

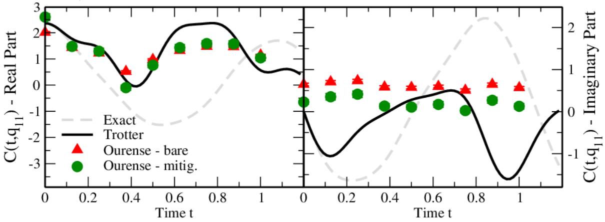


Real time correlators on current generation devices

- First steps toward nuclear response: real-time correlators

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

- Can be done "easily" using one additional qubit (Somma, Ortiz et al. (2001))



Baroni, Carlson, Gupta, Li, Perdue, AR PRD(2022)

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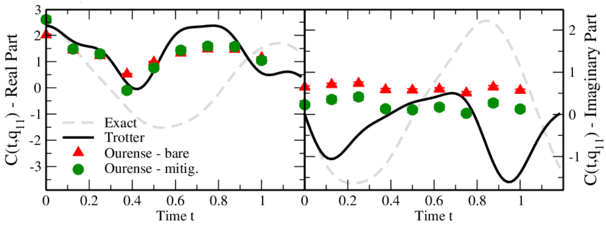


Baroni, Carlson, Gupta, Li, Perdue, AR PRD(2022)

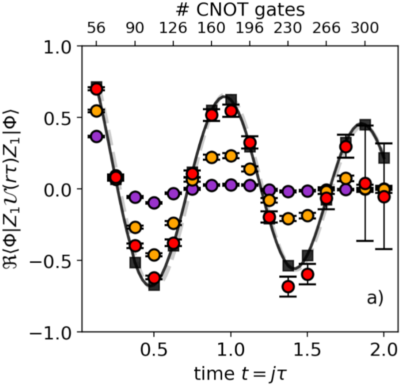
- expensive to control some systematic errors

$$\langle \widetilde{\Psi_0} | O e^{-it(H-E_0)} O | \widetilde{\Psi_0} \rangle \neq \langle \widetilde{\Psi_0} | O(t) O(0) | \widetilde{\Psi_0} \rangle \quad \text{if} \quad | \widetilde{\Psi_0} \rangle \neq | \Psi_0 \rangle$$

Fourier moments on (more) current generation devices

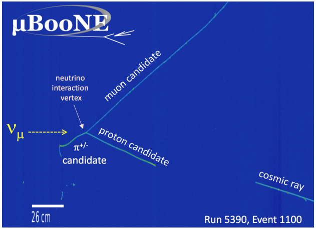
$$R(\omega) \approx \sum_k c_k(\omega) M(t_k) \quad \text{with} \quad M(t) = \langle \Psi_0 | O e^{-iHt} O | \Psi_0 \rangle$$

Both devices and error mitigation have come a long way in last few years



Kiss, Grossi, **AR** arXiv:2401.13048 (2024)

Exclusive cross sections in neutrino oscillation experiments



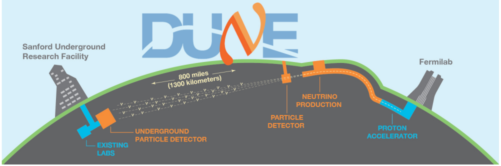
Goals for ν oscillation exp.

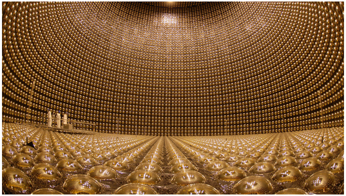
- neutrino masses
- accurate mixing angles
- CP violating phase

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

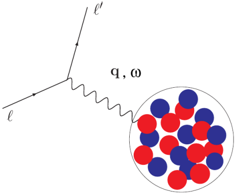
- need to use measured reaction products to constrain E_ν of the event

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





Towards exclusive scattering using quantum computing



- response $R(\omega) \Leftrightarrow$ probability for events at fixed ω
- exclusive x-sec $\rightarrow$ events with specific final states

IDEA: prepare the following state on QC

$$|\Phi\rangle = \sum_\omega \sqrt{R(\omega)}\, |\omega\rangle \otimes |\psi_\omega\rangle$$

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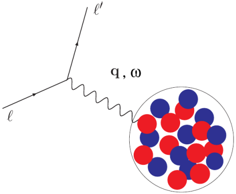

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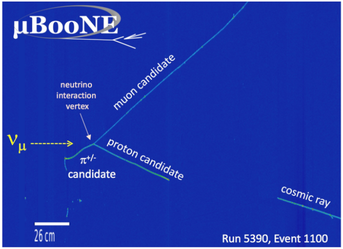
- measurement of first register returns ω with probability $R(\omega)$!
- after measurement, the second register contains final states at ω!

Blume-Kohout et al. (2013)



AR & Carlson PRC(2019)

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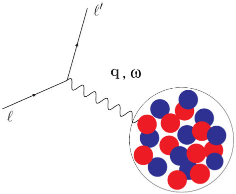

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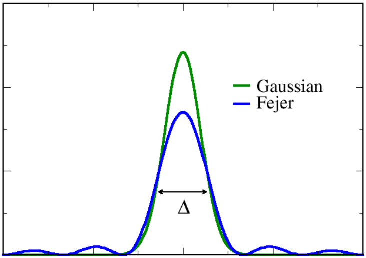
Difficult to prepare $|\Phi\rangle$ but we can prepare instead the following state

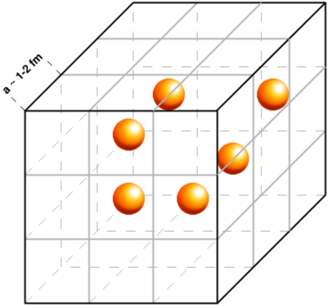
$$|\Phi_\Delta\rangle = \sum_\omega \sqrt{R_\Delta(\omega)}\, |\omega\rangle \otimes |\psi_\omega\rangle$$

with R_Δ an integral transform of the response with energy resolution Δ



AR & Carlson PRC(2019), **AR** PRA(2020)

Prospects of impact of QC on Nuclear Reactions



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 $T \approx 1/\Delta\omega$

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

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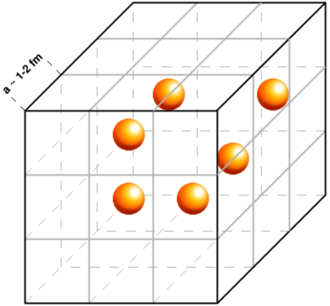

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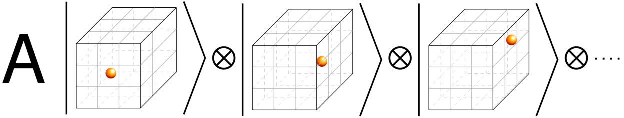

- $10^7 - 10^9$ operations and $\approx 150 - 300$ qubits [**AR**, Spagnoli, Lissoni (in prep.)]

Prospects of impact of QC on Nuclear Reactions

Cost estimates for realistic response in medium mass nuclei

We need $\approx 10^2 - 10^4$ qubits and push the gate buttons $\approx 10^7 - 10^{12}$ times

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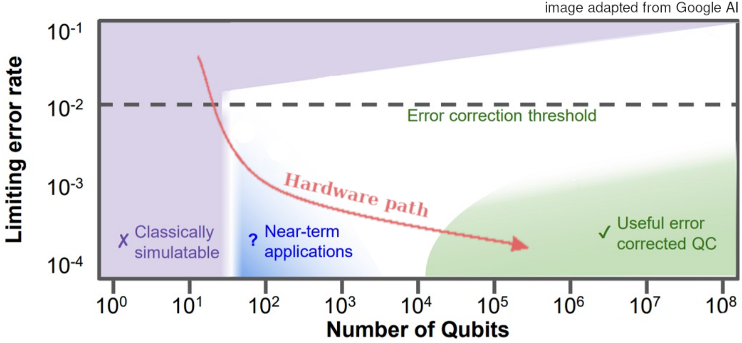

Prospects of impact of QC on Nuclear Physics

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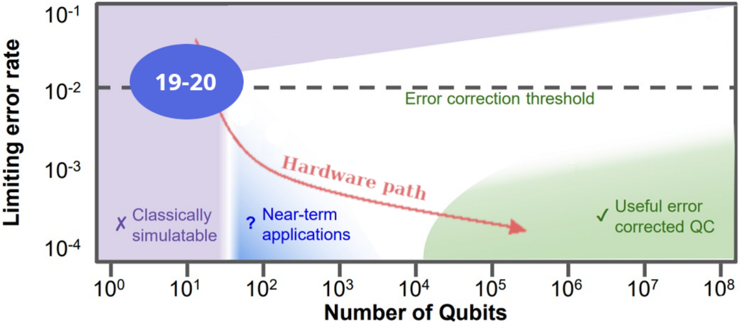
image adapted from Google AI



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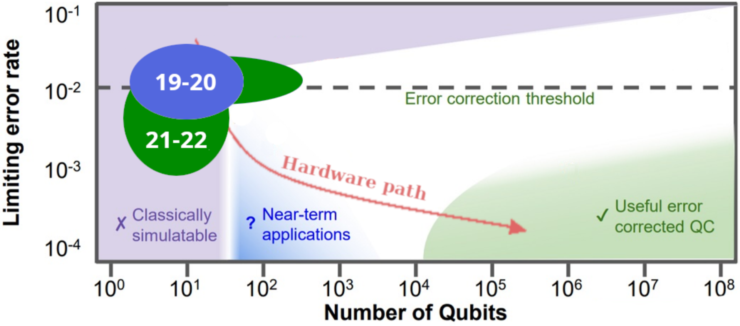

Prospects of impact of QC on Nuclear Physics

Cost estimates for realistic response in medium mass nuclei

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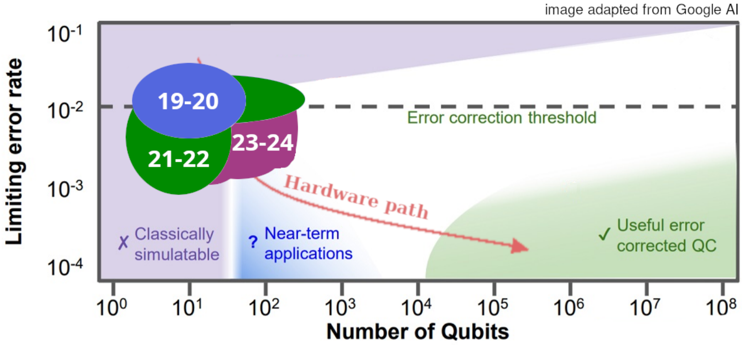

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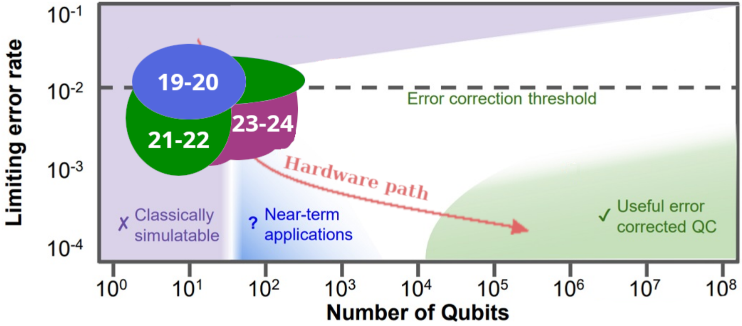


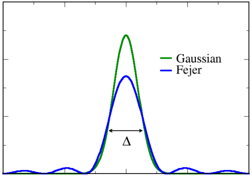
- Still possible to optimize further (bounds are loose)
- Insights for classical methods could come before we have a large QC!

Nuclear dynamics with quantum (inspired) computing?

We can prepare the following state

$$|\Phi_\Delta\rangle = \sum_\omega \sqrt{R_\Delta(\omega)}\,|\omega\rangle \otimes |\psi_\omega\rangle$$

with R_Δ an integral transform of the response with energy resolution Δ



AR & Carlson PRC(2019), **AR** PRA(2020)

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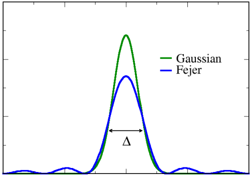

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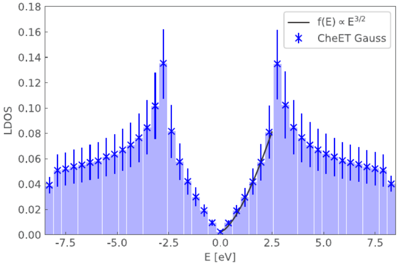
- Gaussian approach uses the fact that Chebyshev polynomials can be evaluated efficiently on quantum computers (Berry, Childs, Low, Chuang, ...)

We can approximate expectation values like

$$\langle\Phi_0|P_n(H)|\Phi_0\rangle$$

using classical many-body methods like Coupled Cluster



Sobczyk, **AR** PRE(2022)

Spin response of bulk neutron matter

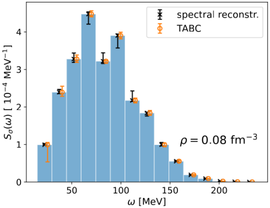
Dynamic spin structure factor

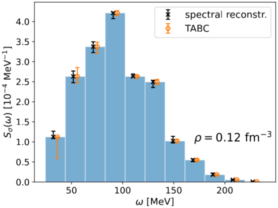
$$S_\sigma(\vec{q},\omega) = \int dt e^{i\omega t} \langle \vec{s}(t,\vec{q}) \cdot \vec{s}(0,\vec{q}) \rangle$$

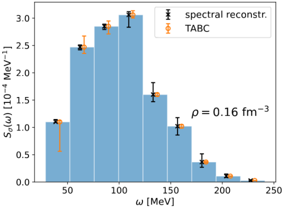
νN scattering and ν pair-production emissivity dominated by $S_\sigma(\vec{q},\omega)$ for small wave-lenghts $|\vec{q}| \to 0$

Ab-initio calculation of $|\vec{q}| = 0$ response with up to $N = 114$ neutrons and realistic nuclear interactions

Sobczyk, Jiang, **AR** arXiv:2407.20986







Summary & Conclusions

- Advances in theory and computing are opening the way to ab-initio calculation of equilibrium properties in the medium-mass region
- New ideas are needed to study nuclear dynamics in large open-shell nuclei, exclusive processes and out-of-equilibrium dynamic
- Quantum Computing has the potential to bridge this gap and increasingly better experimental test-beds are being built
- Error mitigation techniques will be critical to make the best use of these noisy near-term devices
- Early impact of QC on nuclear physics might come as insights into classical many-body methods

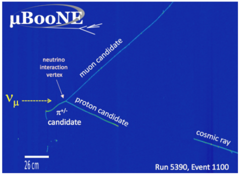


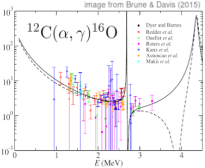
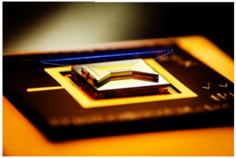
image from Brune & Davis (2015)



image from Chandra collab.



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- Chiara Lissoni (Trento)
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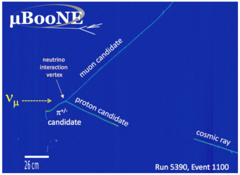
- Oriel Kiss (CERN)



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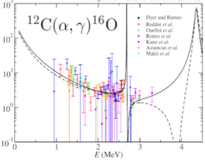

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