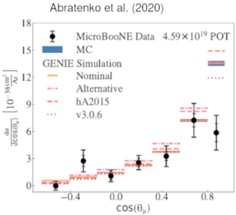
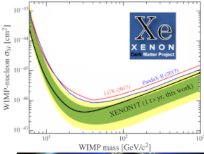
Towards quantum simulation of nuclear reactions

Alessandro Roggero





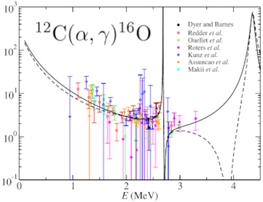
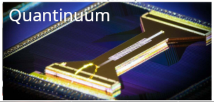
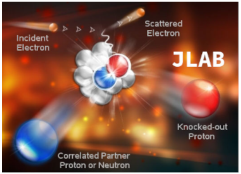


image from Brune & Davis (2015)





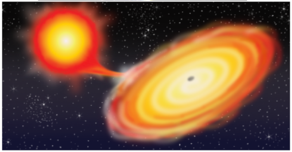


image from Chandra collab.

Montpellier – 18 Nov, 2025

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

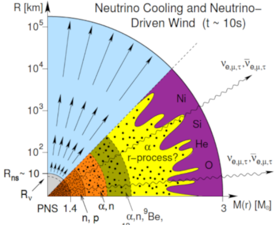
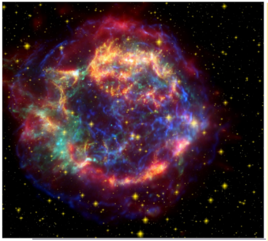


image from T.Janka



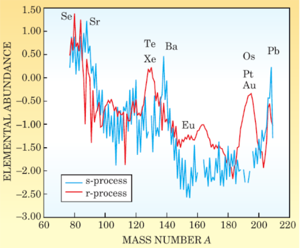
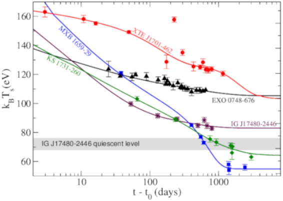
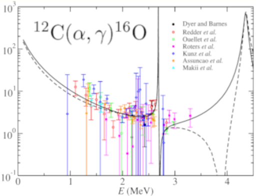


image from Cowan & Thielemann (2004)





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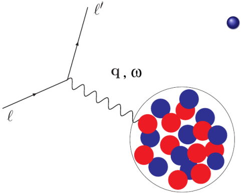
Inclusive cross section and the response function



- 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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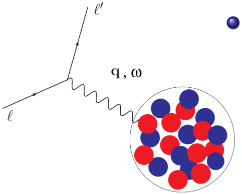

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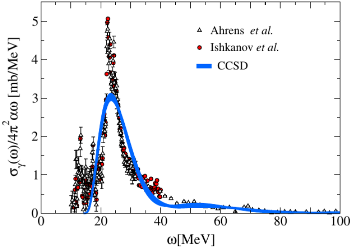
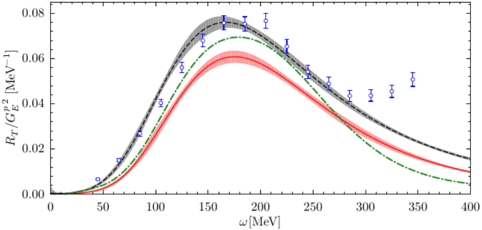
Extremely challenging classically for strongly correlated quantum systems

- 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**

Many body dynamics with Integral Transforms

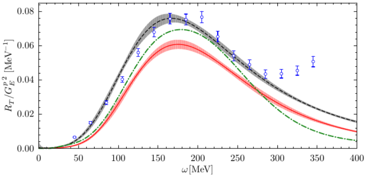
A possible way out with integral transform techniques

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

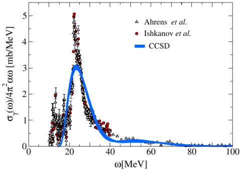
$$K(\sigma,\omega) = e^{-\sigma\omega}$$



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

Lorentz

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



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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

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

$$T(\sigma) = \langle 0|\hat{O}^\dagger \exp\left(-i\sigma(\hat{H} - E_0)\right)\hat{O}|0\rangle = \langle 0|\hat{O}^\dagger(\sigma)\hat{O}(0)|0\rangle$$

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

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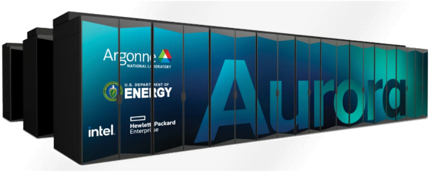
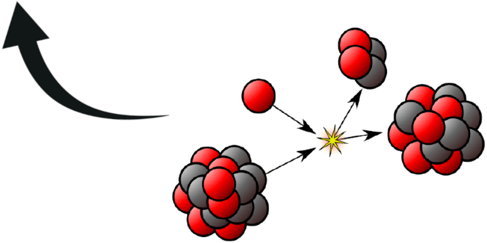
Simulations of nuclear dynamics

Classical simulations





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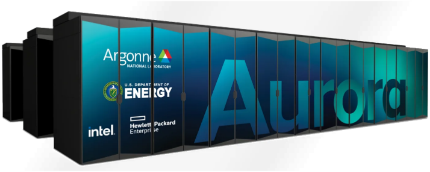
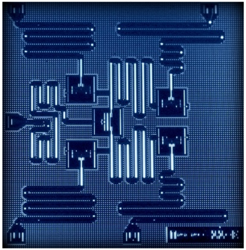
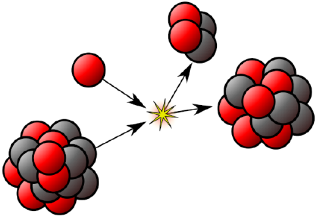


Quantum simulations



IBM



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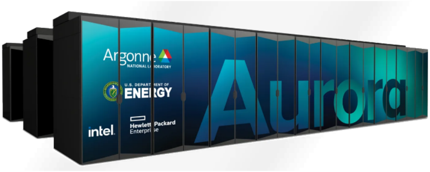

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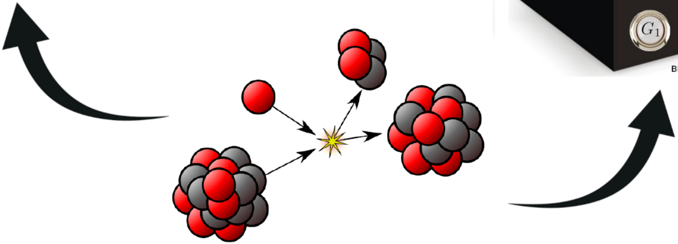

Inclusive cross section from QC

For inclusive scattering seems reasonable to get real-time correlators

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

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

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Turns out it is much more convenient to compute moments

Somma(2019), AR et al.(2020), AR(2020), Rall(2020), Baroni et al.(2021), AR&Sobczyk(2022), Kiss et al.(2023)

$$M_F(t) = \langle \Psi_0 | O e^{-itH} O | \Psi_0 \rangle \qquad M_C(n) = \langle \Psi_0 | O \mathsf{T}_n(H) O | \Psi_0 \rangle$$

- Chebyshev Polynomials T_n appear naturally [e.g. in QSP/QSVT]

$$f(H)|\Phi\rangle = \sum_{n=0}^{\infty} c_k \mathsf{T}_n(H)|\Phi\rangle \approx \sum_{n=0}^{M} c_k \mathsf{T}_n(H)|\Phi\rangle$$

- Very popular recently for early fault-tolerant ground state energy estimation (and preparation) [Lin & Tong (2022), Dong et al. (2022), Wan et al. (2022)]

Progress on time evolution for NP

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

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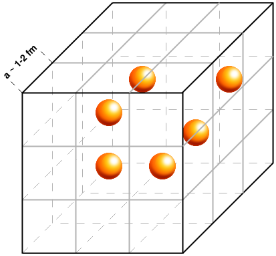
We then place nucleons on a spatial lattice to regularize them



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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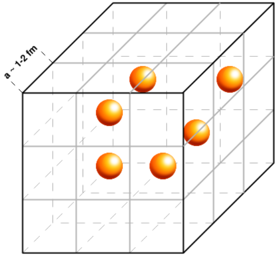

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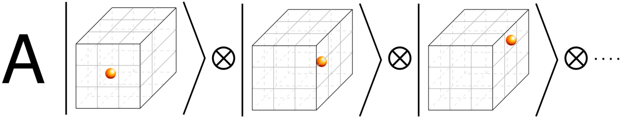
- $10^{11} - 10^{12}$ operations and ≈ 4000 qubits [Roggero et al. PRD (2020)]
- $10^9 - 10^{11}$ operations and ≈ 6000 qubits [J.Watson et al. arXiv:2312.05344]

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?



Should cost $N \log(V)$ qubits and hopefully not too many more gates

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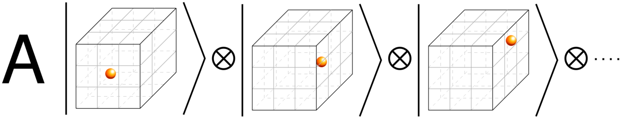

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Long history of first-quantization methods for quantum simulations of chemistry [Abrams & Lloyd (1997), Kassal et al. (2008), Jones et al. (2012), Babbush et al. (2019),. . .]

- anti-symmetrization costs $\mathcal{O}(N\log(N)\log(V))$ [D.Berry et al. (2018)]
- kinetic energy simple in momentum space costing $\mathcal{O}(N\log^2(V))$

The main bottleneck is evolving under the potential energy

$$e^{-it\hat{U}}\left|x\right\rangle = e^{-itU(x)}\left|x\right\rangle$$

Progress on time evolution for NP: Trotter

The main bottleneck is evolving under the potential energy

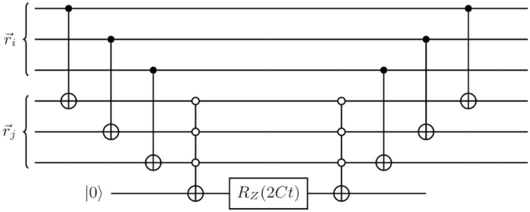
$$e^{-it\hat{U}}|x\rangle = e^{-itU(x)}|x\rangle$$

In a contact theory this is not necessarily true anymore. For instance

$$\hat{U}|x\rangle = \left[\sum_{ij}^{N} U_{ij}(x_i, x_j)\right]|x\rangle = \left[C\sum_{ij}^{N}\delta(x_i - x_j)\right]|x\rangle$$

but then all pairs commute with each other and for one pair

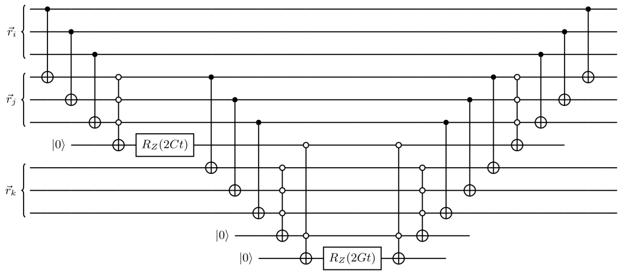
$$\exp(-itC\delta(x_i - x_j))|x\rangle =$$



Spagnoli, Lissoni, Roggero, arXiv:2507.22814

Progress on time evolution for NP: Trotter II

The same idea can be extended to three-body contacts too



With this implementation, the step cost is $\mathcal{O}(N^3 \log(V))$

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

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

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Progress on time evolution for NP: post-Trotter

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

In order to use QSP we need a **block-encoding** of the Hamiltonian

$$\langle 0|U_H|0\rangle = H/\Lambda$$

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- for the potential we exploit again the fact it is a contact

$$U(x) = C\sum_{i<j}\delta(x_i - x_j) + G\sum_{i<j<k}\delta(x_i - x_j)\delta(x_i - x_k)$$
$$= \frac{3C-G}{6}\sum_i\Big(\sum_{j\neq i}\delta(x_i - x_j)\Big) + \frac{G}{6}\sum_i\Big(\sum_{j\neq i}\delta(x_i - x_j)\Big)^2$$

for any given i, the sum in parenthesis is bounded by 4.

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$$

for any given i, the sum in parenthesis is bounded by 4. But then that can be done in $\mathcal{O}(N\log(V))$ and outer sum another $\mathcal{O}(N)$

Progress on time evolution for NP II

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

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

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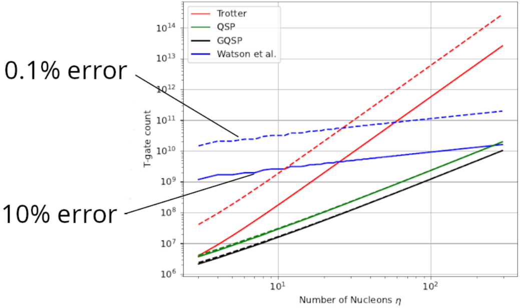

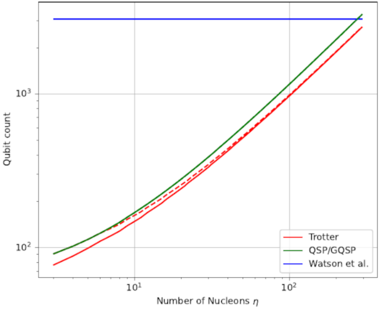

- $10^7 - 10^9$ operations and $\approx 70 - 500$ qubits [Spagnoli, Lissoni, Roggero (2025)]

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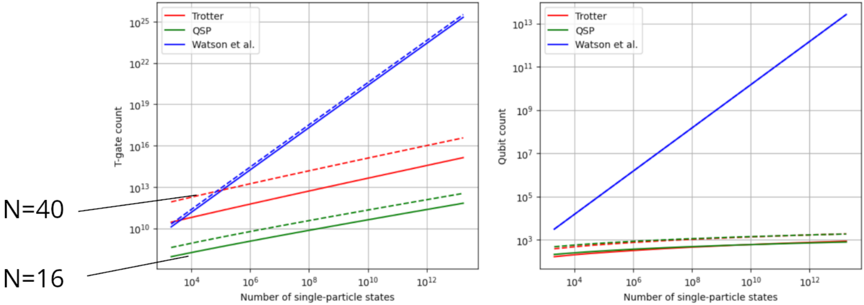

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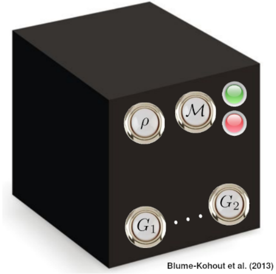
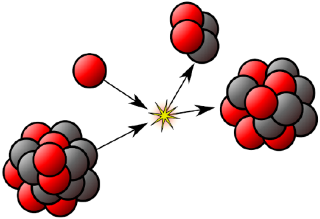
Simulations of nuclear dynamics II

Classical simulations

Quantum simulations





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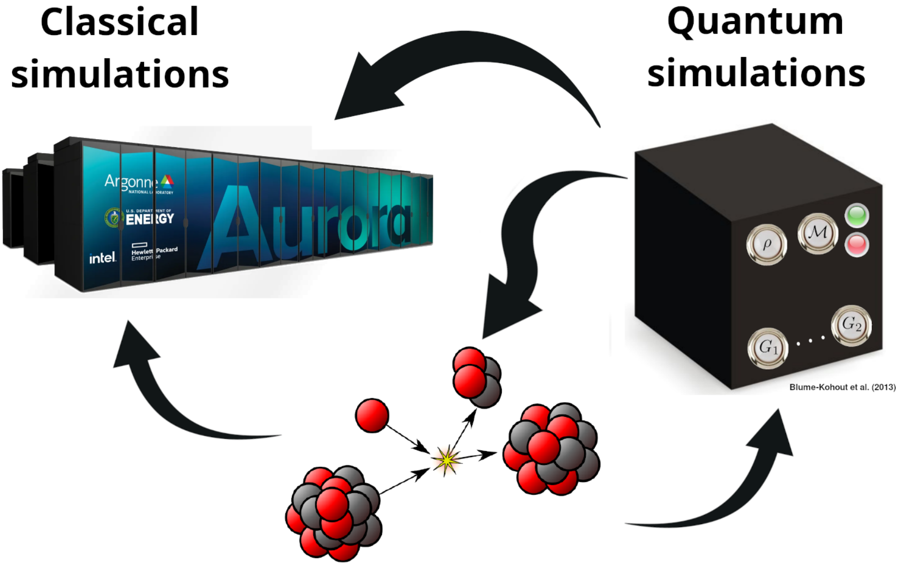

Quantum inspired simulation of reactions

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

Orthogonal polynomials satisfy recurrence relations, for Chebyshev

$$\mathsf{T}_0(H) = 1 \quad \mathsf{T}_1(H) = H \quad \Rightarrow \quad \mathsf{T}_{n+1}(H) = 2H\mathsf{T}_n(H) - \mathsf{T}_{n-1}(H)$$

To get Chebyshev moments we need a many-body method such that

- we can prepare a good approximation to the ground state $|\Psi_0\rangle$
- we can apply the Hamiltonian efficiently

$$|\phi_0\rangle = |\Psi_0\rangle \quad |\phi_1\rangle = H|\Psi_0\rangle$$
$$|\phi_n\rangle \quad \rightarrow \quad |\phi_{n+1}\rangle = 2H|\phi_n\rangle - |\phi_{n-1}\rangle$$

- we can calculate overlaps efficiently $m_k = \langle\phi_0|\phi_k\rangle = \langle\phi_k|\phi_0\rangle$

Once we have the moments, all the post processing is carried out as if we obtained them from a quantum computer

Quantum inspired simulation of reactions with CC-theory

Sobczyk & Roggero (2022), Sobczyk, Jiang, Roggero (2025)

Coupled-cluster theory allows for accurate nuclear ground states to be prepared efficiently. We can use EOM-CC to study excited-states/moments

$$|\Psi_0\rangle = e^T |HF\rangle \qquad \langle\widetilde{\Psi}_0| = \langle HF|(1+\Lambda)e^{-T}$$

the natural construction uses a similarity transformed Hamiltonian

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Within EOM the excited states are parametrized as

$$|\phi_{n+1}\rangle = 2\overline{H}|\phi_n\rangle - |\phi_{n-1}\rangle = \mathcal{R}_n |\Psi_0\rangle$$

Once we collected the parameters of $\mathcal{R}_n$ we can get moments as

$$m_k = \langle\widetilde{\Psi}_0|\phi_k\rangle$$

Spin response of bulk neutron matter

Dynamic spin structure factor

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

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

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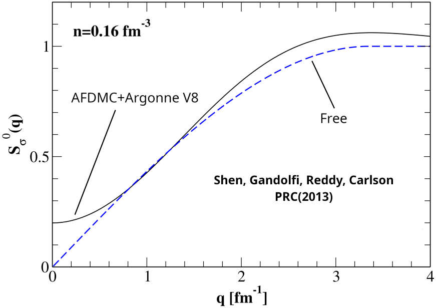
Total strength given by sum rule

$$S^0_\sigma(\vec{q}) = \int d\omega S_\sigma(\vec{q},\omega)$$

Tensor & Spin-orbit terms lead to

$$S^0_\sigma(0) = \frac{4}{3N}\langle \mathsf{S}^2\rangle \neq 0$$



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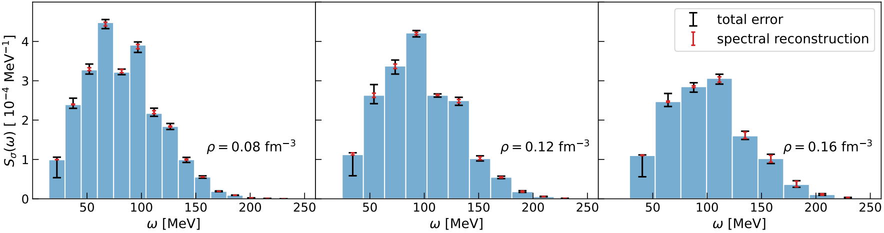

First ab-initio calculation of the frequency dependent spin response of neutron matter with **controllable errors**

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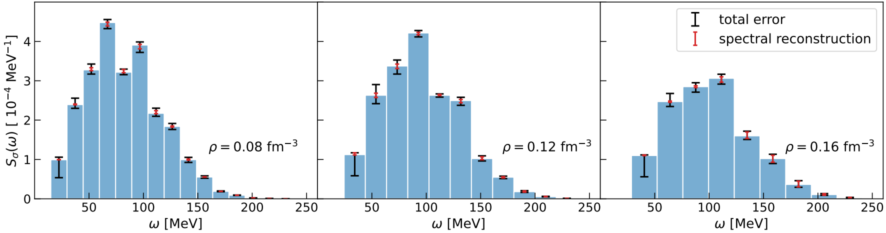

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TOTAL THEORY ERROR = **MANY-BODY METHOD** + **NUCLEAR INTERACTION** + **FREQUENCY RESPONSE RECONSTRUCTION**

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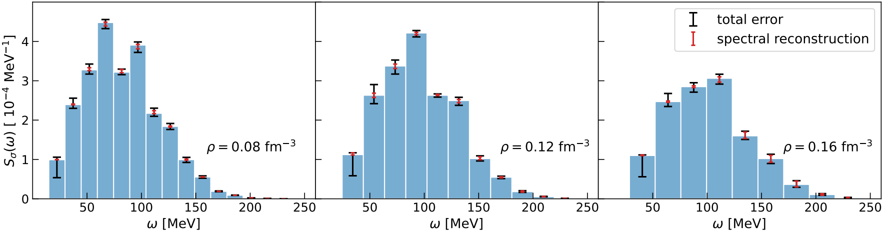

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Summary and perspective

- Ab-initio treatement of nuclear dynamics is important for both terrestrial experiments and extreme astrophysical sites
- Quantum computing is a strong candidate to considerably improve our simulations of nuclear physics, especially dynamical properties
- Substantial advances in the last years in the implementation of time evolution for simple nuclear Hamiltonians. Recent results seem to suggest that a **first-quantization** formulation could be advantageous
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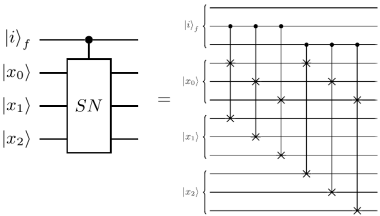
Thanks to my collaborators

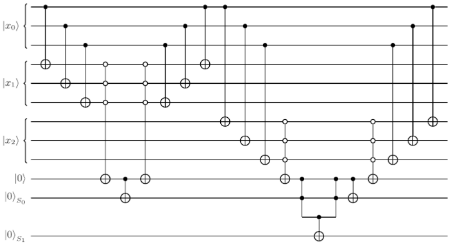
- J. Sobczyk (Chalmers)
- W. Jiang (Mainz)
- L. Spagnoli (Trento)
- C. Lissoni (Trento)

Block encoding of the potential

- we use a SWAP network to place in first place the particle i flagged by ancilla register $|i\rangle$ (which we start in superposition)

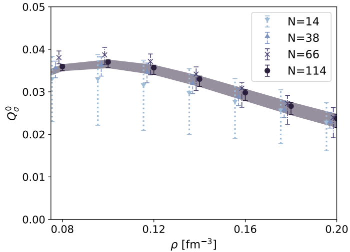


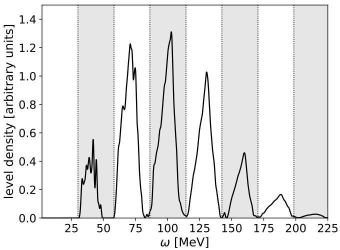
- evaluate the inner sum in the parenthesis on the swapped register



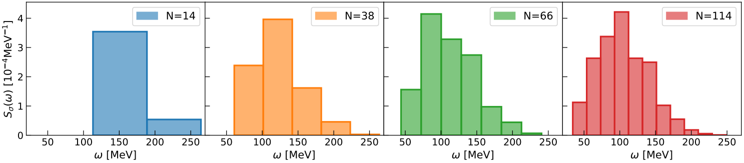
Finite size systematics

We use TABC to minimize finite size effects. This works well for sum rules but residual N dependence in the density of states (and thus the response)





Clustering can be explained as a shell effect: at fixed density $\rho = N/L^3$ so the free single particle energies are $E_n \propto n(2\pi/L)^2$

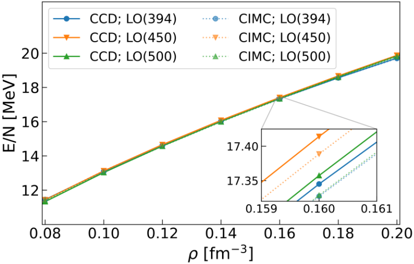


Spin response of bulk neutron matter from CC

Despite being a low energy observable, important interaction dependence

We tested three different Chiral potentials at LO using CC and CIMC

- energy per particle has negligible dependence on method/model



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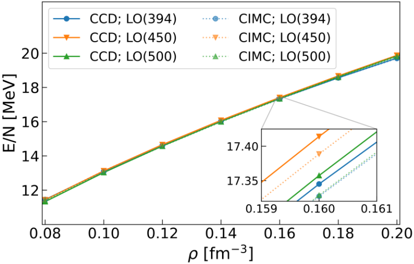

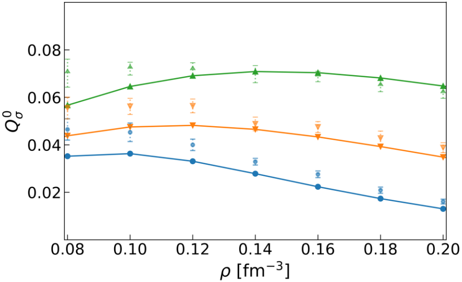

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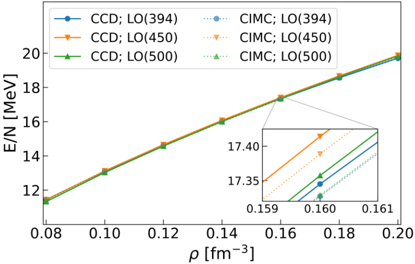

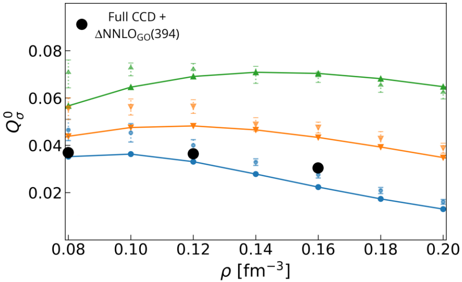

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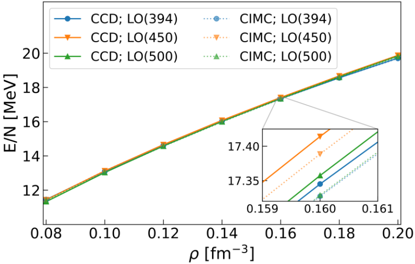

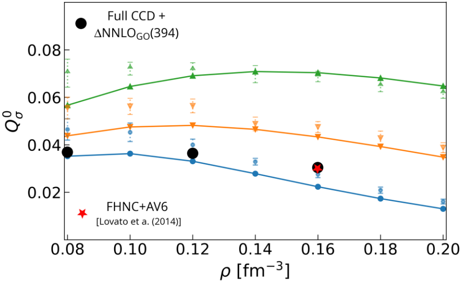

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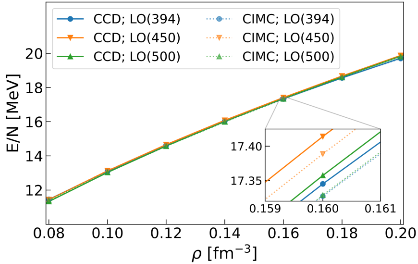

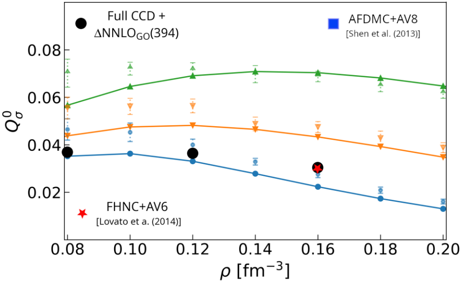

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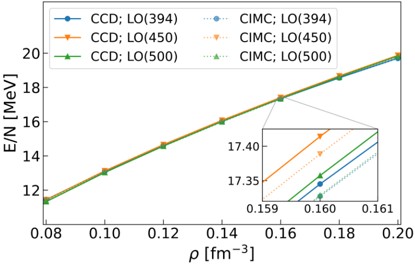

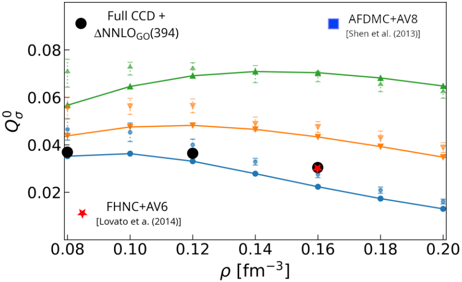

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What is the value of $\langle S^2 \rangle$ in zero temperature neutron matter?