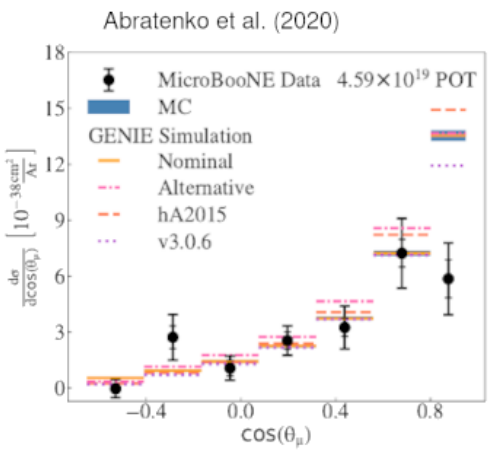
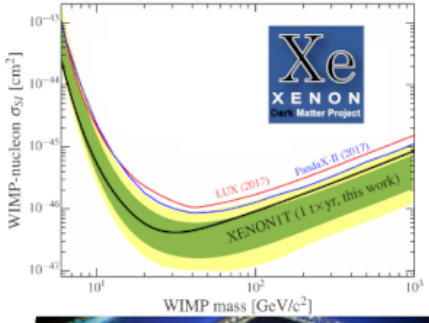
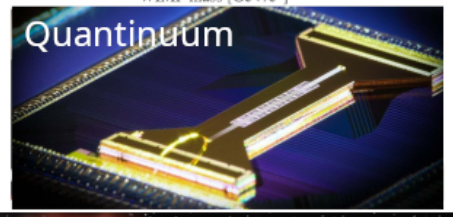
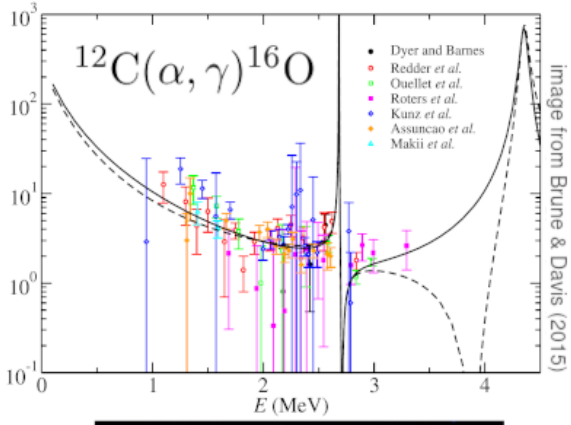
Ab-initio nuclear response functions with quantum (inspired) algorithms

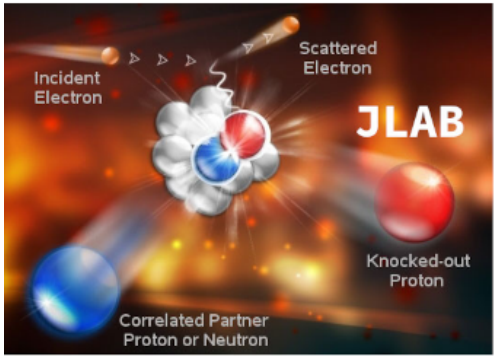
Alessandro Roggero

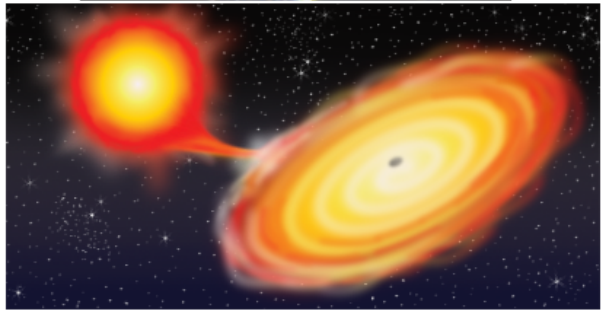












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Ischia – 22 May, 2025

UNIVERSITAS ATHESINA STUDIORUM

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

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

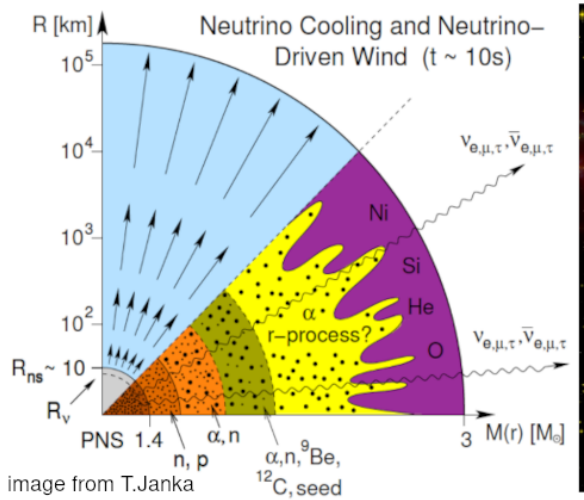
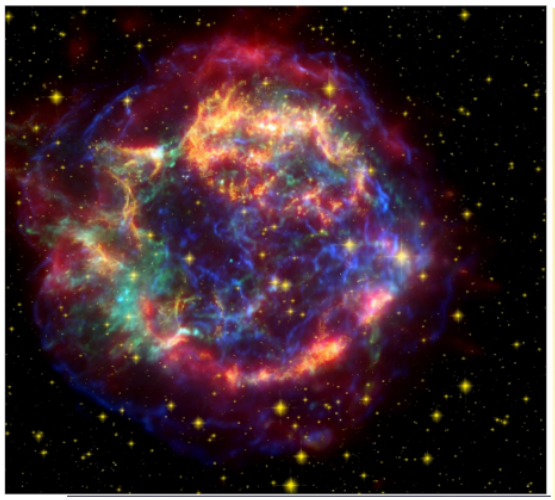


image from T.Janka



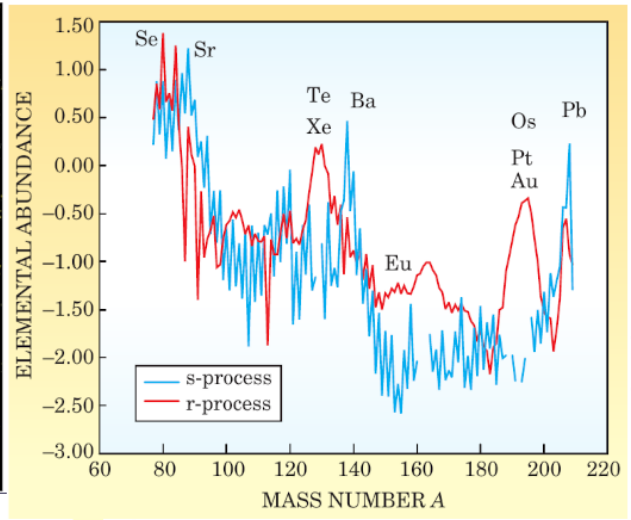
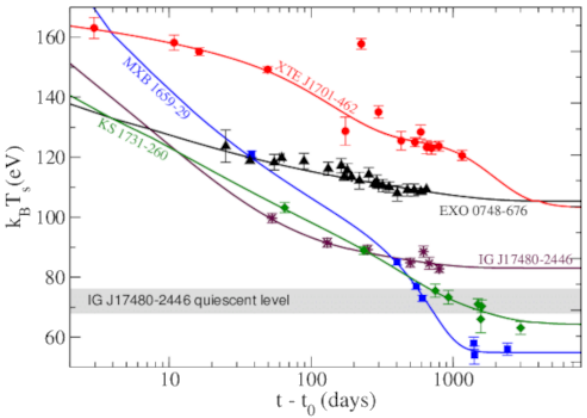
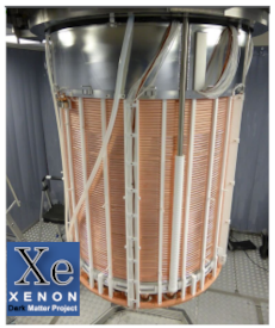


image from Cowan & Thielemann (2004)





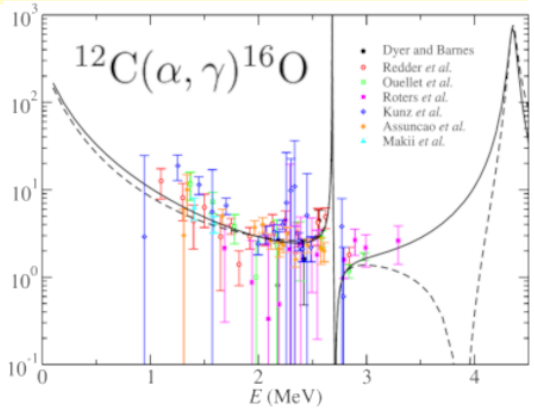
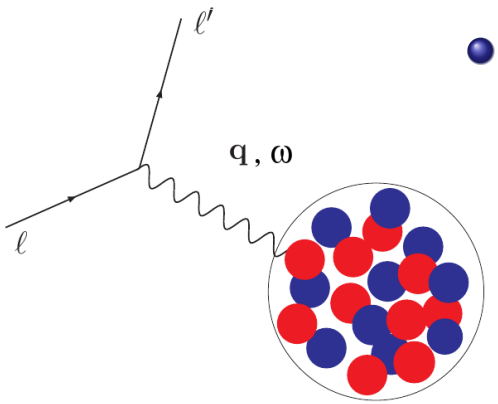


image from Brune & Davis (2015)

Inclusive cross section and the response function



- 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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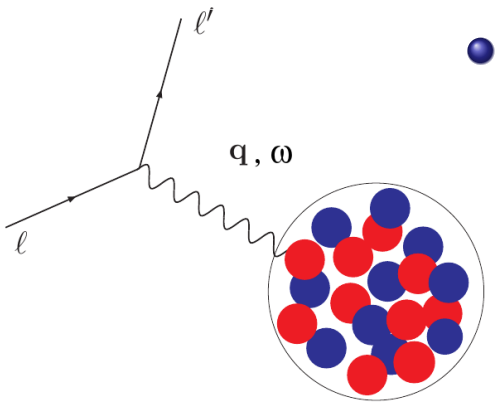

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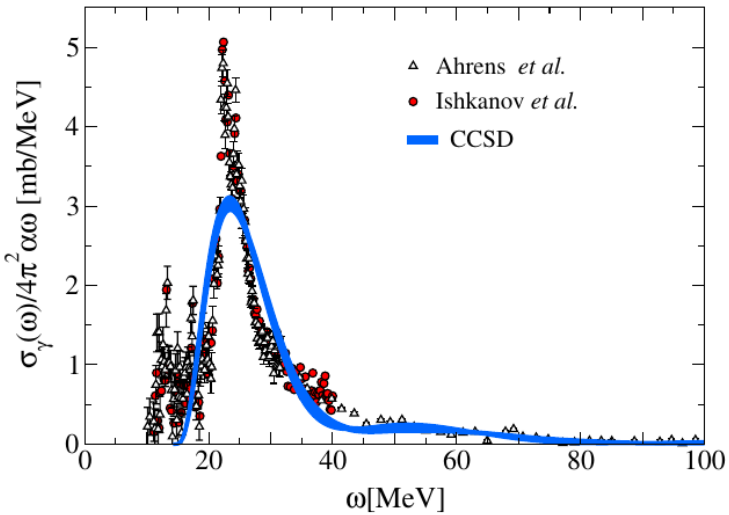
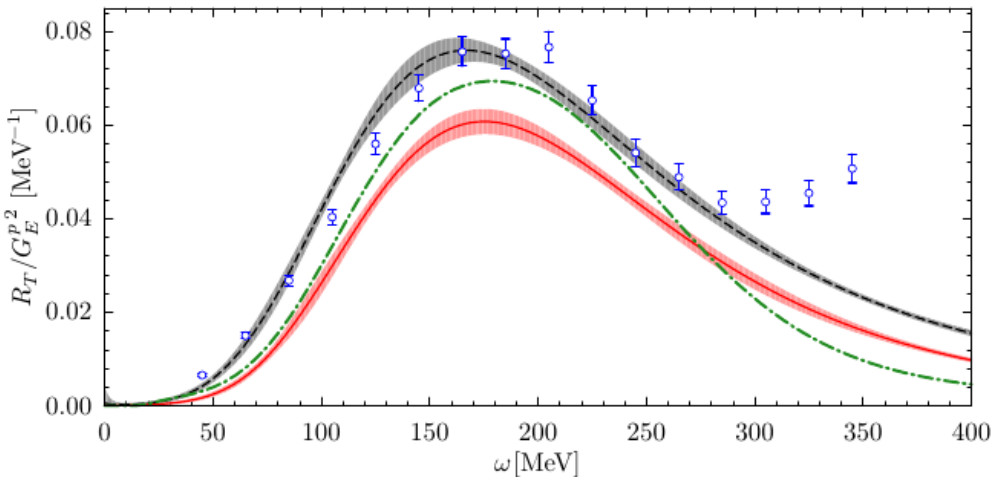
Extremely challenging classically for strongly correlated quantum systems

- 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**

(see also F.Marino's and G.King's talks)

Many body dynamics with Integral Transforms

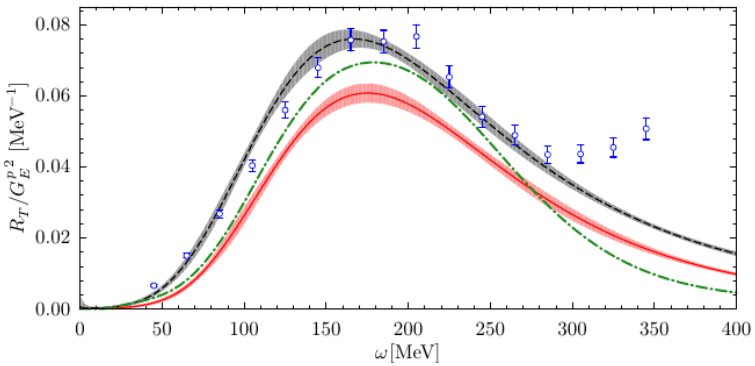
A possible way out with integral transform techniques

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

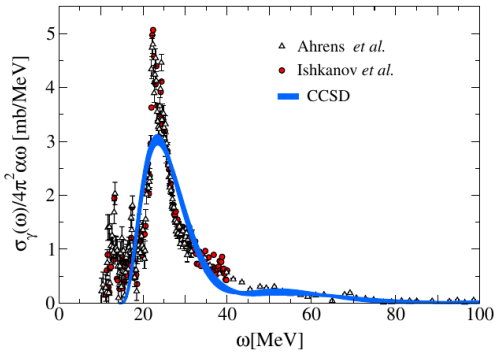
$$K(\sigma,\omega) = e^{-\sigma\omega}$$



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

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

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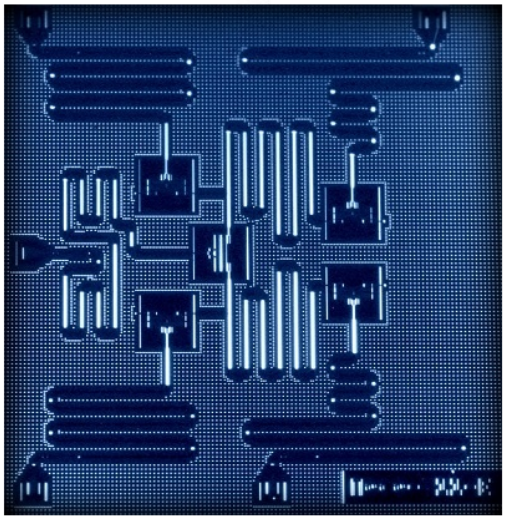
ADVANTAGE: if we did, we could do more than linear response!

Simulations of nuclear dynamics

Classical simulations

Quantum simulations



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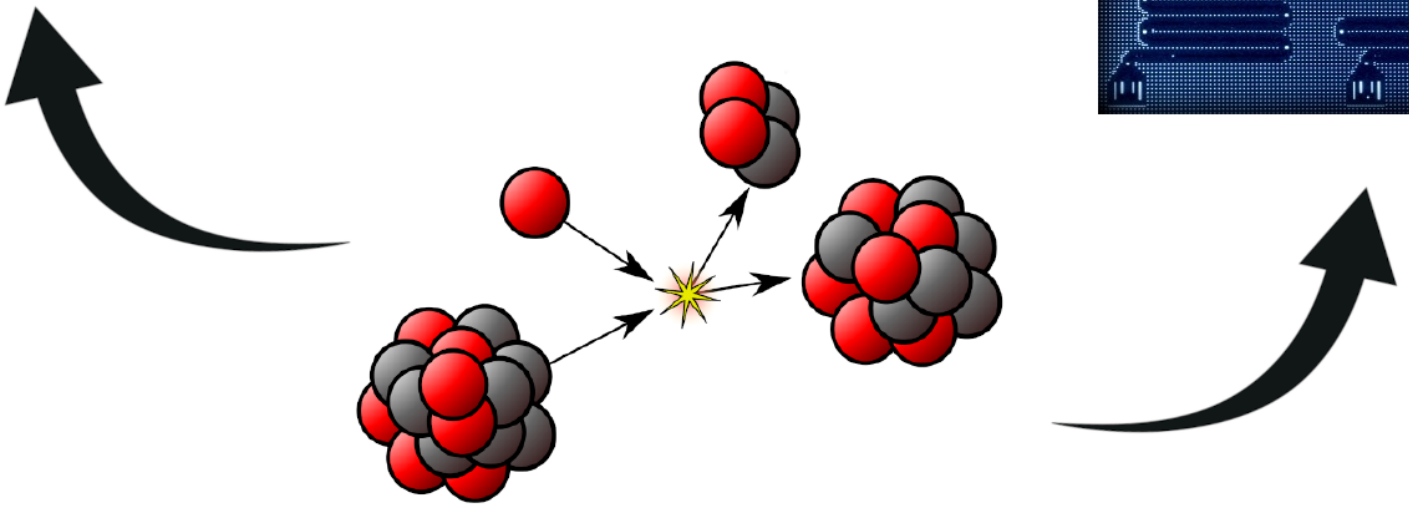

several talks in Ischia: D. Lacroix, J. Menendez, E. Costa

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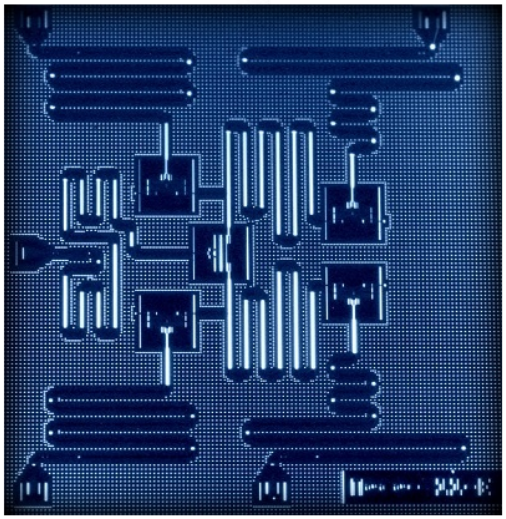

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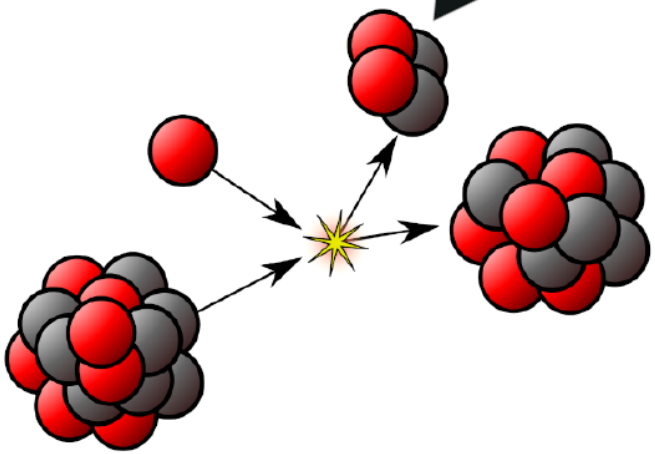

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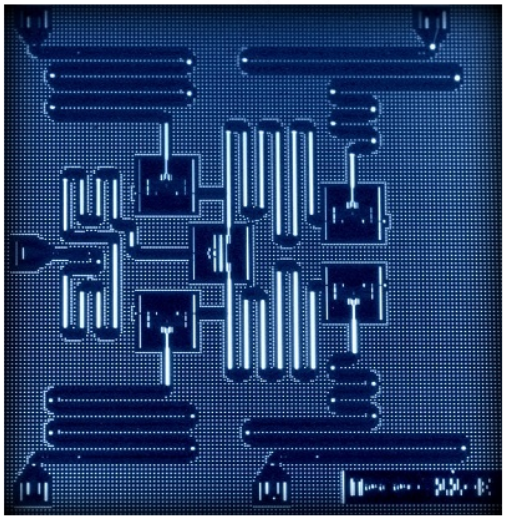
Simulations of nuclear dynamics

"Quantum inspired"

Classical simulations

Quantum simulations



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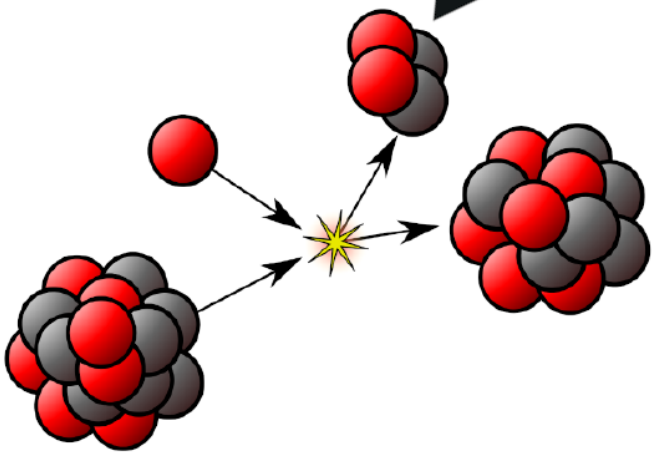

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Inclusive cross section from QC

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 (see also S. Wang's talk)

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

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

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 take 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

$$\overline{H} = e^{-T} H e^T \qquad \text{in CCSD operator } T \text{ contains 1p1h and 2p2h}$$

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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

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

Reasonably similar to the LIT-CC method (see F.Marino's talk)

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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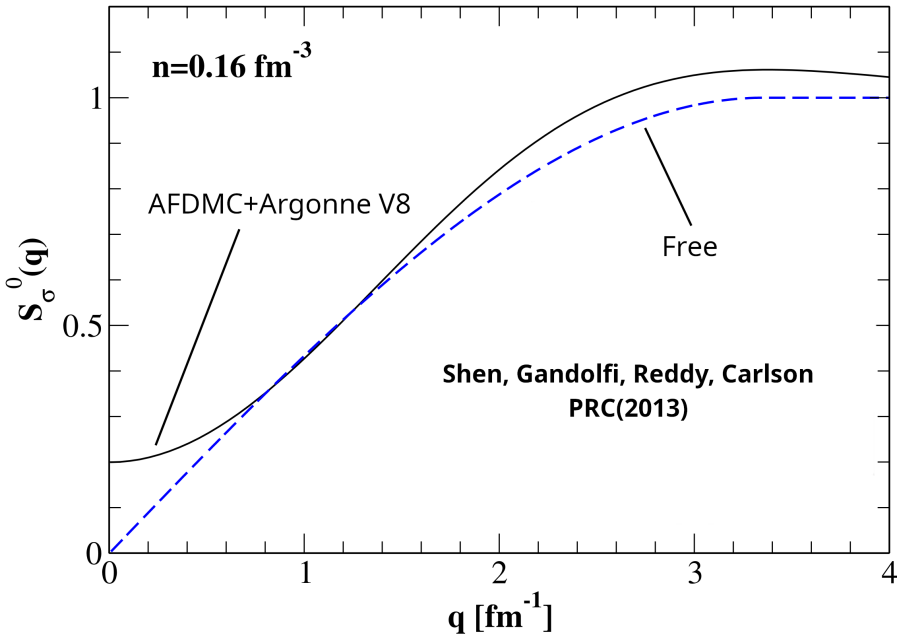
Total strength given by sum rule

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

Tensor & Spin-orbit terms lead to

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



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

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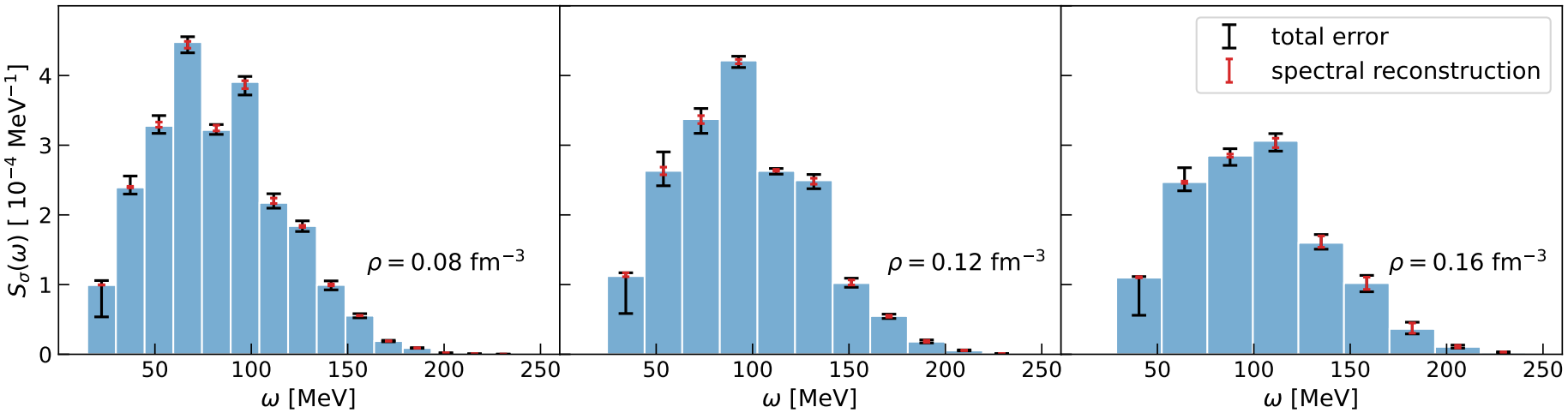

First ab-initio calculation of the frequency dependent spin response of neutron matter with **controllable errors**

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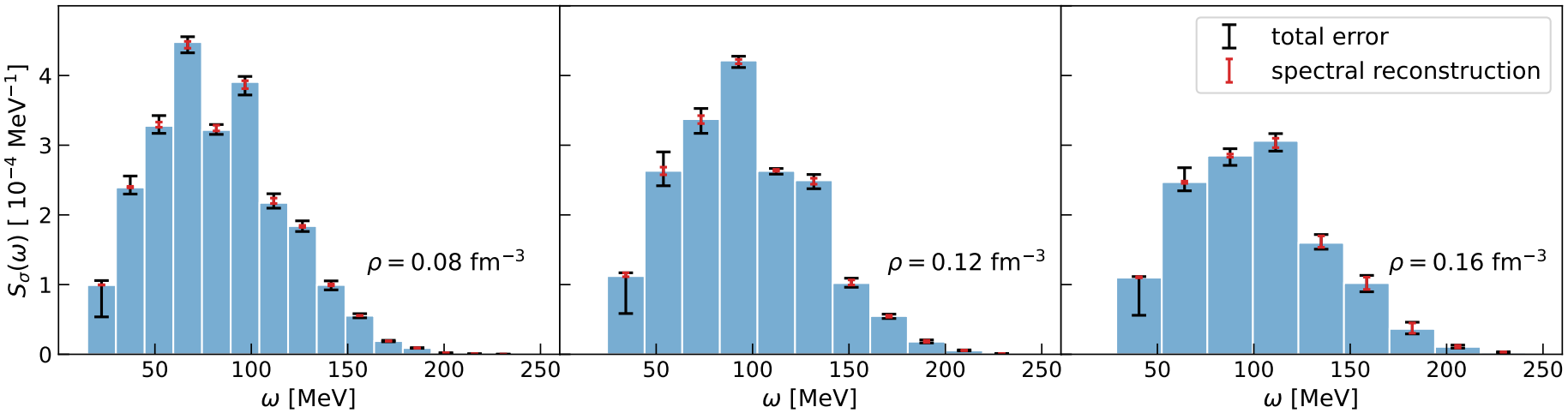

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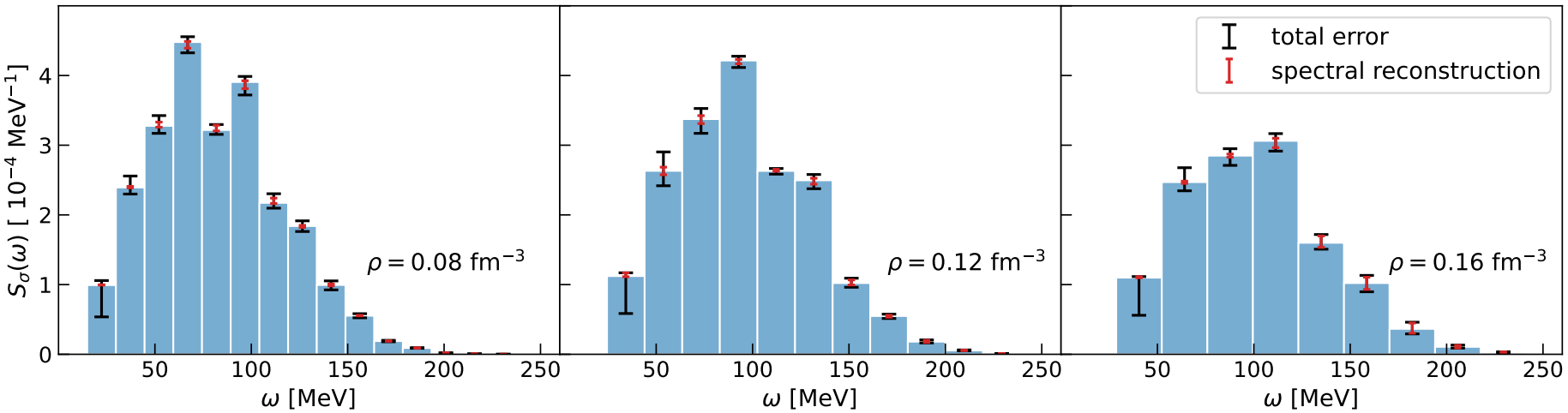

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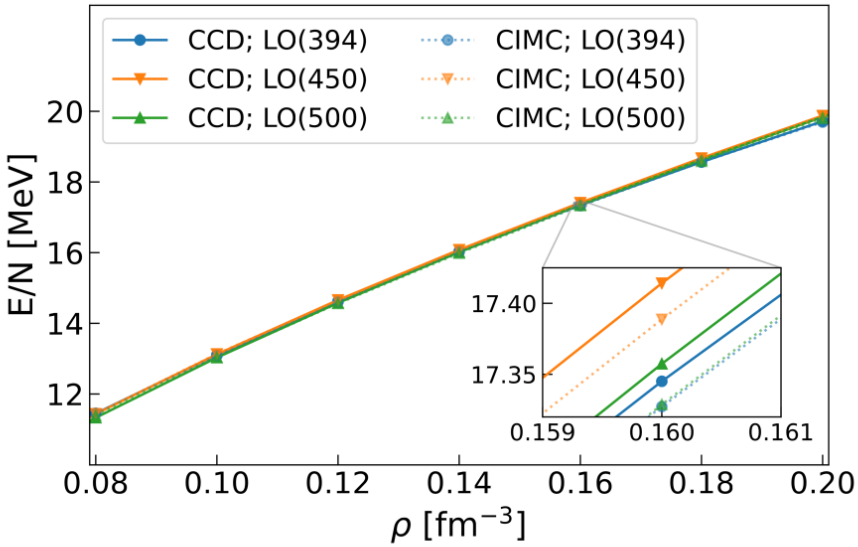
Spin response of bulk neutron matter from CC

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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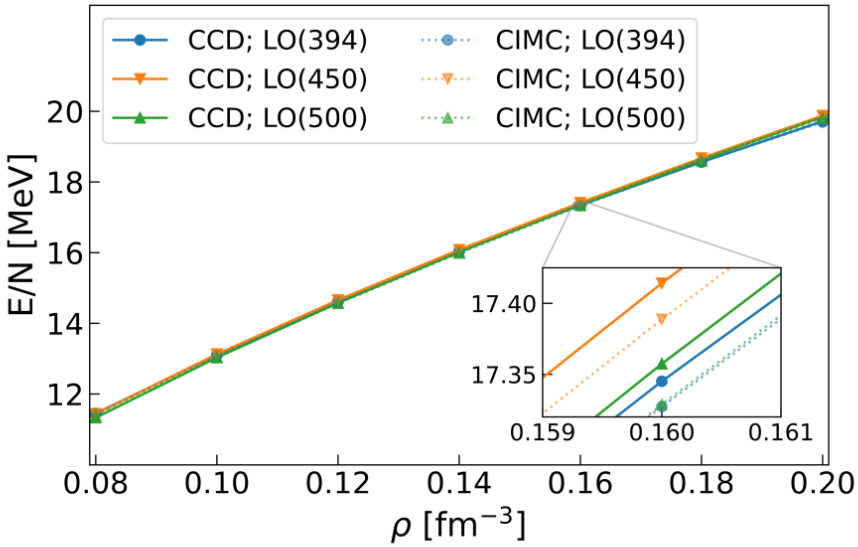

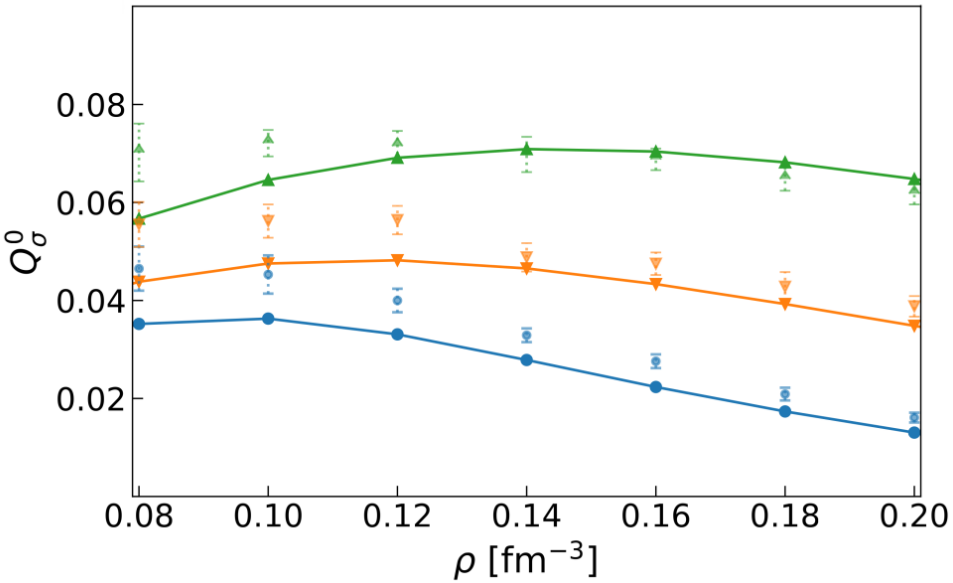

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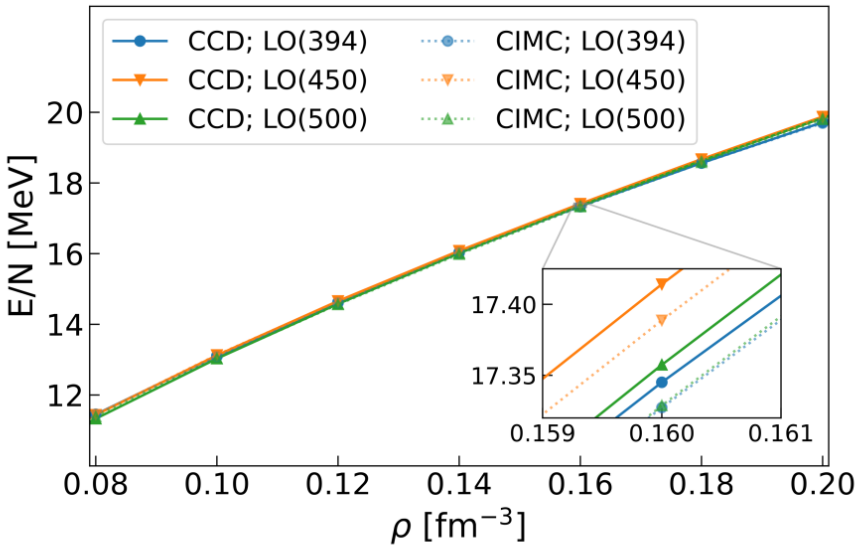
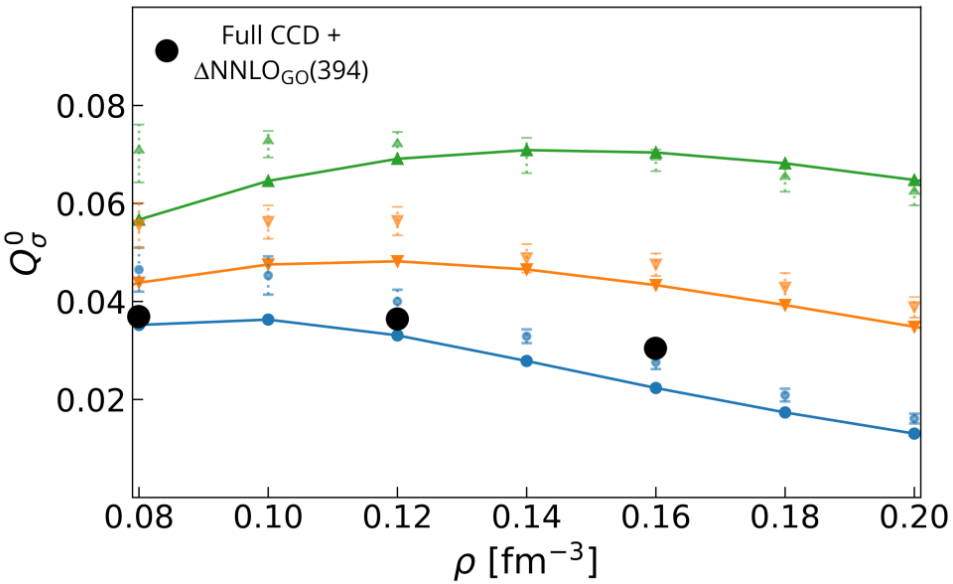


- Small effect in going NNLO



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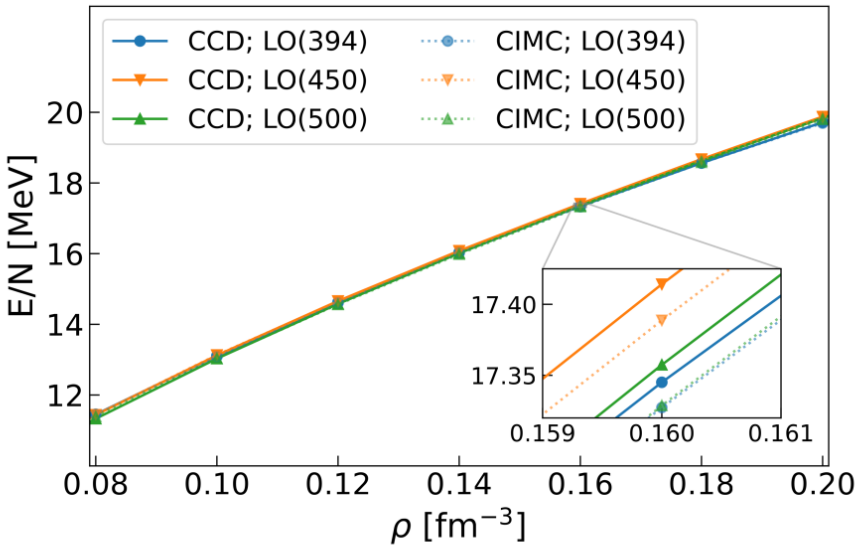

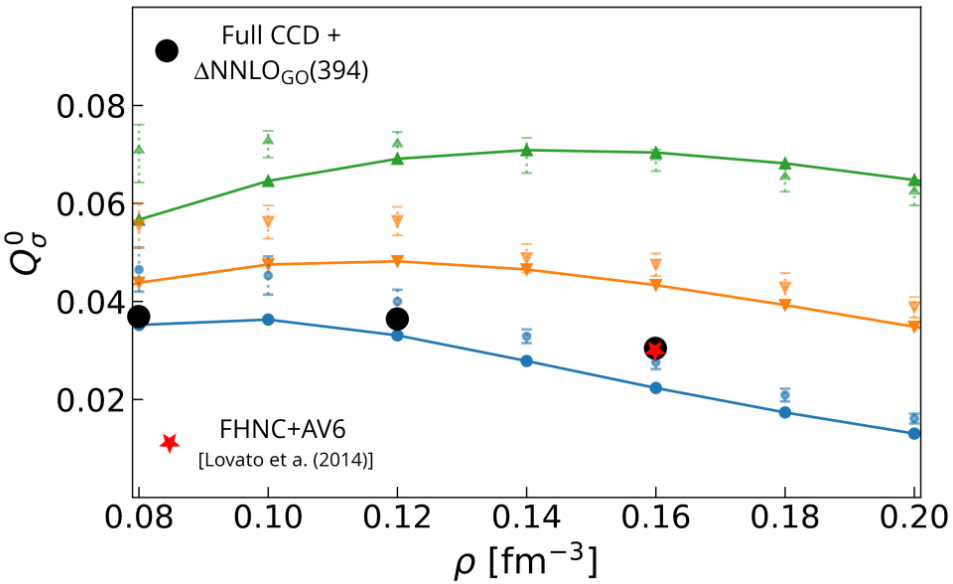

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Spin response of bulk neutron matter from CC

Despite being a low energy observable, important interaction dependence

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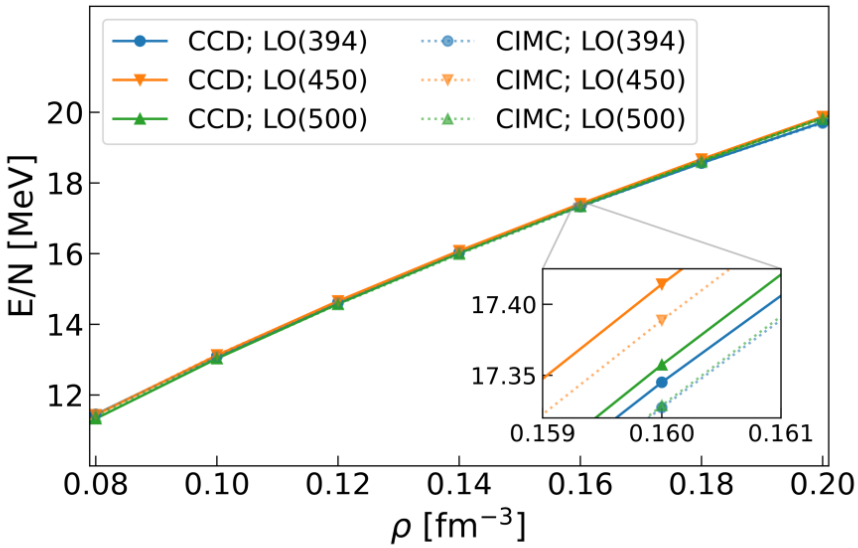

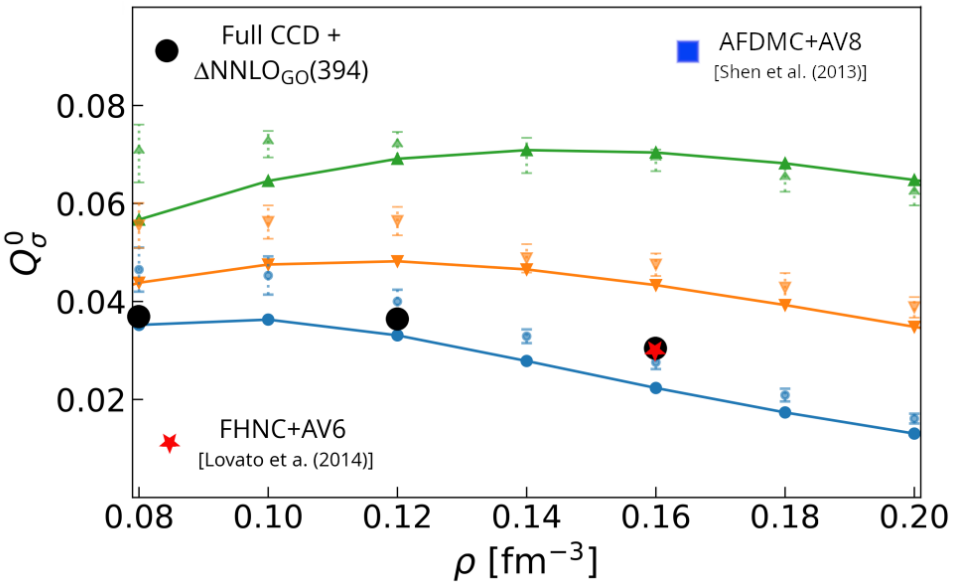

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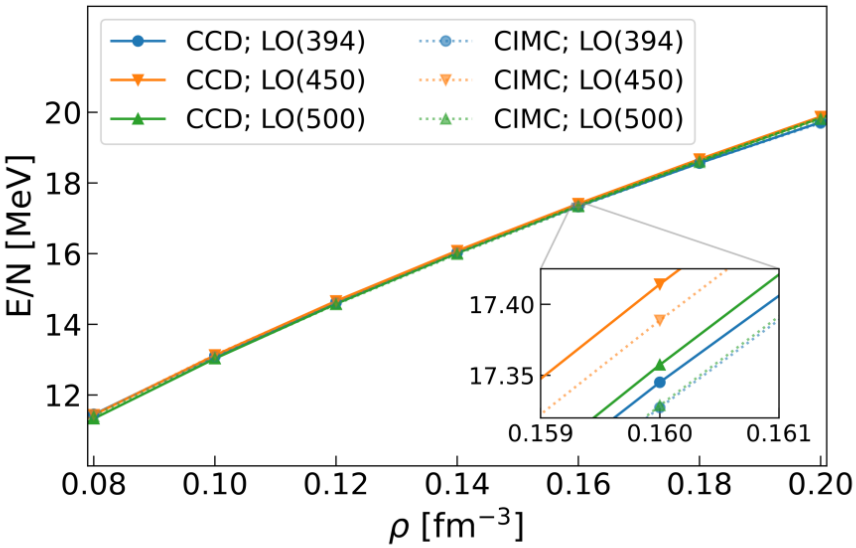

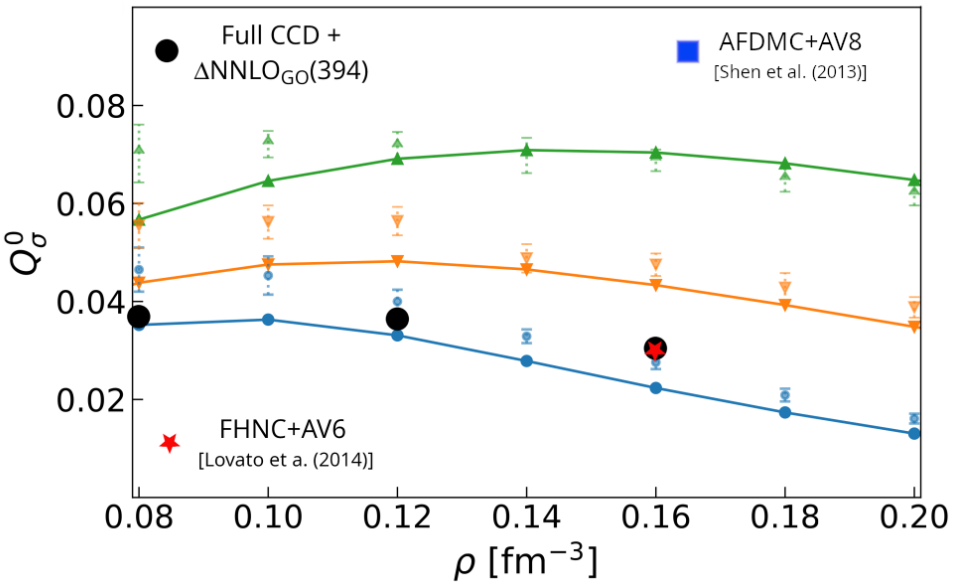

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What is the value of $\langle S^2 \rangle$ in zero temperature neutron matter?

Summary and perspective

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- incredible recent progress especially for static nuclear properties but new tools might be needed for some dynamical processes
- quantum computing is a strong candidate to considerably improve our simulations of nuclear physics, especially dynamical properties
- some of the techniques developed for use on future large scale quantum computers can be employed now on classical HPC!
- calculation of spin response shows important interaction/method dependence: **neutron matter around ρ_0 not boring anymore!**

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Thanks to my collaborators

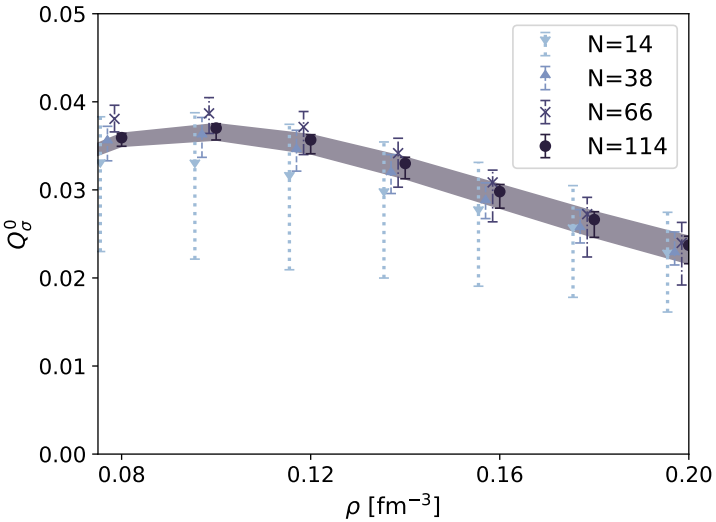
- J. Sobczyk (Mainz $\rightarrow$ Chalmers)
- W. Jiang (Mainz)

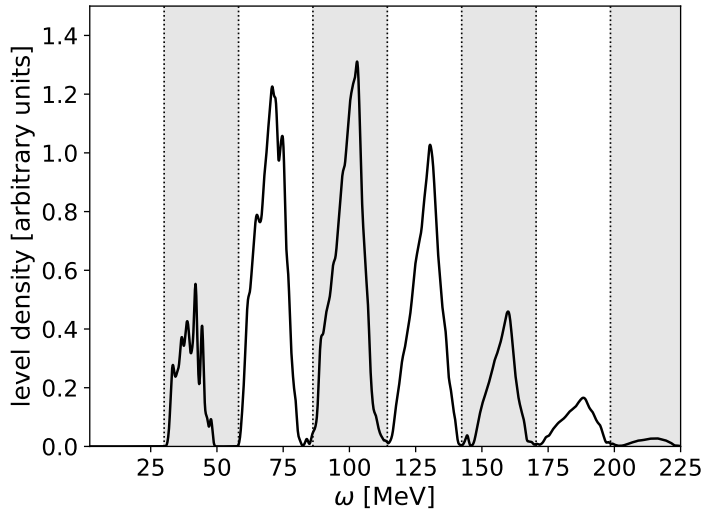
CHALMERS UNIVERSITY OF TECHNOLOGY

mitp Mainz Institute for Theoretical Physics

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 $E_n \propto n(2\pi/L)^2$