DIAGRAMMATIC MONTE CARLO: AB INITIO BE BUBBLING

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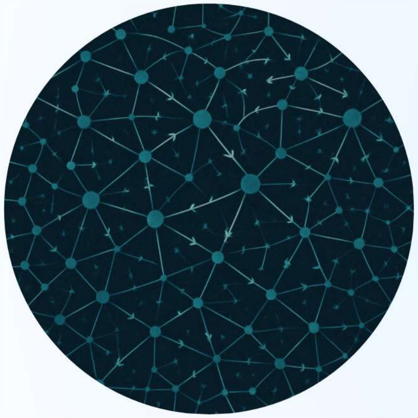
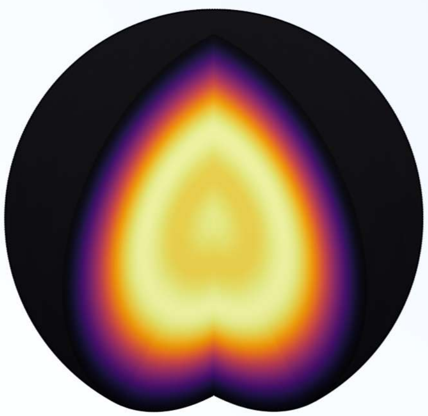




OUTLINE

Quick overview of Self-Consistent Green's Function (SCGF) Theory.

Diagrammatic Monte Carlo:

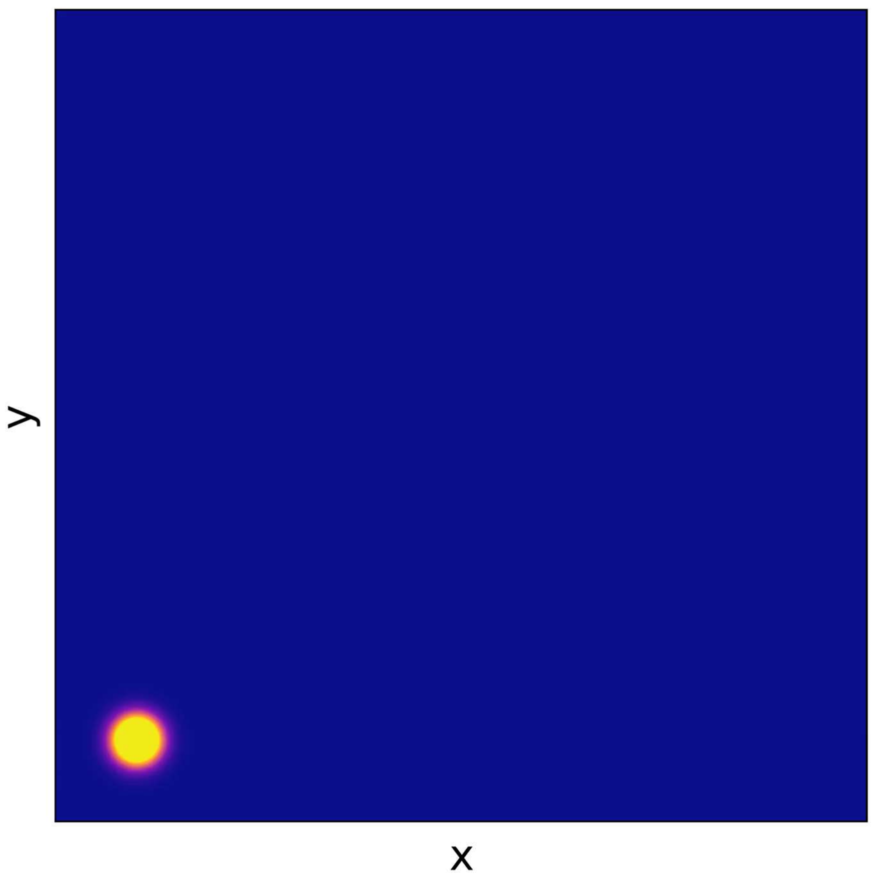
- Nuclear pairing model
- Chiral interaction in a small space

SCGF calculations for nuclei in large model spaces:

- Shell inversion in Argon 46

SELF-CONSISTENT GREEN'S FUNCTION THEORY

$iG_{\alpha\beta}(t,t') \stackrel{\text{def}}{=} \langle \Psi_0^A | T c_\alpha(t) c_\beta^\dagger(t') | \Psi_0^A \rangle$



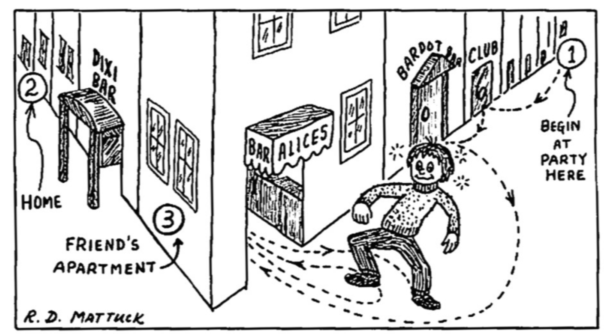


Fig. 1.1 *Propagation of Drunken Man*

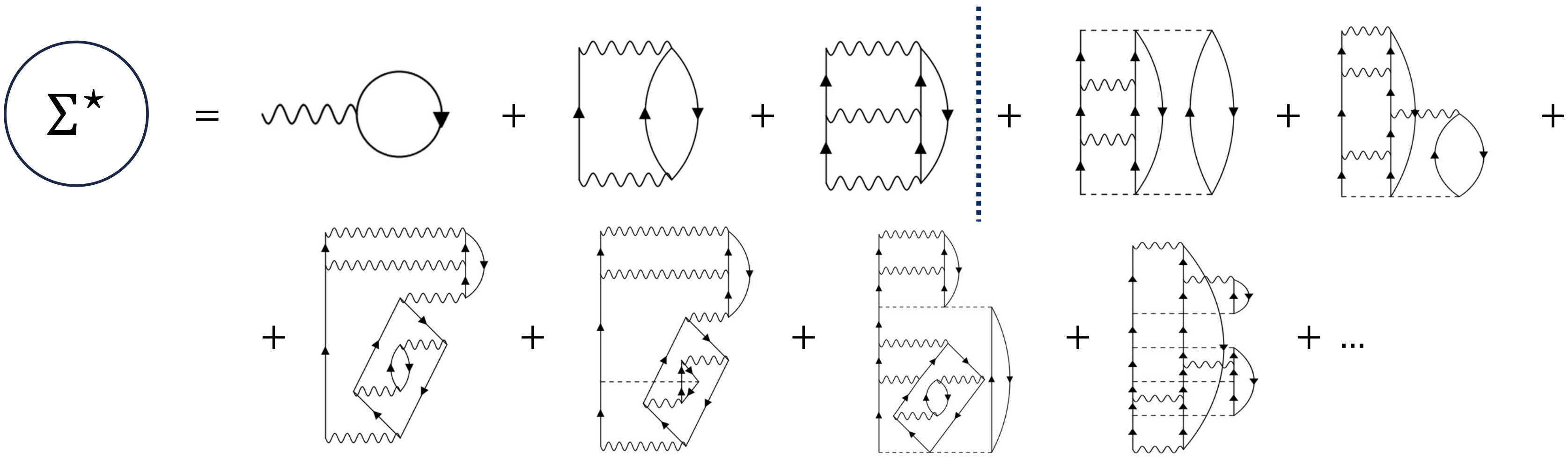
Mattuck, A Guide to Feynman Diagrams in the Many-Body Problem (1992)

DYSON EQUATION

$$G_{\alpha\beta}(\omega) = G^{(0)}_{\alpha\beta}(\omega) + G^{(0)}_{\alpha\gamma}(\omega)\Sigma^{\star}_{\gamma\delta}(\omega)G_{\delta\beta}(\omega)$$

Unperturbed propagator

Irreducible self-energy

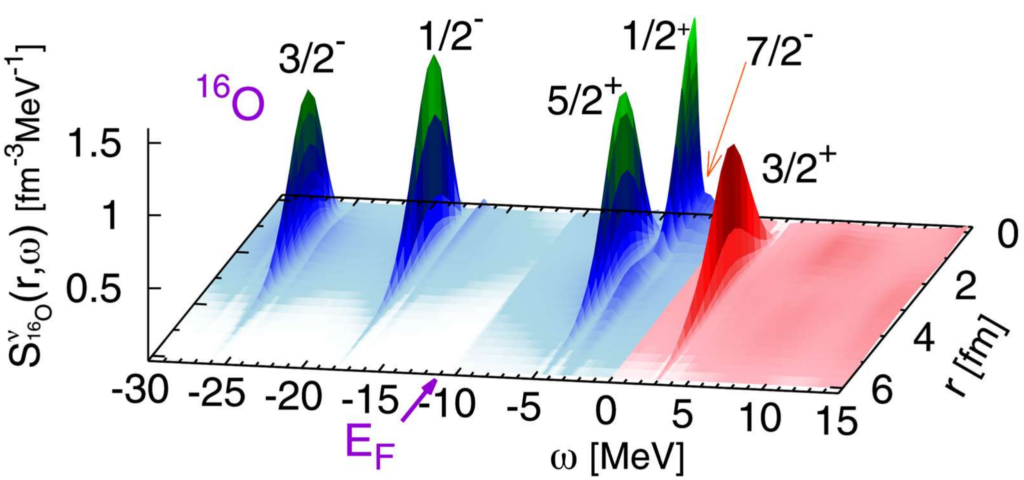


STRUCTURE INFORMATION

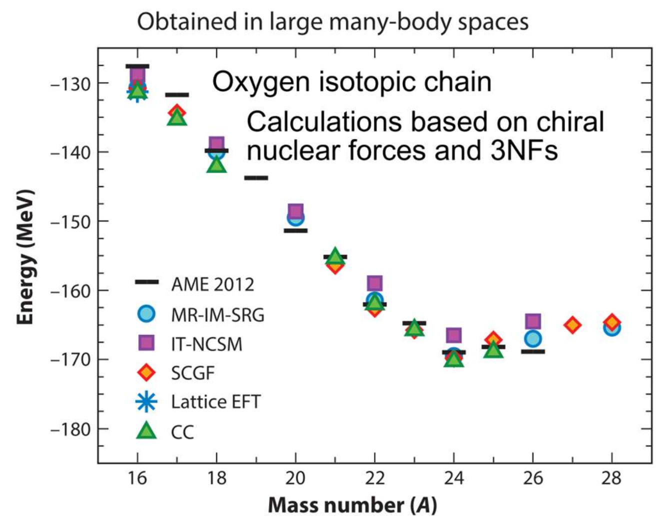
$$G_{\alpha\beta}(\omega) = \sum_n \frac{(\mathcal{X}_\alpha^n)^* \mathcal{X}_\beta^n}{\omega - \varepsilon_n^+ + i\eta} + \sum_k \frac{\mathcal{Y}_\alpha^k \left(\mathcal{Y}_\beta^k\right)^*}{\omega - \varepsilon_k^- - i\eta}$$

$$(\mathcal{X}_\alpha^n)^* = \langle \Psi_0^A | c_\alpha | \Psi_n^{A+1} \rangle \qquad \mathcal{Y}_\alpha^k = \langle \Psi_k^{A-1} | c_\alpha | \Psi_0^A \rangle$$

$$\varepsilon_n^+ = E_n^{A+1} - E_0^A \qquad \varepsilon_k^- = E_0^A - E_k^{A-1}$$



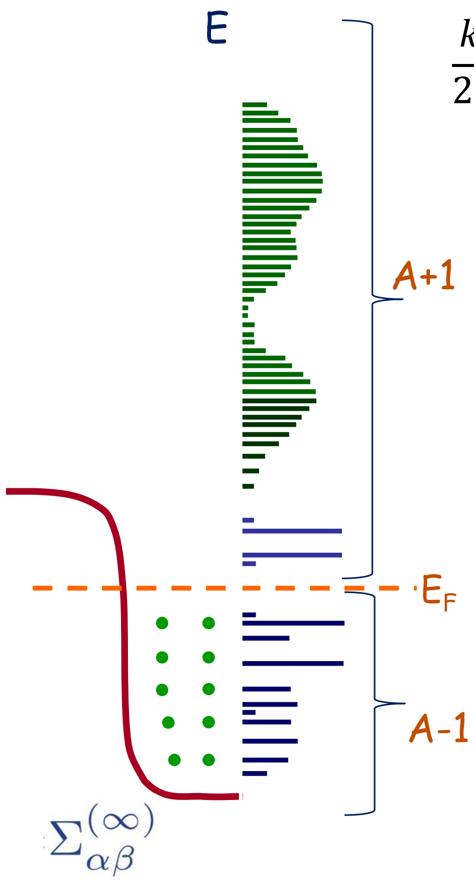
Cipollone et al., Phys. Rev. C, 92, 014306 (2015)

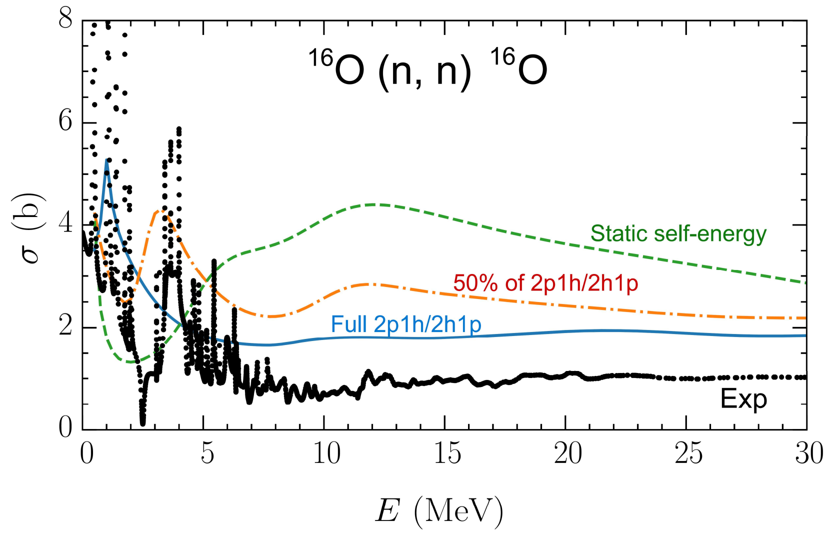


Hebeler et al., Annu. Rev. Nucl. Part. Sci. (2015)

OPTICAL POTENTIAL

$$\frac{k^2}{2m}\psi^{l,j}(k) + \int dk' k'^2 \Sigma^{l,j\star}(k,k',E_{c.m.},\eta)\psi^{l,j}(k') = E_{c.m.}\psi^{l,j}(k)$$





Idini et al., Phys. Rev. Lett., 123, 092501 (2019)

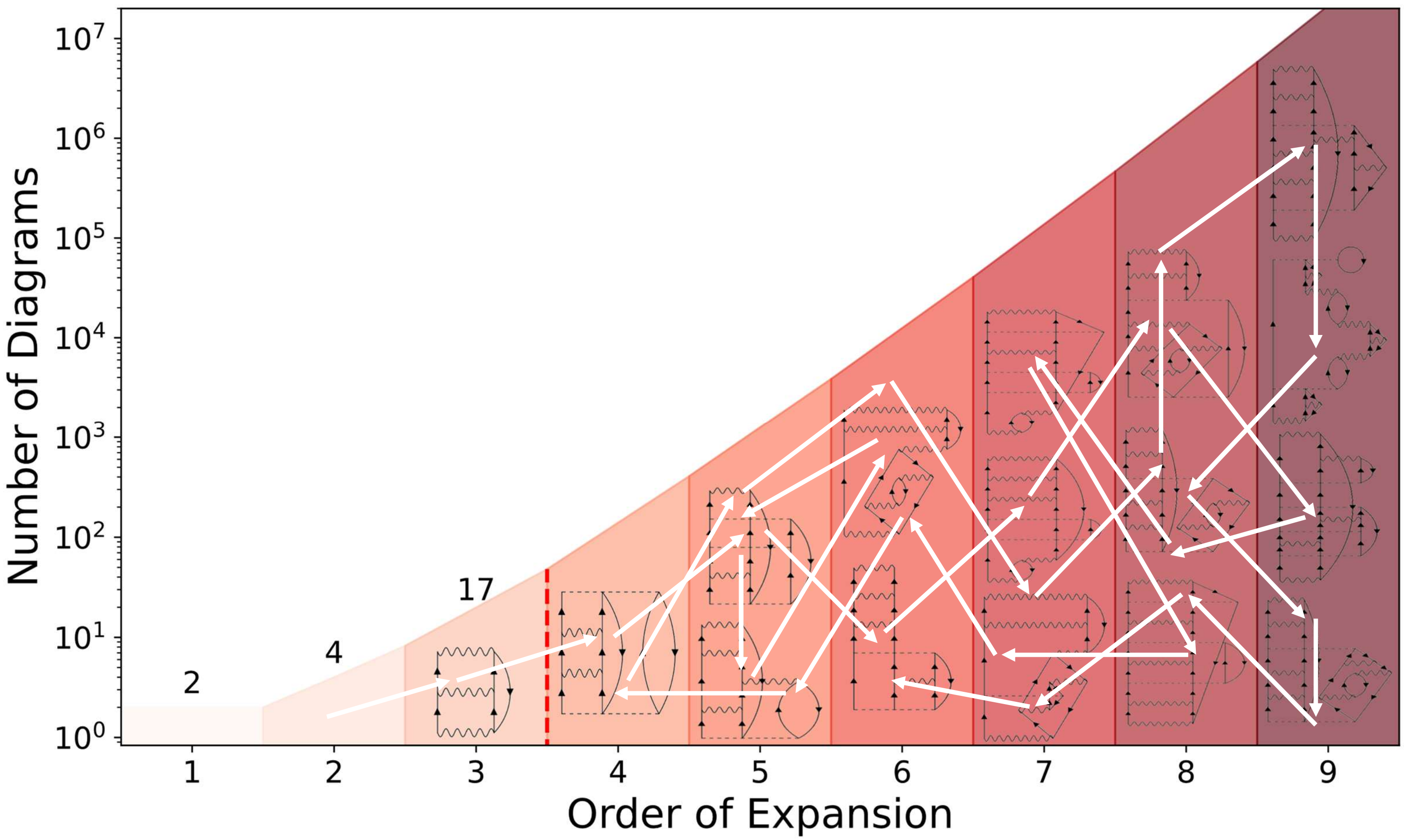
- We do not include ISCs beyond $2p1h$ and the cross section is overestimated.
- We need to include high order diagrams ($\gg 3$).

Notable work towards high order diagrams:

C. Drischler et al., Phys. Rev. Lett. 122, 042501 (2019)

P. Arthuis et al., Comp. Phys. Comm. 240, 202 (2019)

SAMPLING THE DIAGRAMMATIC SPACE



DIAGRAMMATIC MONTE CARLO

Diagrammatic Monte Carlo was developed for condensed matter systems.

- It can sum up (very) high order Feynman diagrams of the self-energy expansion[1].
- Applied for infinite systems at finite temperature.

How does it work?

- Each diagram (at fixed internal frequencies and quantum numbers) is assigned a weight.
- This creates a probability distribution W over the space of diagrams.
- We build a Markov chain with carefully tuned Metropolis-Hastings update ratios designed to reproduce the PDF W.
- The Markov chain "moves" thanks to updates on the topology and quantum numbers of the diagrams.

Can it work for nuclear physics?

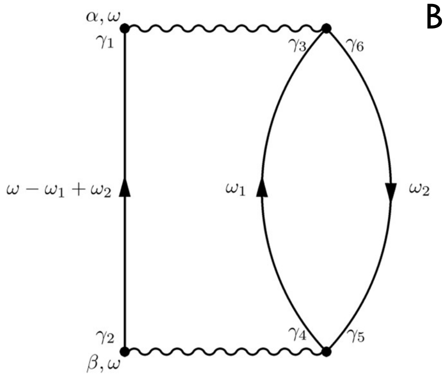
1. DiagMC included diagrams up to order 9 for the unitary Fermi gas, see K. Van Houcke et al., Phys. Rev. B., 99, 035140 (2019)

A BIT OF MATHEMATICAL MACHINERY

$$\Sigma^{\star}_{\alpha\beta}(\omega) = \sum_n \Sigma^n_{\alpha\beta} B_n(\omega)$$

Basis functions

$$\Sigma^n_{\alpha\beta} = \int d\omega\, B_n(\omega) \Sigma^{\star}_{\alpha\beta}(\omega)$$



$$\mathrm{C} = (\mathcal{T};\ \gamma_1, \ldots, \gamma_n;\ \omega_1, \ldots, \omega_m)$$

Topology

Internal single-particle quantum numbers

Internal frequencies

Diagrams of the self-energy expansion

Normalization factor

$$\Sigma^n_{\alpha\beta} = \int d\omega \int dC\, B_n(\omega) D_{\alpha\beta}(\omega, C) 1_{\mathcal{T}\in S_\Sigma} = Z_{\alpha\beta} \int d\omega \int dC\, B_n(\omega) \boxed{\frac{|D_{\alpha\beta}(\omega, C)|}{Z_{\alpha\beta}}} e^{i arg[D_{\alpha\beta}(\omega, C)]} 1_{\mathcal{T}\in S_\Sigma}$$

$$= Z_{\alpha\beta} \lim_{N\to\infty} \frac{1}{N} \sum_{j=1}^{N} B_n(\omega_j) e^{i arg[D_{\alpha\beta}(\omega_j, C_j)]} 1_{\mathcal{T}_j\in S_\Sigma}$$

$w_{\alpha\beta}(\omega, C)$, probability distribution function

DEALING WITH $Z_{\alpha\beta}$

$$\Sigma_{\alpha\beta}^{n} = Z_{\alpha\beta} \lim_{N\to\infty} \frac{1}{N} \sum_{j=1}^{N} B_n(\omega_j) e^{i arg[D_{\alpha\beta}(\omega_j, C_j)]} 1_{\mathcal{T}_j \in S_\Sigma}$$

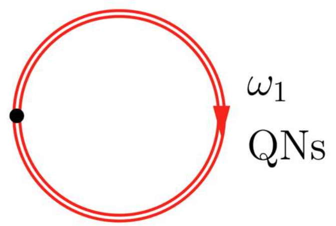
$$= \int d\omega \int dC \, |D_{\alpha\beta}(\omega)|$$

If the weight of a subset S_N of diagrams is known ($Z_{N\,\alpha\beta}$), we can use the number of times S_N is visited ($\mathcal{N}$) to compute the normalization.

$$\lim_{N\to\infty} \frac{\mathcal{N}}{N} = \frac{Z_{N\,\alpha\beta}}{Z_{\alpha\beta}}$$

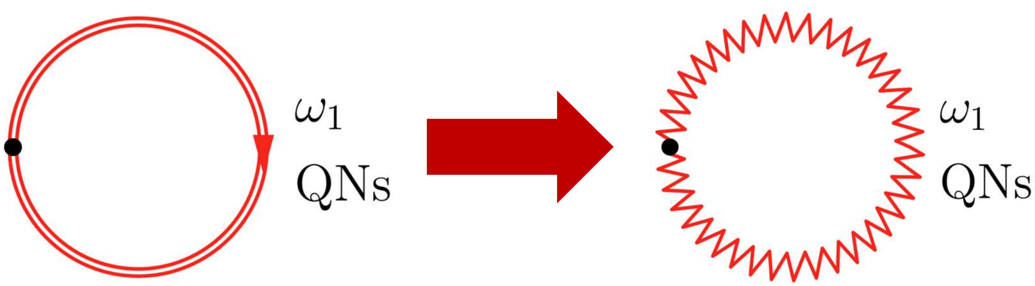
$$\Sigma_{\alpha\beta}^{n} = Z_{N_{\alpha\beta}} \lim_{N\to\infty} \frac{1}{\mathcal{N}} \sum_{j=1}^{N} B_n(\omega_j) e^{i arg[D_{\alpha\beta}(\omega_j, C_j)]} 1_{\mathcal{T}_j \in S_\Sigma}$$

NORMALIZATION SECTOR



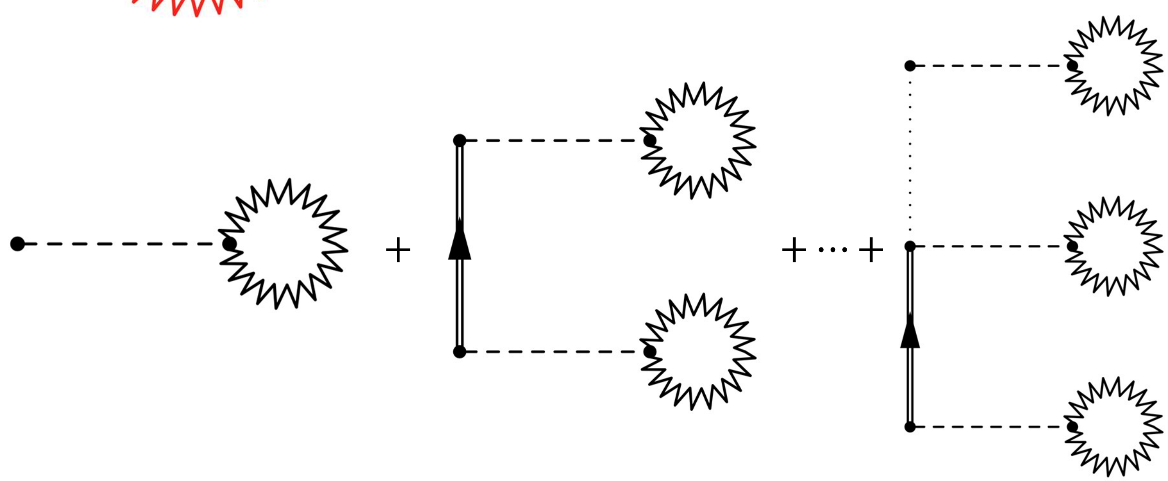
Self-closing propagators need convergence factors $e^{i\omega_1\eta}$.

They can be included automatically at all orders by using a HF reference propagator.

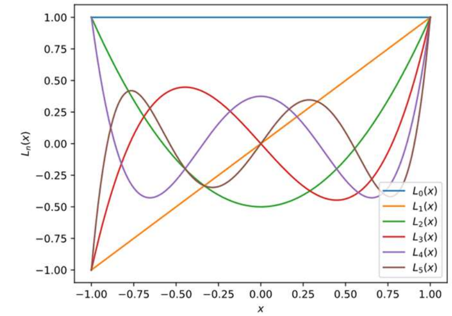


$$\stackrel{\text{def}}{=} \frac{iA}{\omega_1^2 + \gamma^2}$$

We choose as normalization sector:



BASIS FUNCTIONS



$$\Sigma^n_{\alpha\beta} = Z_{N_{\alpha\beta}} \lim_{N\to\infty} \frac{1}{\mathcal{N}} \sum_{j=1}^{N} B_n(\omega_j) e^{i \arg[D_{\alpha\beta}(\omega_j, C_j)]} 1_{\mathcal{T}_j \in S_\Sigma}$$

$B_n(x)$ are normalized Legendre polynomials.

Recursion formulas are used to generate higher order $\Sigma^n_{\alpha\beta}$ during the sampling.

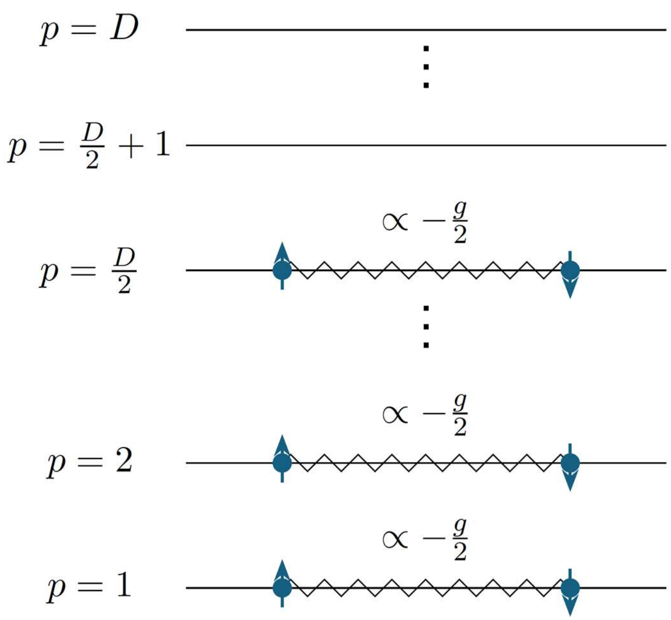
$$A_j \stackrel{\text{def}}{=} e^{i \arg[D_{\alpha\beta}(\omega_j, C_j)]} 1_{\mathcal{T}_j \in S_\Sigma}$$

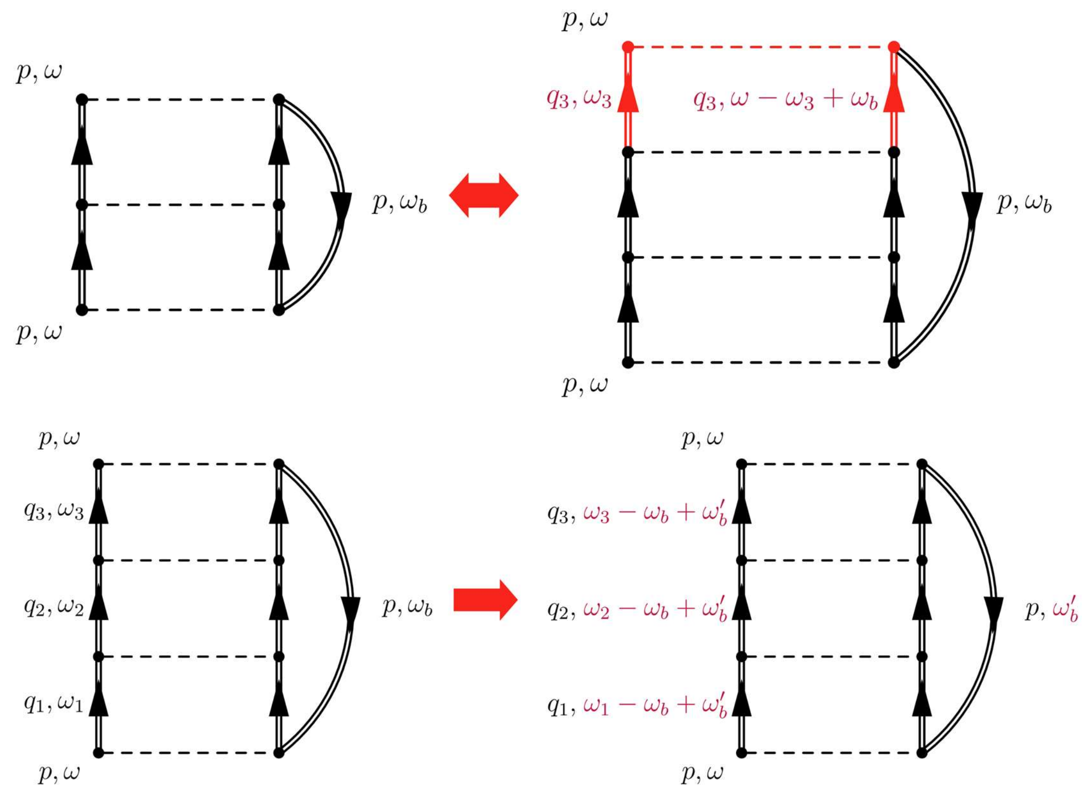
$$(n+1) A_j B_{n+1}(\omega_j) = (2n+1)\omega_j A_j B_n(\omega_j) - n B_{n-1}(\omega_j)$$

- Now we expand up to order ~ 25 with bins of size 5 MeV.
- Currently exploring higher orders and other basis functions. Maybe other polynomial basis (e.g. Chebyshev) have better performance.

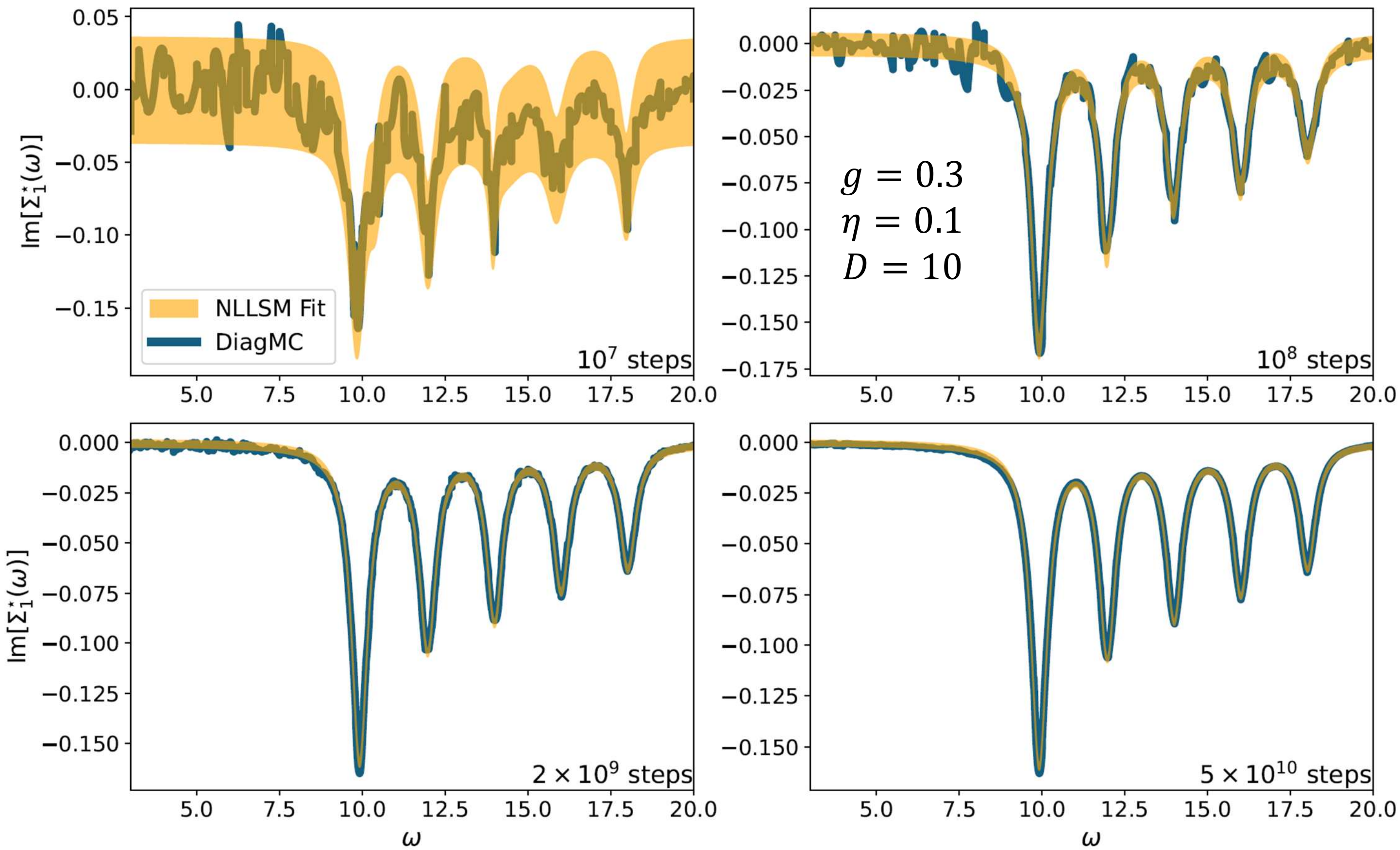
RICHARDSON MODEL

$$H^{(D)} = \sum_{p=1}^{D} \sum_{s=\uparrow,\downarrow} (p-1) c_{ps}^{\dagger} c_{ps} - \frac{g}{2} \sum_{p,q=1}^{D} c_{p\uparrow}^{\dagger} c_{p\downarrow}^{\dagger} c_{q\downarrow} c_{q\uparrow}$$



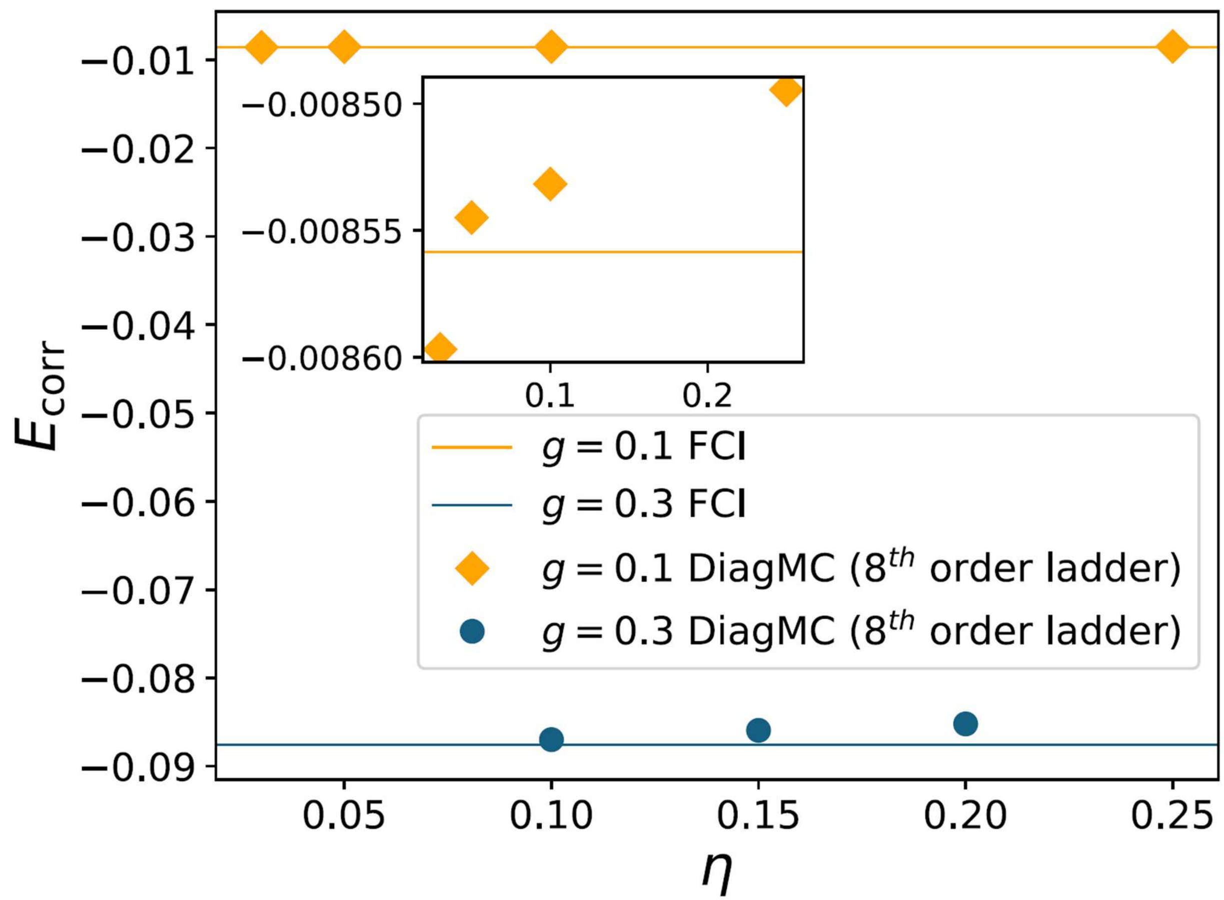


RICHARDSON MODEL: SELF-ENERGY



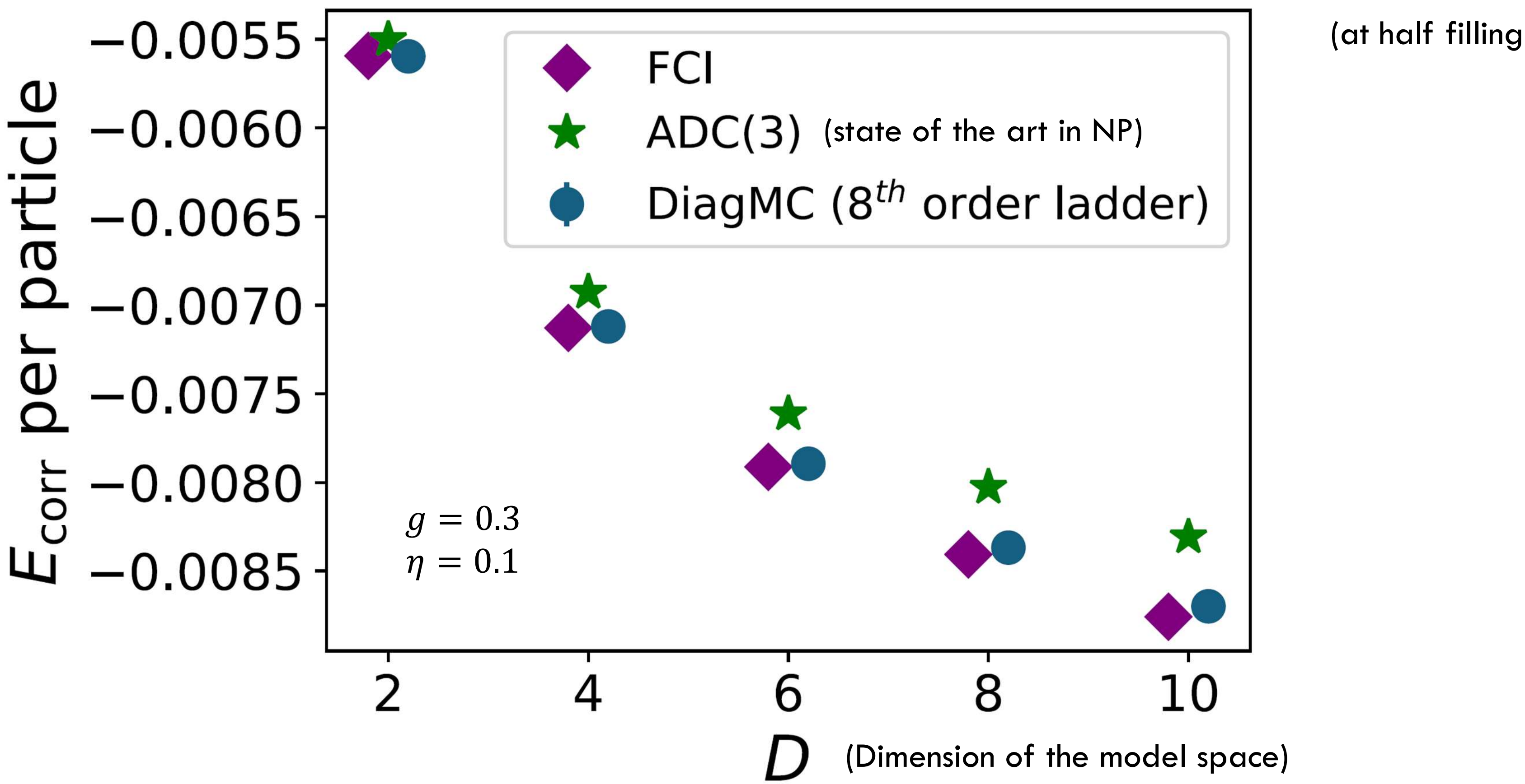
SB, C. Barbieri, and E. Vigezzi, Phys. Rev. Lett. 134, 182502 (2025)

RICHARDSON MODEL: FINITE REGULATOR ERROR



SB, C. Barbieri, and E. Vigezzi, Phys. Rev. Lett. 134, 182502 (2025)

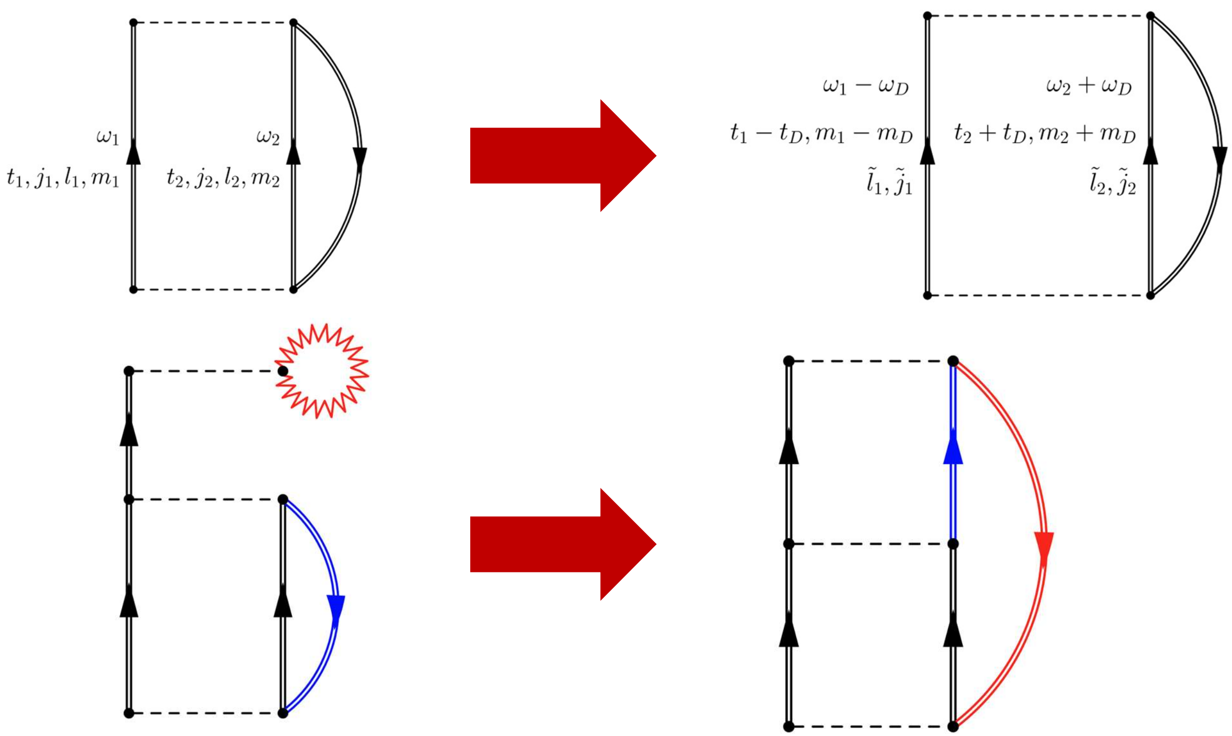
RICHARDSON MODEL: GROUND STATE ENERGY



SB, C. Barbieri, and E. Vigezzi, Phys. Rev. Lett. 134, 182502 (2025)

CHIRAL POTENTIALS

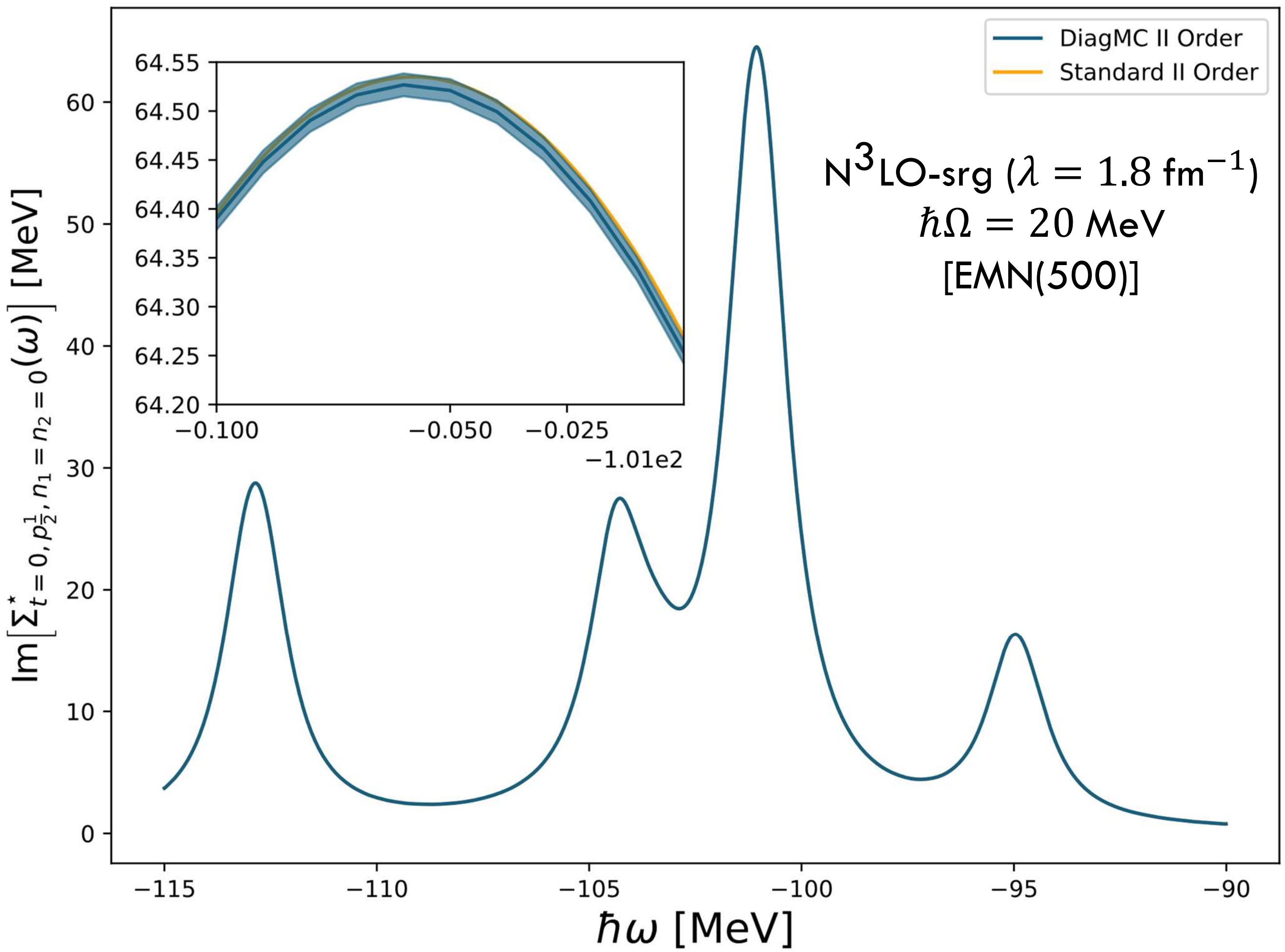
- To our knowledge DiagMC calculations with such difficult potentials have never been attempted.
- They require a much more complicated updating scheme that can keep track of all the conservation laws at each vertex (to avoid sampling too many zero diagrams).



SECOND ORDER RESULTS

^{16}O

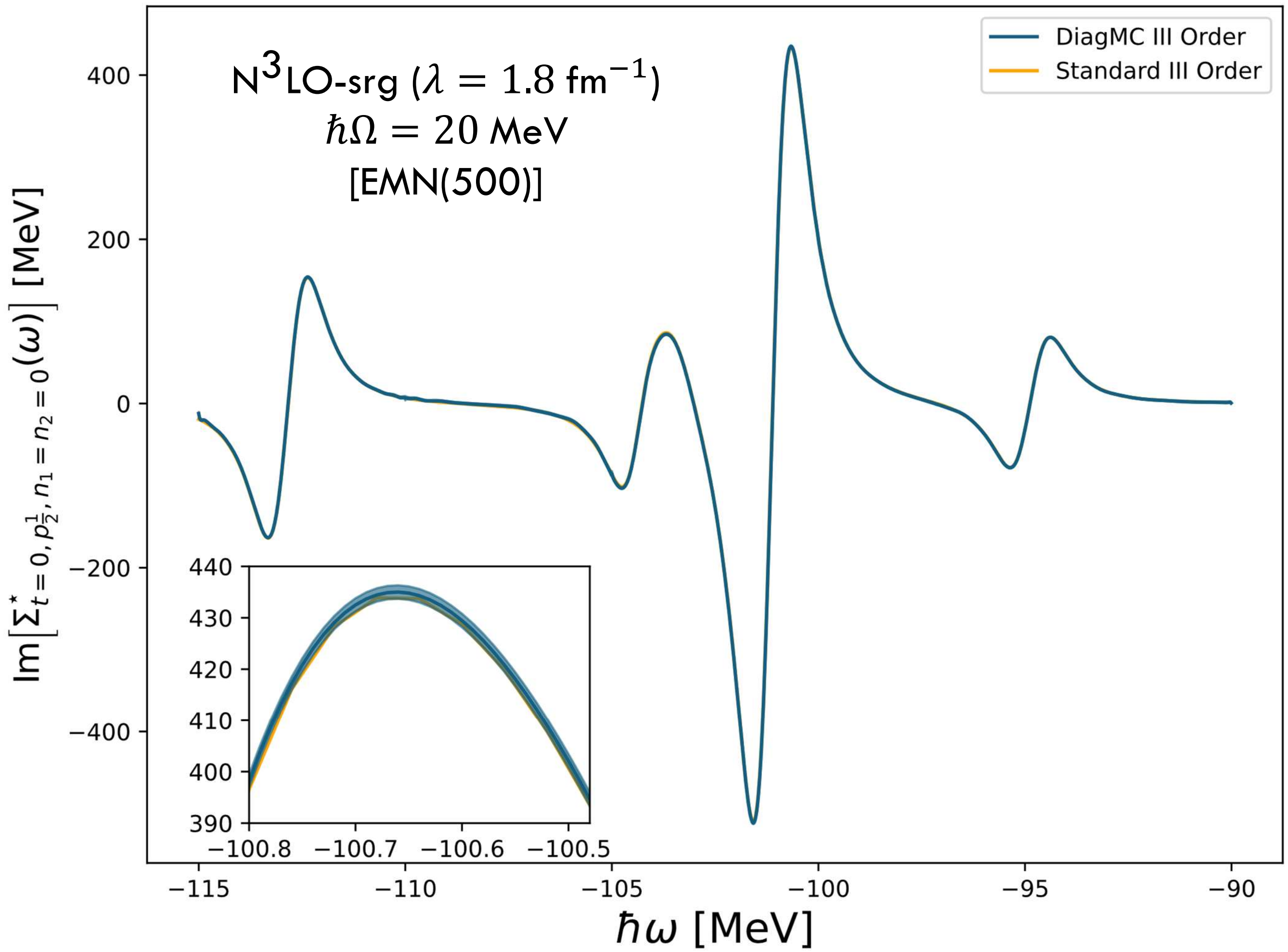
$N_{max} = 2$



THIRD ORDER RESULTS

^{16}O

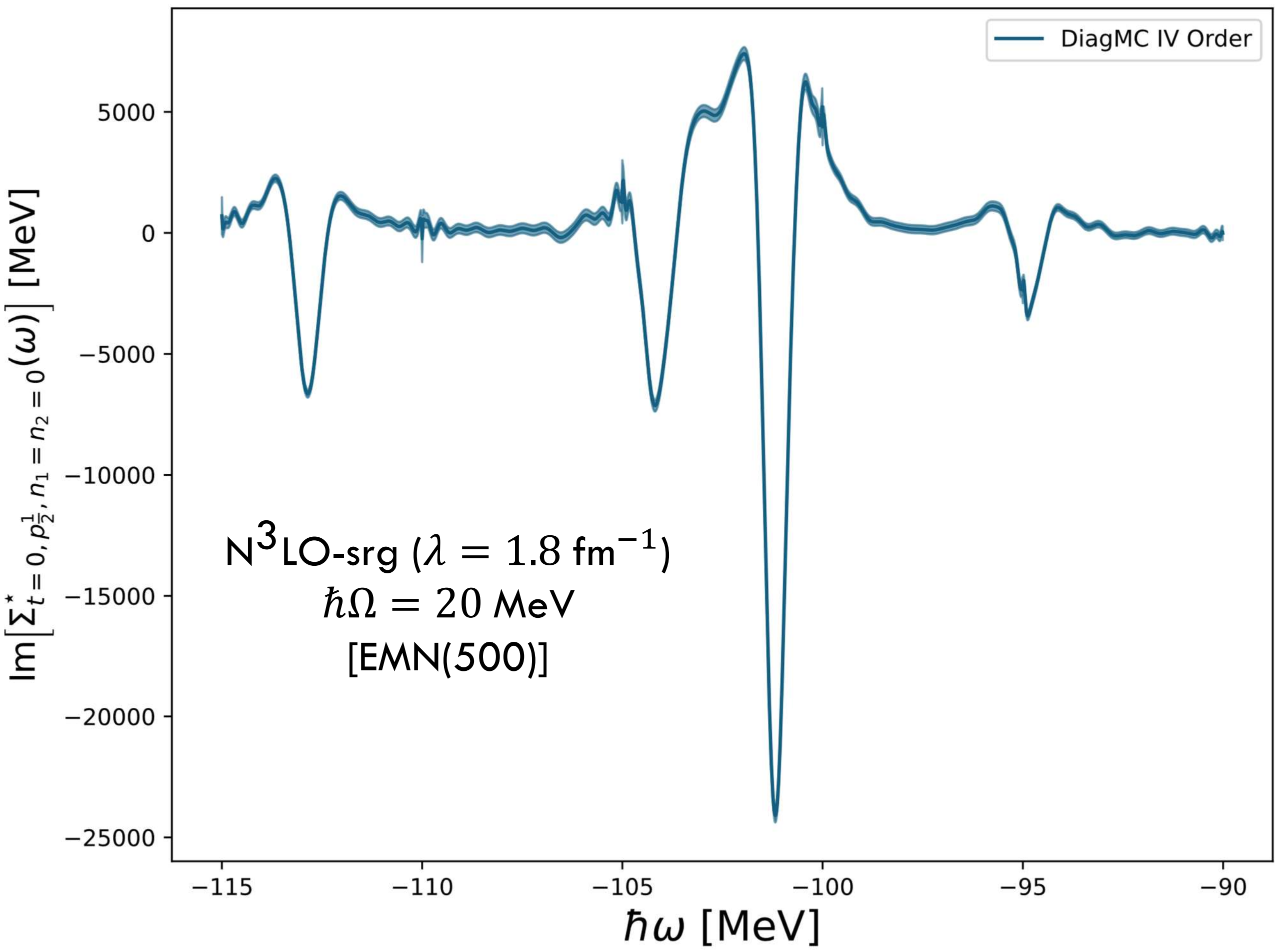
$N_{max} = 2$



FOURTH ORDER RESULTS

^{16}O

$N_{max} = 2$



RECOVERING CAUSALITY

There are ways to recover the causality principle from the perturbation theory expansion:

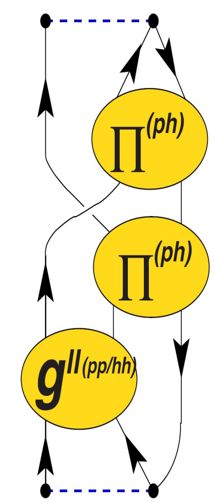
- Resummation techniques (Borel resummation) → Already used in solid state physics

- ADC-like schemes natively retain causality → State of the art techniques in nuclear physics, never integrated with DiagMC

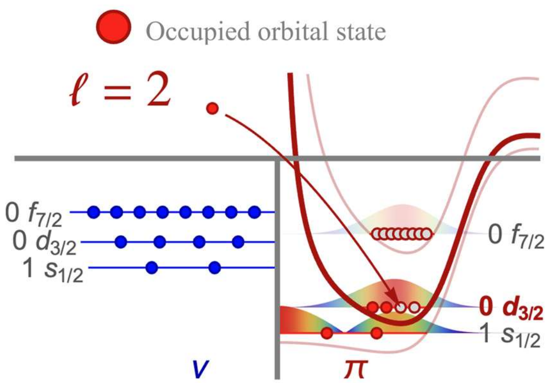
Particle-vibration couplings

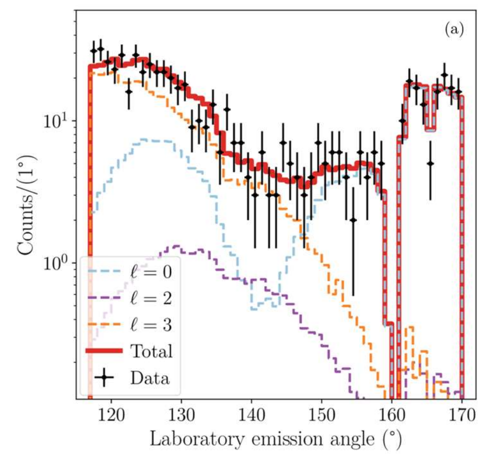
$$\Sigma^{\star}_{\alpha\beta}(\omega) = \Sigma^{(\infty)}_{\alpha\beta} + M^{\dagger}_{\alpha,r} \frac{1}{\omega - [E^{>} + C]_{r,r'} + i\eta} M_{r',\beta} + N_{\alpha,s} \frac{1}{\omega - [E^{<} + D]_{s,s'} - i\eta} N^{\dagger}_{s',\beta}$$

Mean field

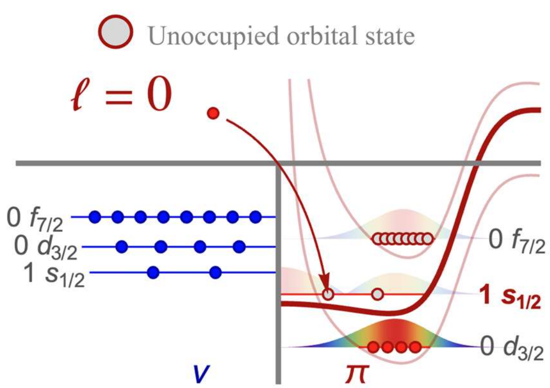


SHELL INVERSION IN ARGON 46





The $^{46}Ar(\,^{3}He,d)^{47}K$ reaction shows a smaller-than-expected exclusive cross section for the $l = 2$ component and a larger $l = 0$ component.



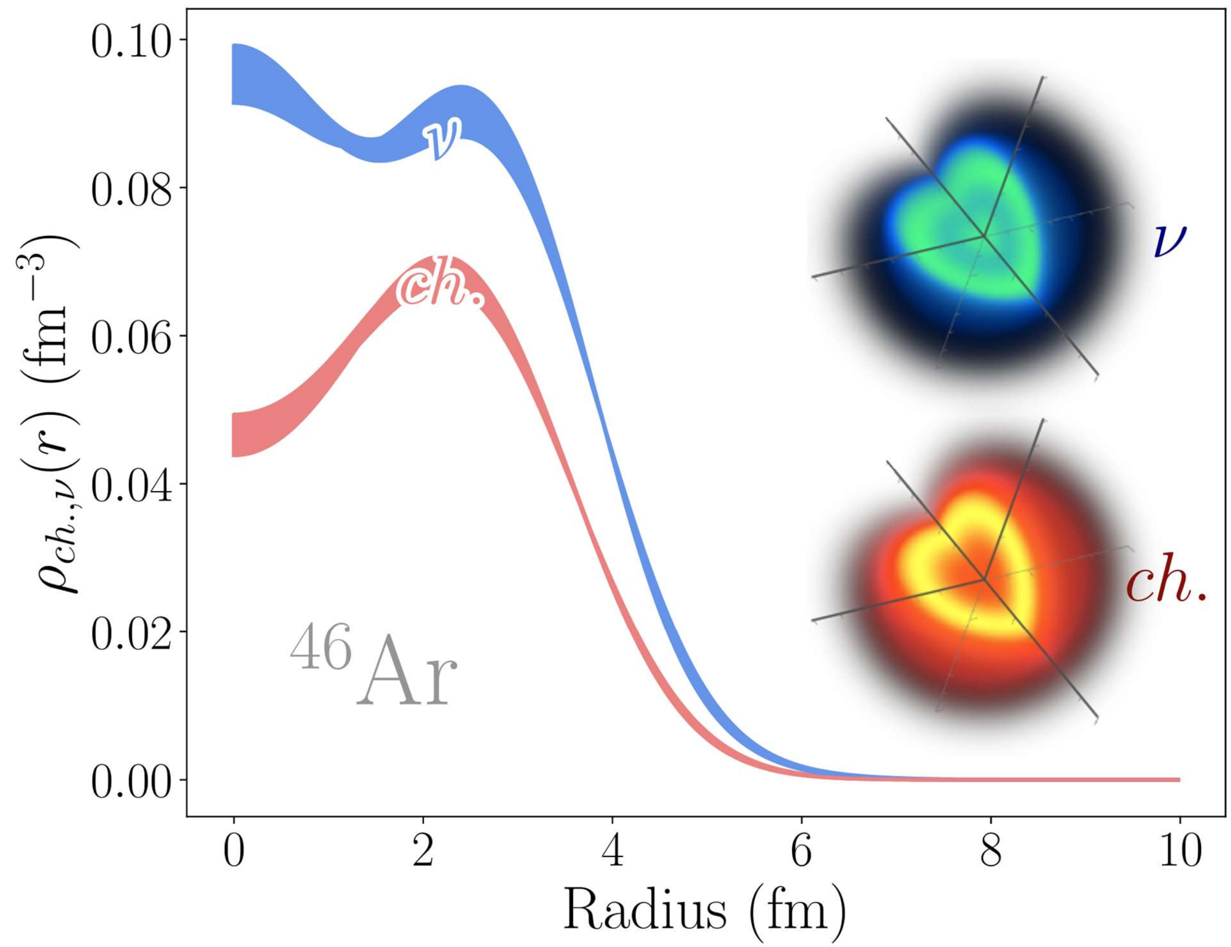
This points toward shell inversion.

SCGF calculations with the interactions $NNLO_{sat}$, $\Delta NNLO_{GO}(394, 450)$ and 1.8/2.0(EM7.5) [1, 2, 3] all confirm this shell inversion.

1: A. Ekström et al., Phys. Rev. C 91, 051301 (2015)
2: A. Ekström et al., Phys. Rev. C 97, 024332 (2018)
3: P. Arthuis et al., arXiv: 2401.06675 (2024)

D. Brugnara et al., arXiv:2506.23228v2 (2025)

CHARGE BUBBLE IN ARGON 46



D. Brugnara et al., arXiv:2506.23228v2 (2025)

THANK YOU

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