# A Diagrammatic Monte Carlo Approach for Nuclear Structure and Reactions

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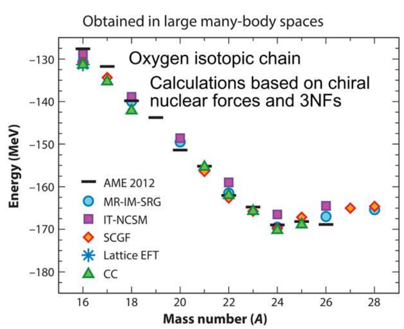
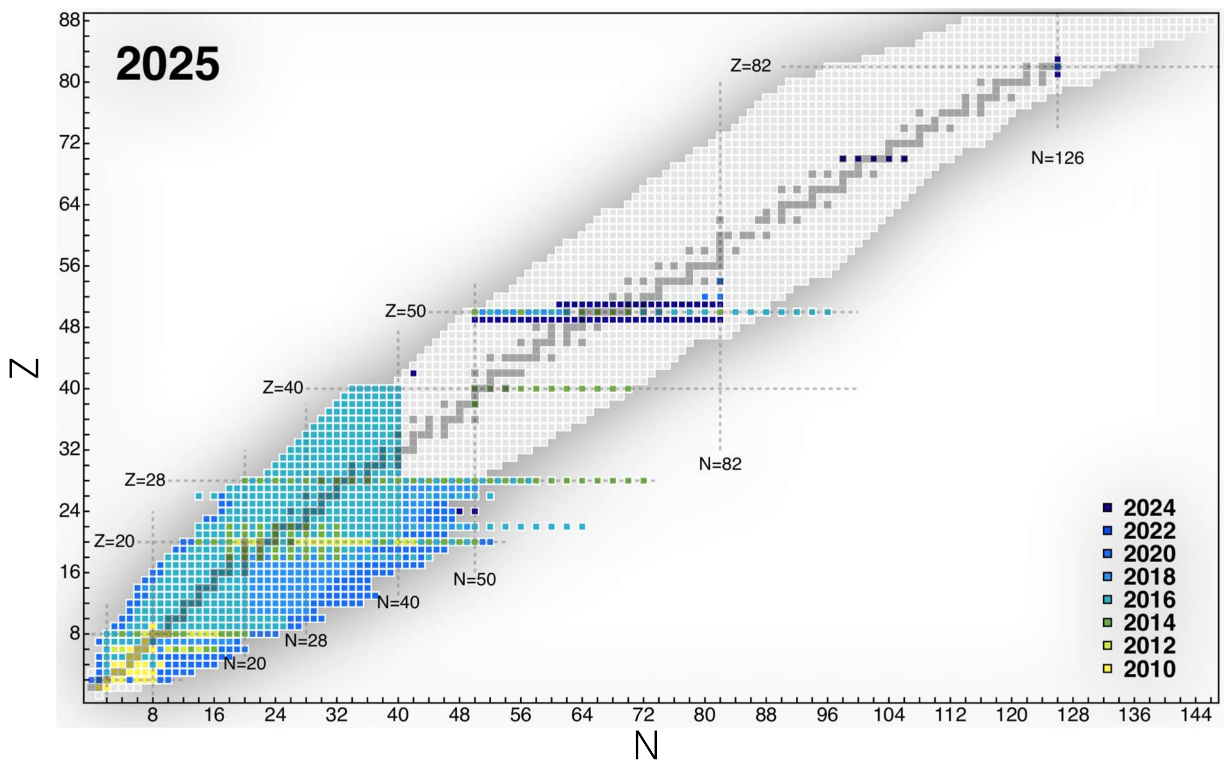
# *AB INITIO* STRUCTURE CALCULATIONS

- Medium-light mass nuclei (and a few heavy ones) are well described.
- Many-body methods (SCGF, NCSM, MBPT, IMSRG, CC, …) agree on ground state structure.
- Most of the uncertainty comes from the Hamiltonian.
- More recently: push for heavy and deformed nuclei.



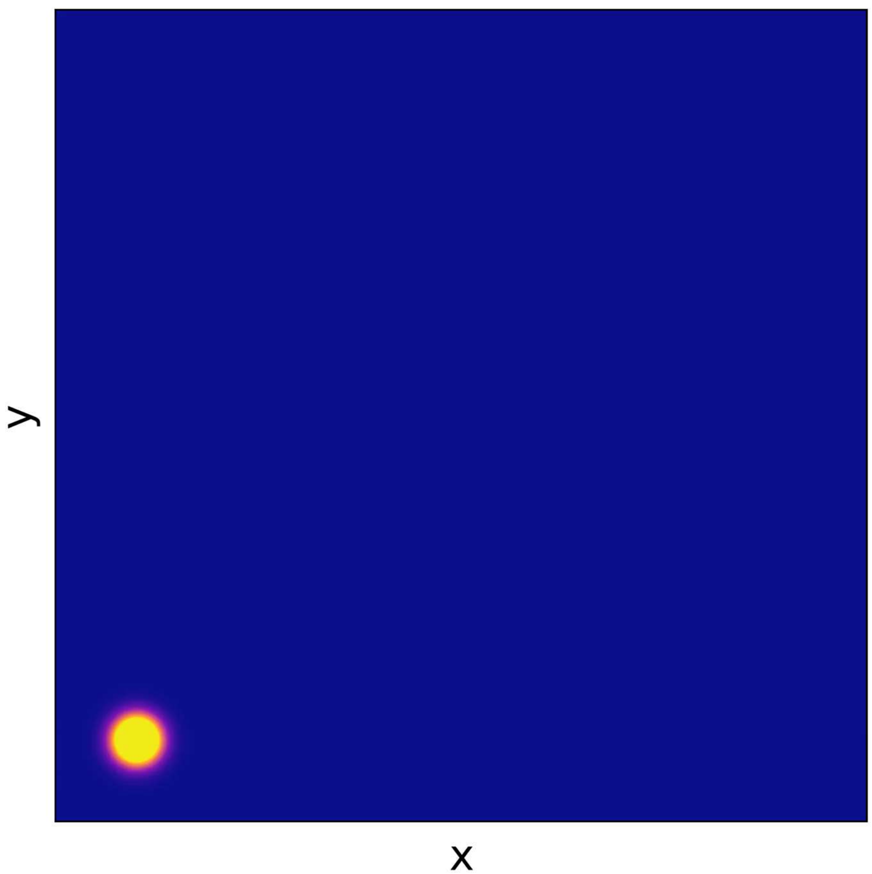

Hebeler et al., Annu. Rev. Nucl. Part. Sci. (2015)




*Hergert, A Guided Tour of ab initio Nuclear Many-Body Theory, Front. Phys. 8 (2020)*

# SELF-CONSISTENT GREEN'S FUNCTION

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



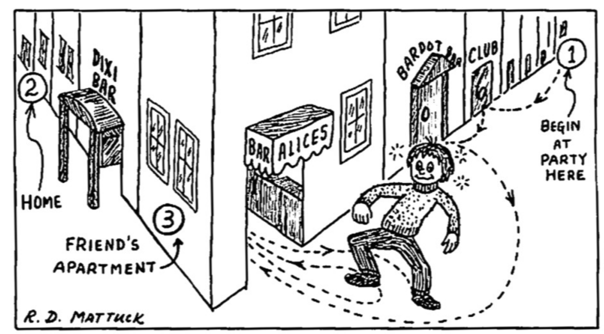




Fig. 1.1 *Propagation of Drunken Man*

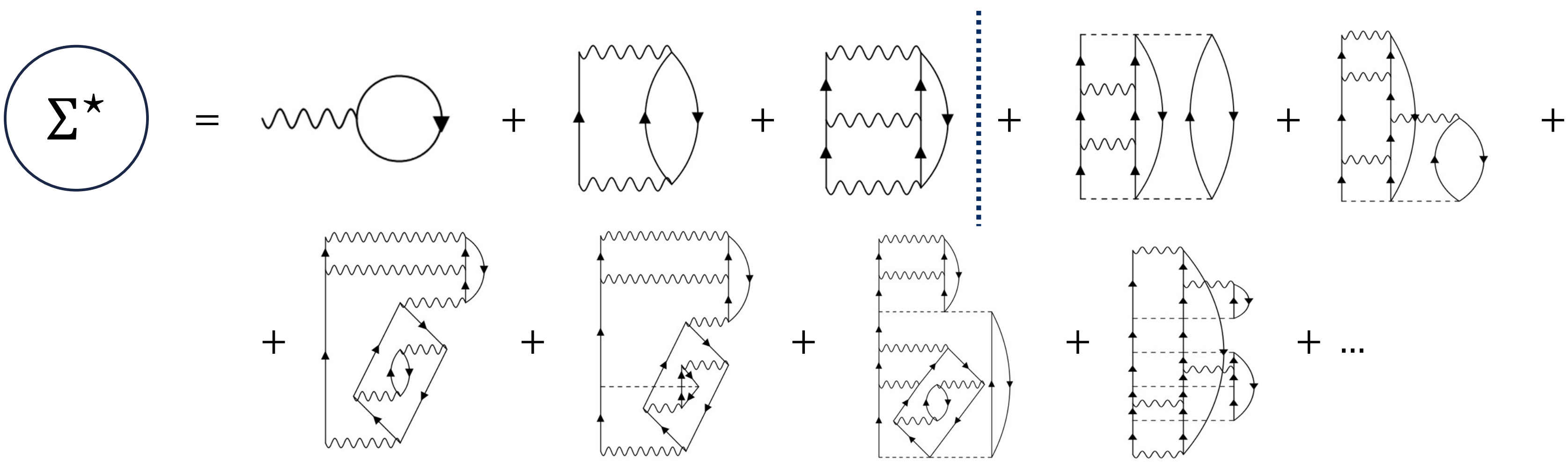
*Mattuck, A Guide to Feynman Diagrams in the Many-Body Problem (1992)*

# DYSON EQUATION

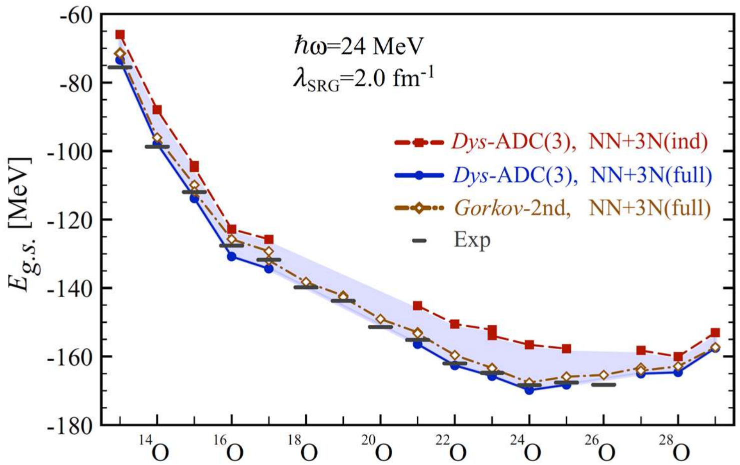
$$G_{\alpha\beta}(\omega) = G^{(0)}_{\alpha\beta}(\omega) + G^{(0)}_{\alpha\gamma}(\omega)\Sigma^{\star}_{\gamma\delta}(\omega)G_{\delta\beta}(\omega)$$

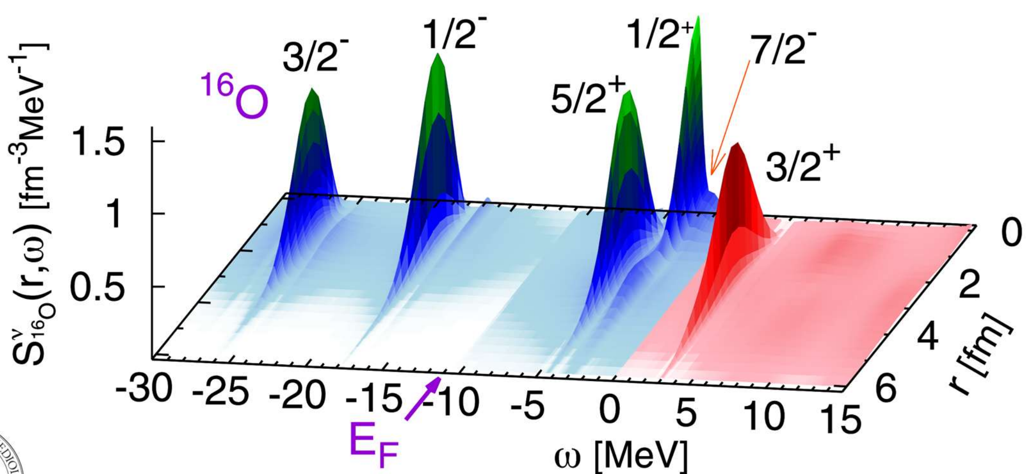
Unperturbed propagator

Irreducible self-energy

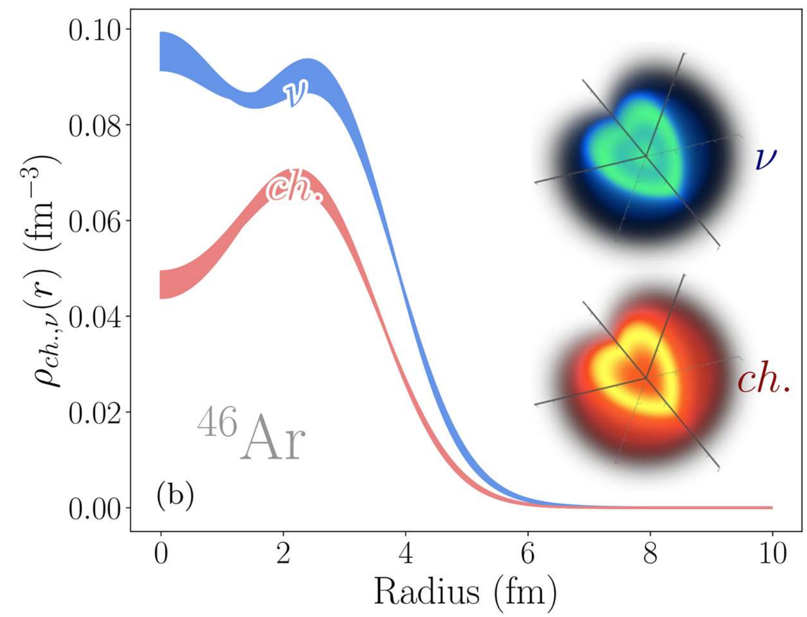


# STRUCTURE INFORMATION



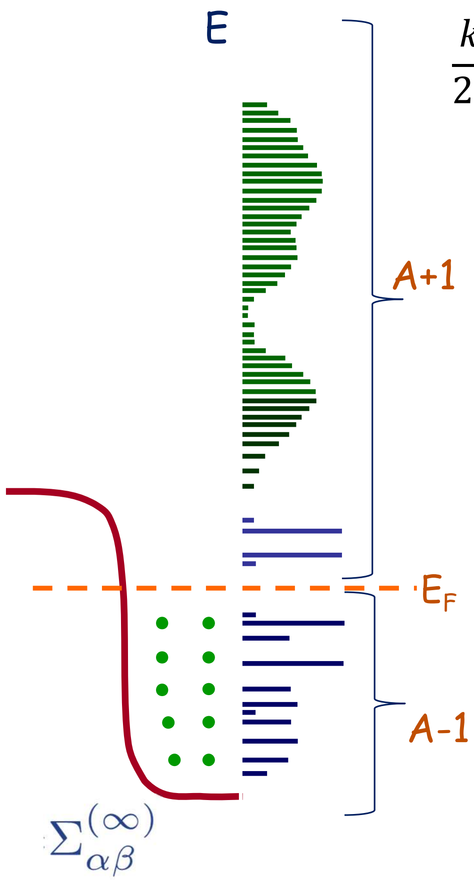




Cipollone et al., Phys. Rev. C, 92, 014306 (2015)

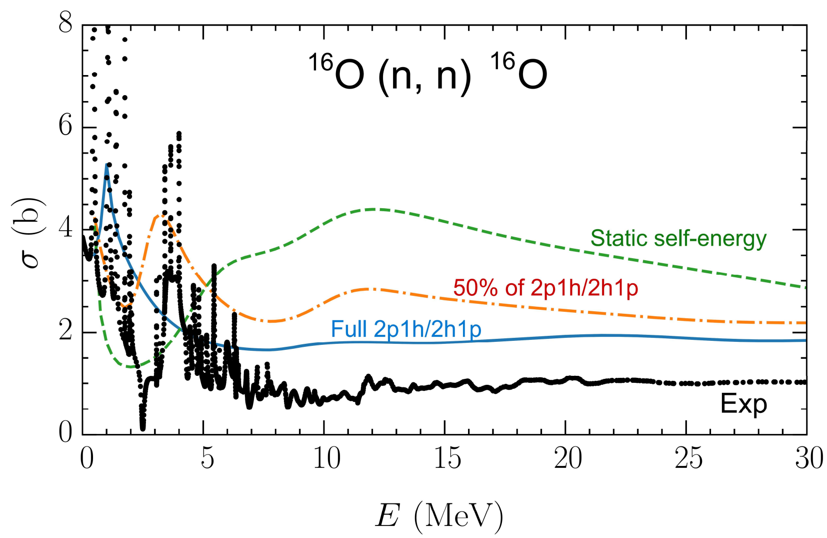



Brugnara et al., arXiv: 2506.23228v2 (2025)

# 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)*

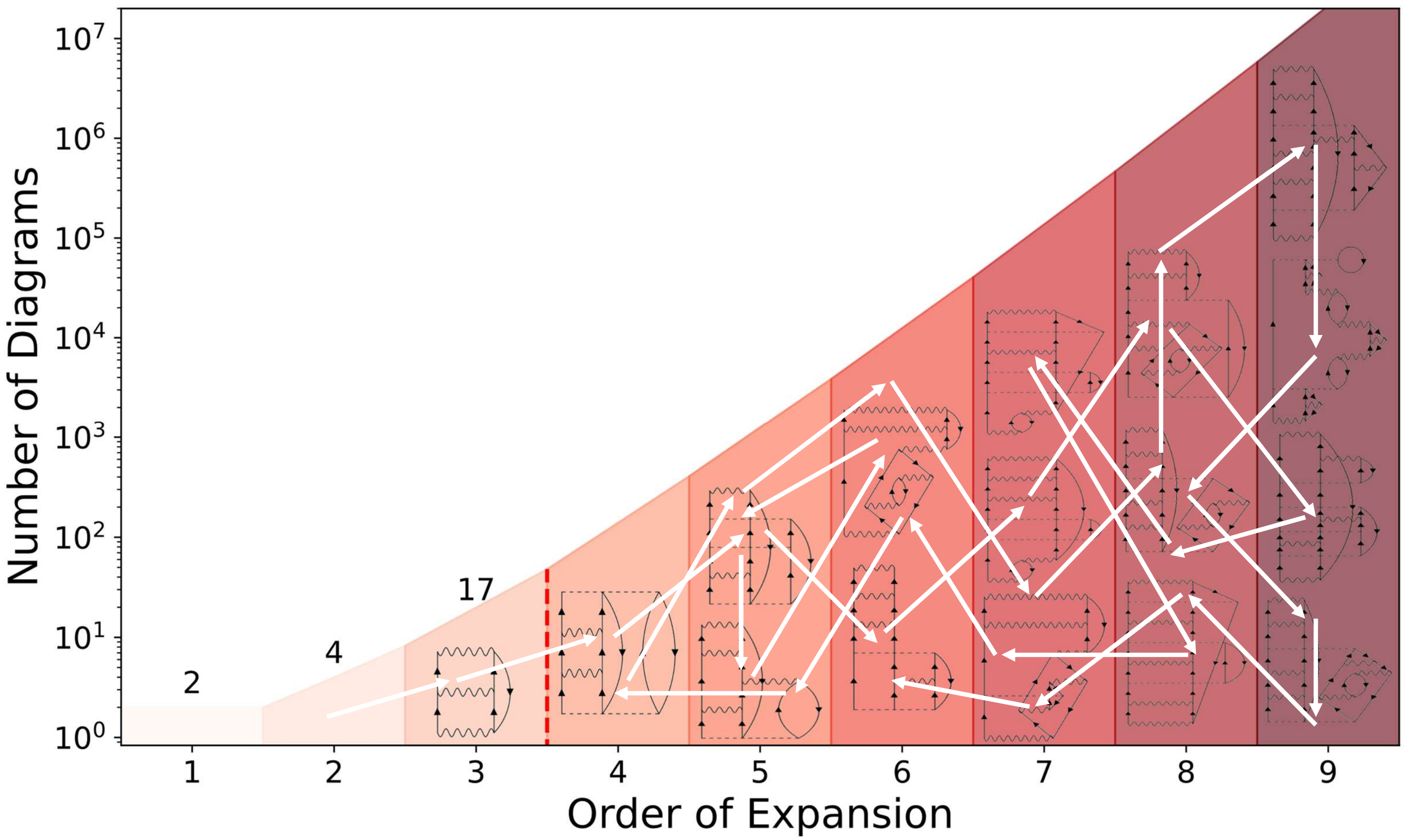
- We do not include ISCs beyond $2p1h$.
- We need to include high-order ($\gg$ 3) diagrams.

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

- 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 (e.g. unitary Fermi gas).

How does it work?

- Each diagram is assigned a weight.
- This creates a probability distribution $\mathcal{W}$ over the space of diagrams.
- A Markov chain with tuned Metropolis-Hastings update ratios reproduces the PDF $\mathcal{W}$.
- The Markov chain "moves" with updates to the topology and quantum numbers of the diagrams.

Can it work for nuclear systems?

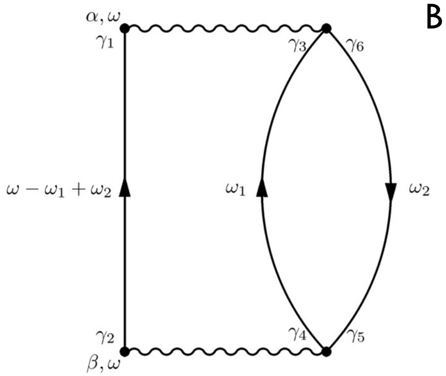
*1. DiagMC included diagrams up to order 9 for the unitary Fermi gas, see K. Van Houcke et al., Phys. Rev. B., 99, 035140 (2019)*

# A BIT OF MATHEMATICAL MACHINERY

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

Basis functions

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




$$\mathrm{C} = (\mathcal{T};\ \gamma_1, \dots, \gamma_{\mathrm{n}};\ \omega_1, \dots, \omega_{\mathrm{m}})$$

Topology

Internal single-particle quantum numbers

Internal frequencies

Diagrams of the self-energy expansion

Normalization factor

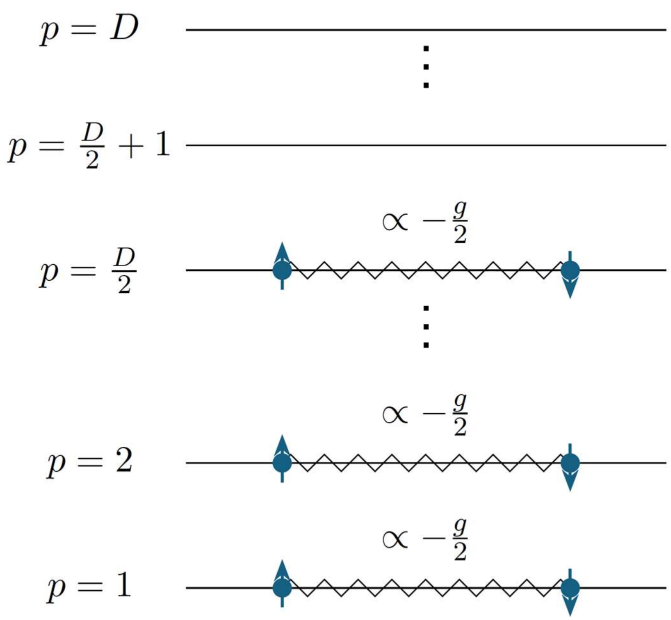
$$\Sigma^n_{\alpha\beta} = \int d\omega \int dC \, B_n(\omega) D_{\alpha\beta}(\omega, C) 1_{\mathcal{T} \in S_\Sigma} = Z_{\alpha\beta} \int d\omega \int dC \, B_n(\omega) \boxed{\frac{|D_{\alpha\beta}(\omega, C)|}{Z_{\alpha\beta}}} e^{i arg[D_{\alpha\beta}(\omega, C)]} 1_{\mathcal{T} \in S_\Sigma}$$

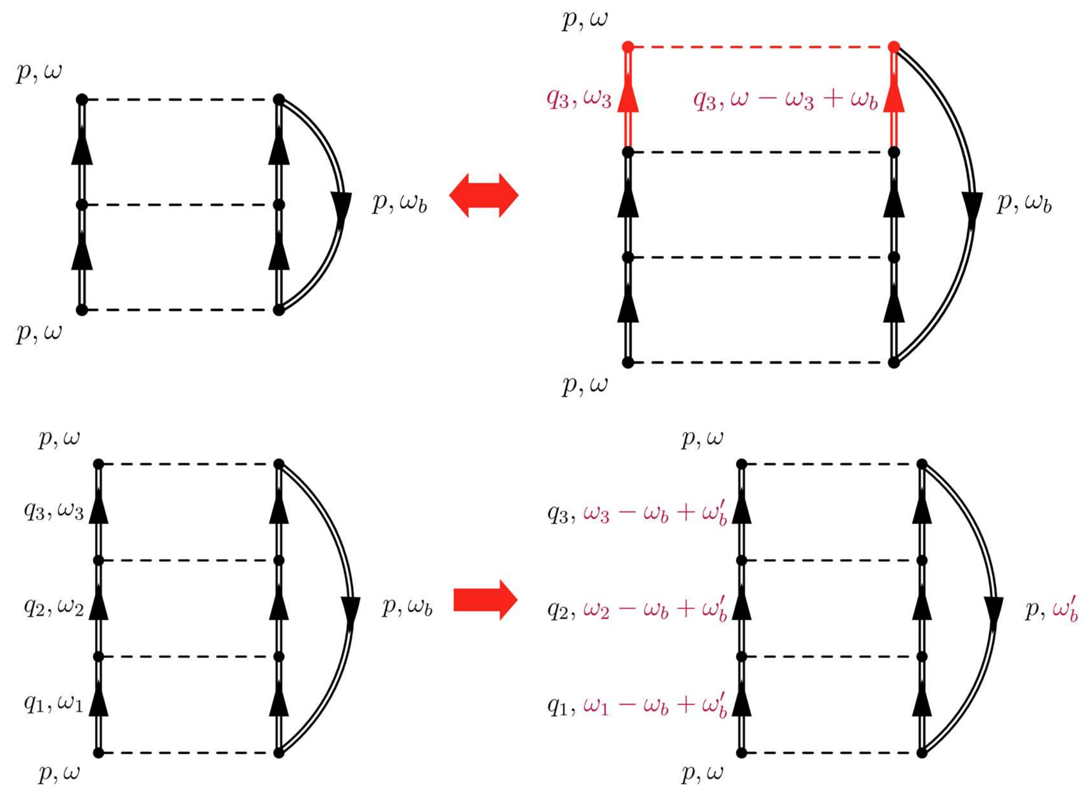
$$= Z_{\alpha\beta} \lim_{N \to \infty} \frac{1}{N} \sum_{j=1}^{N} B_n(\omega_j) e^{i arg[D_{\alpha\beta}(\omega_j, C_j)]} 1_{\mathcal{T}_j \in S_\Sigma}$$

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

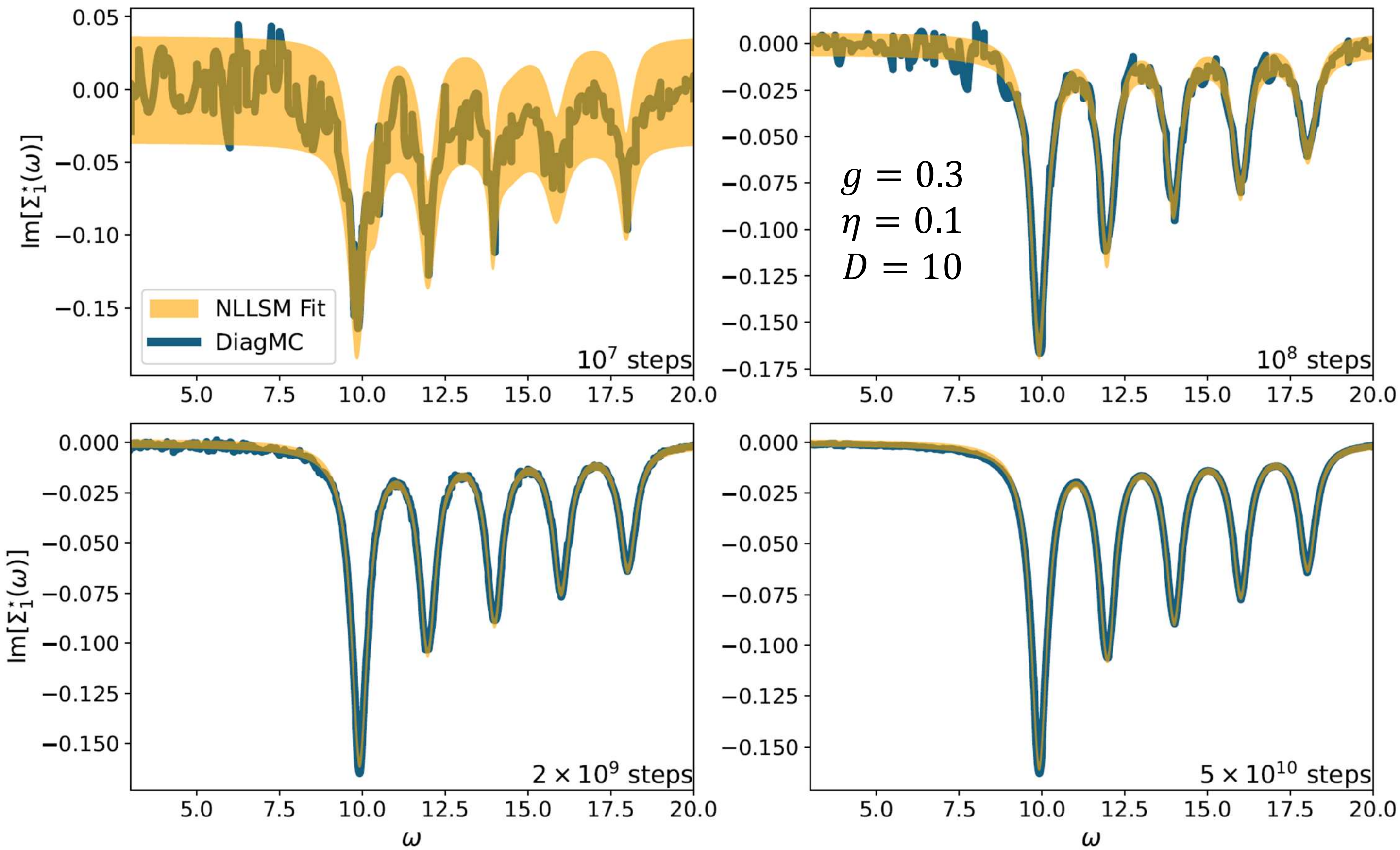
# RICHARDSON MODEL

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



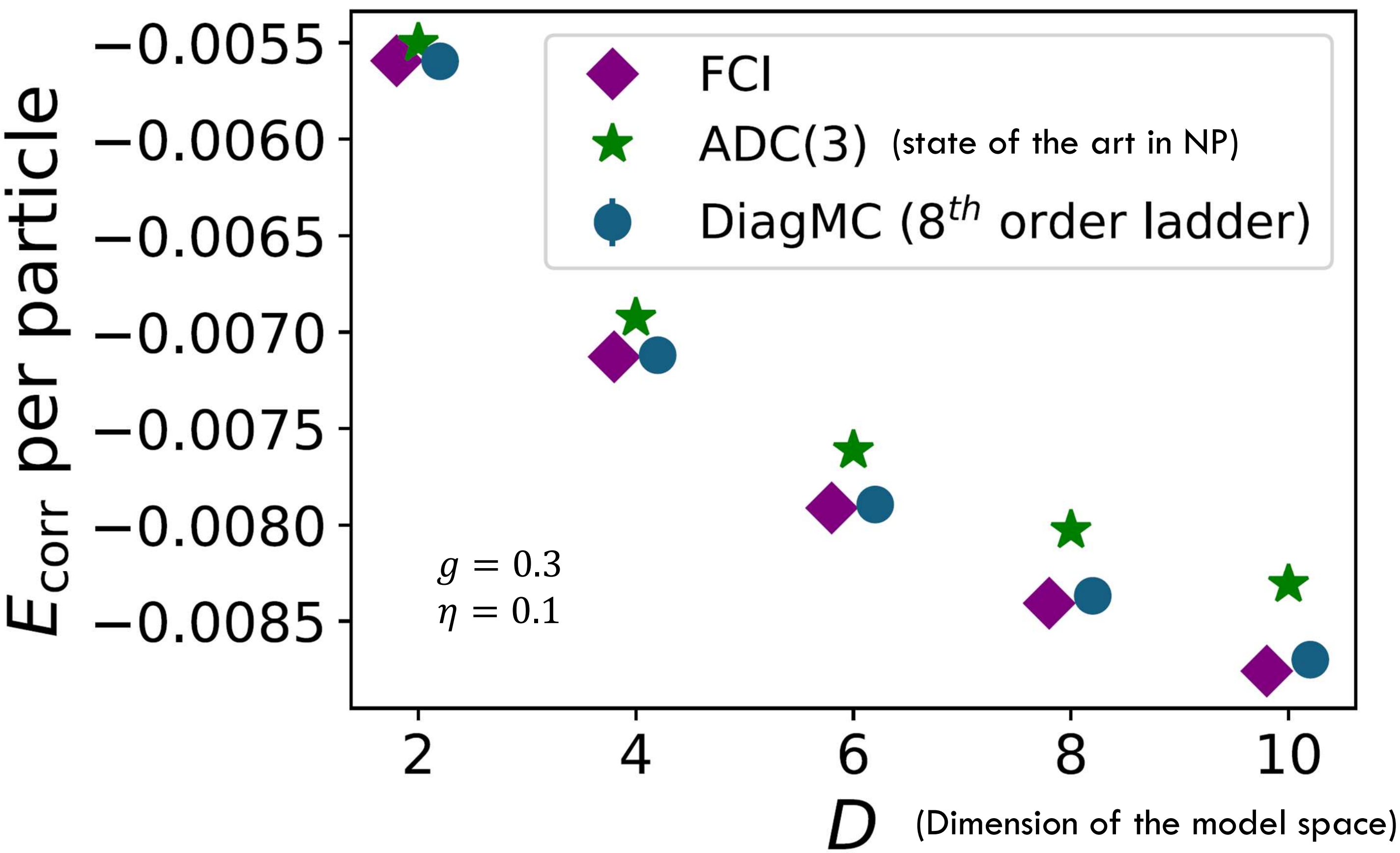



# RICHARDSON MODEL: SELF-ENERGY




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

# RICHARDSON MODEL: GROUND STATE ENERGY

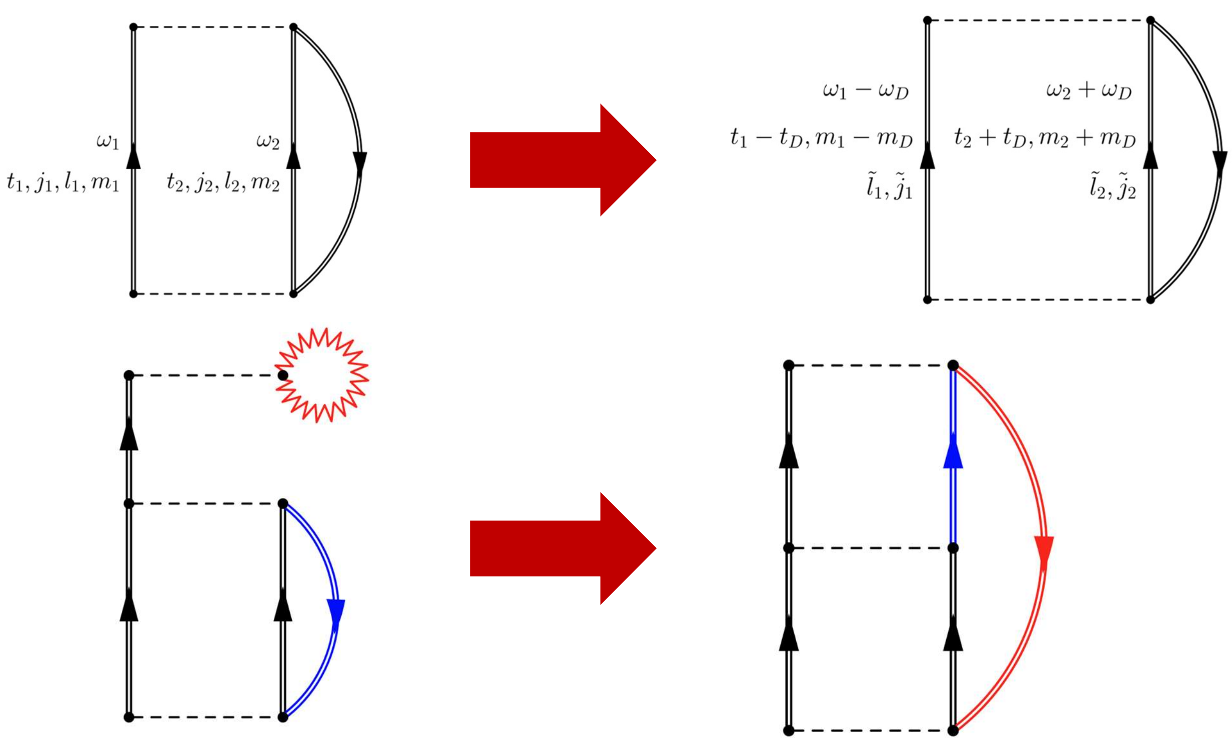



(at half filling)

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

# CHIRAL POTENTIALS

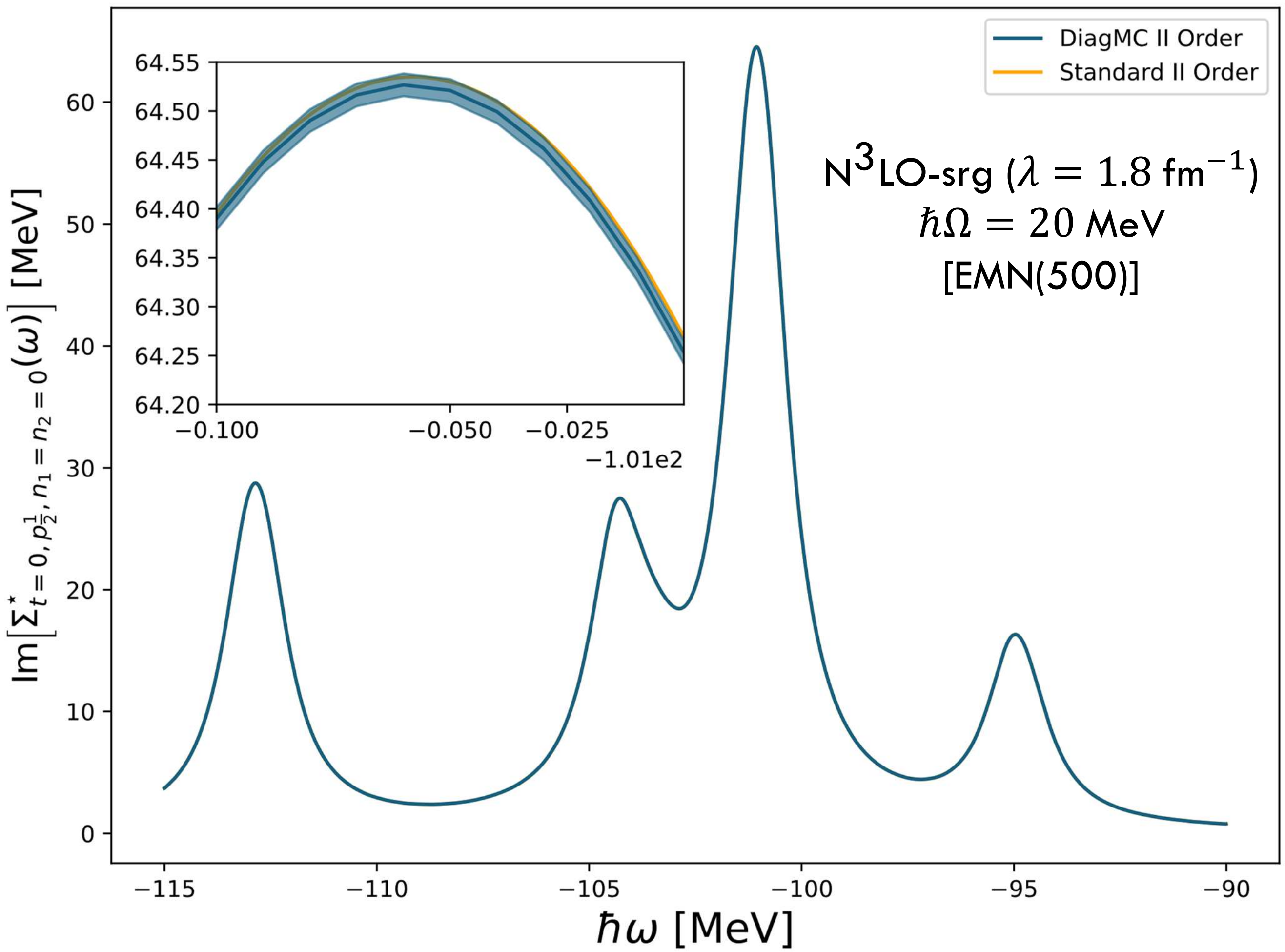
- To our knowledge DiagMC calculations with such difficult potentials have never been attempted.
- They require a much more complicated updating scheme that can keep track of all the conservation laws at each vertex.



# SECOND ORDER RESULTS

$^{16}O$

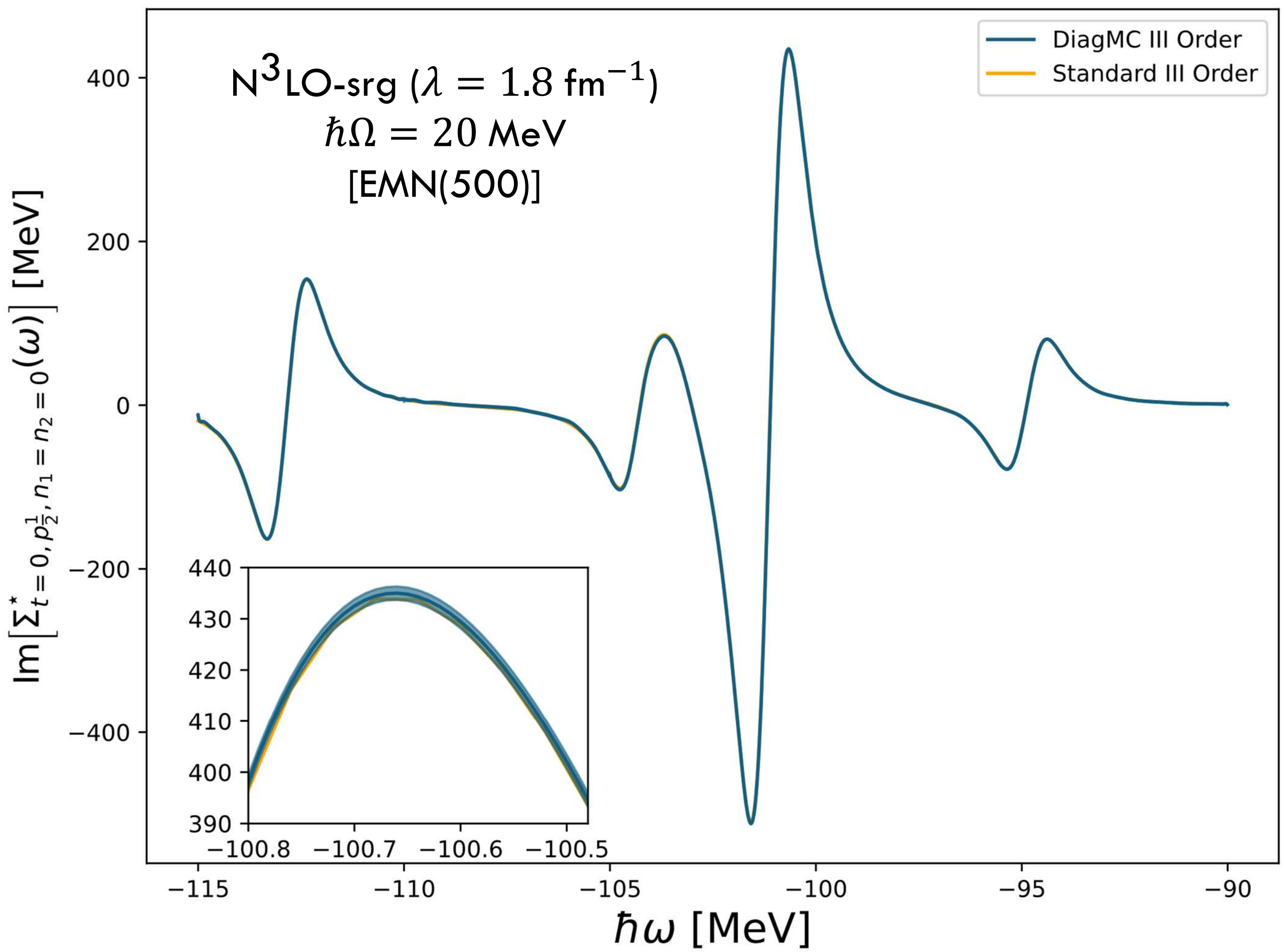
$N_{max} = 2$



# THIRD ORDER RESULTS

$^{16}O$

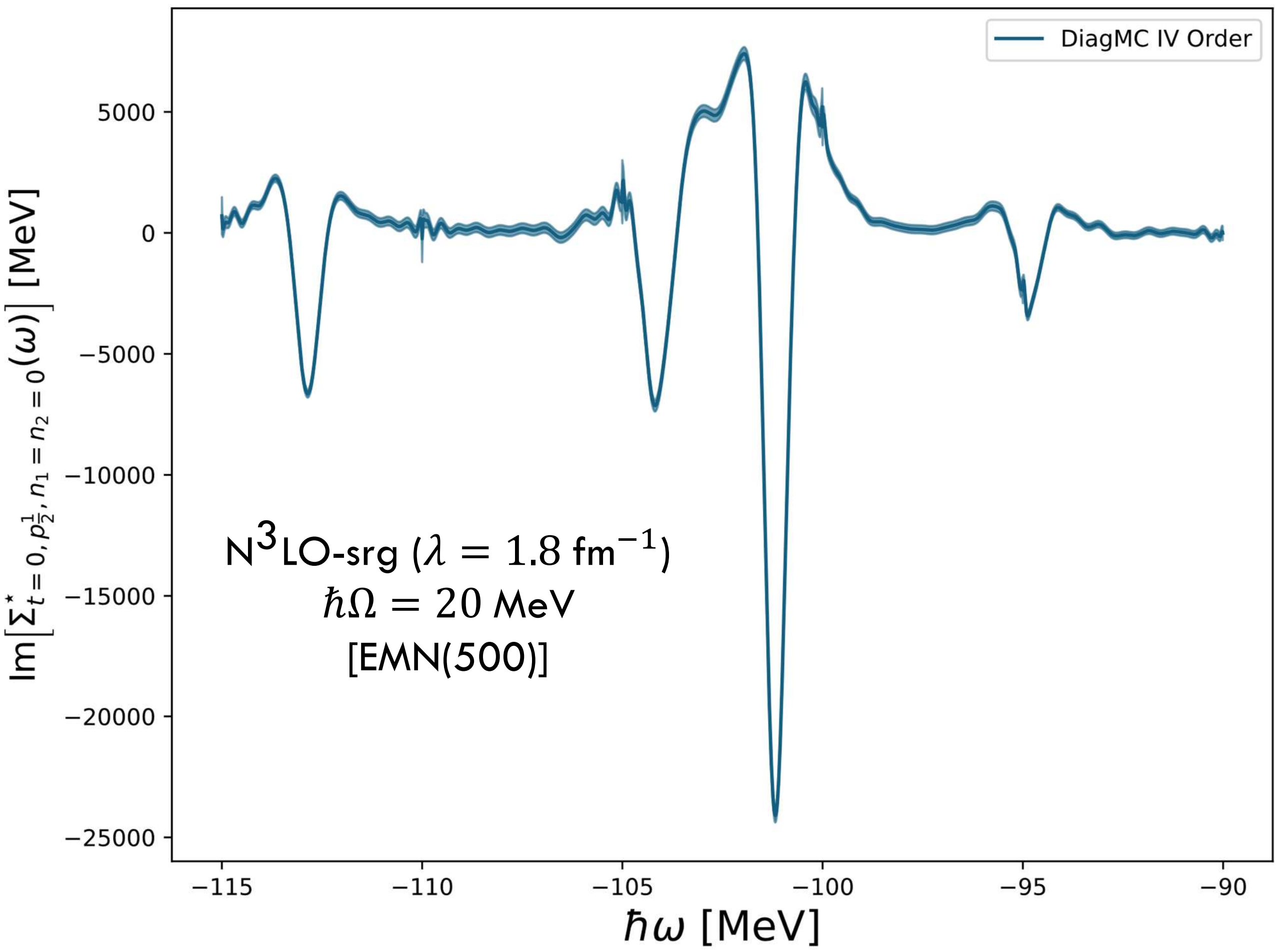
$N_{max} = 2$



# FOURTH ORDER RESULTS

$^{16}$O

$N_{max} = 2$



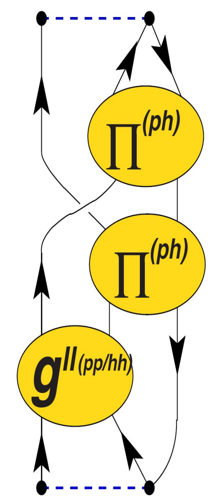
# RECOVERING CAUSALITY

- 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



# THANK YOU

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# BACKUP:

# DEALING WITH $Z_{\alpha\beta}$

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

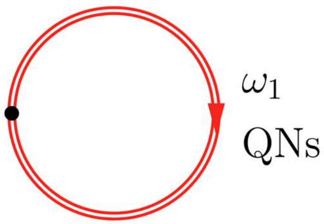
$$= \int d\omega \int dC \, |D_{\alpha\beta}(\omega)|$$

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.

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

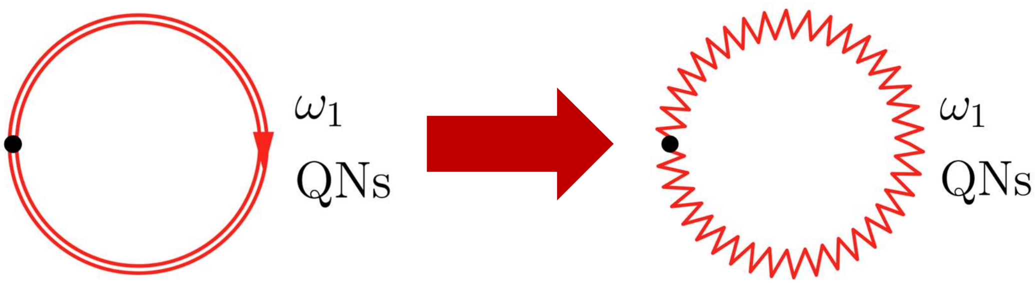
$$\Sigma^n_{\alpha\beta} = Z_{N\,\alpha\beta} \lim_{N\to\infty} \frac{1}{\mathcal{N}} \sum_{j=1}^{N} B_n(\omega_j) e^{i arg[D_{\alpha\beta}(\omega_j, C_j)]} 1_{\mathcal{T}_j \in S_\Sigma}$$

# NORMALIZATION SECTOR



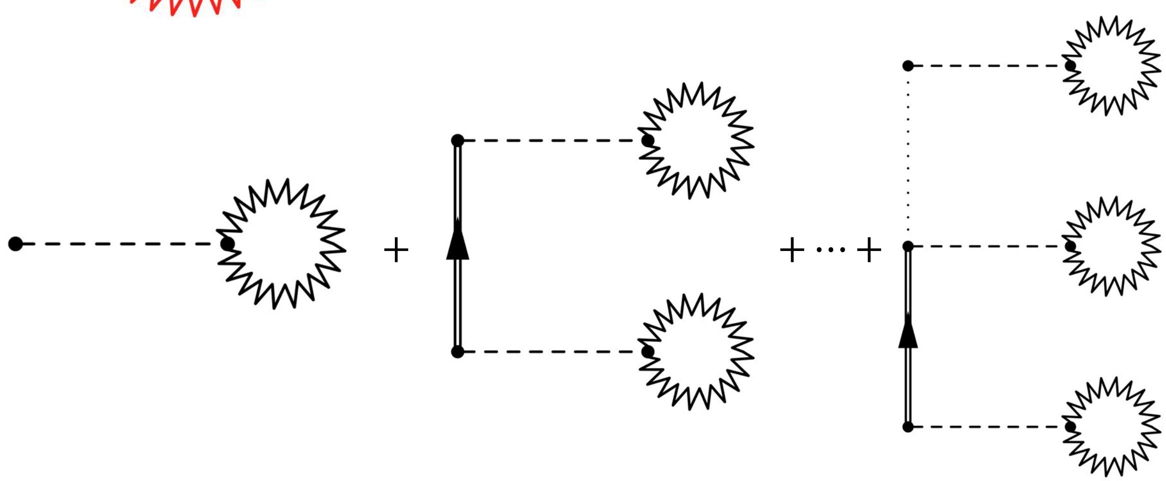

Self-closing propagators need convergence factors $e^{i\omega_1\eta}$.

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

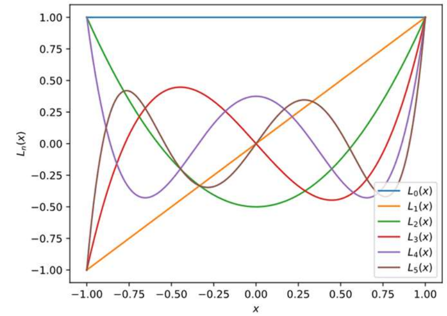



$$\stackrel{\text{def}}{=} \frac{iA}{\omega_1^2 + \gamma^2}$$

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.

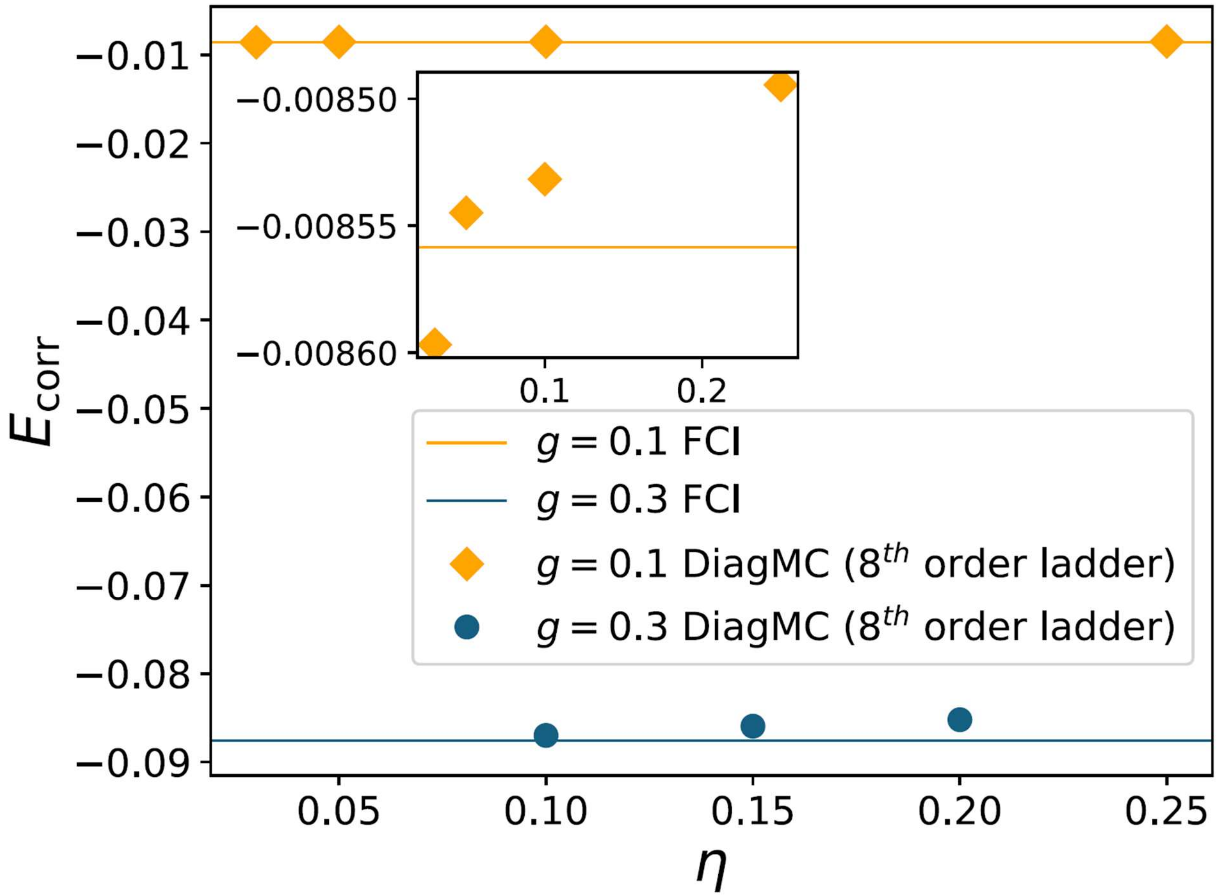
Recursion formulas are used to generate higher order $\Sigma^n_{\alpha\beta}$ during the sampling.

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

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

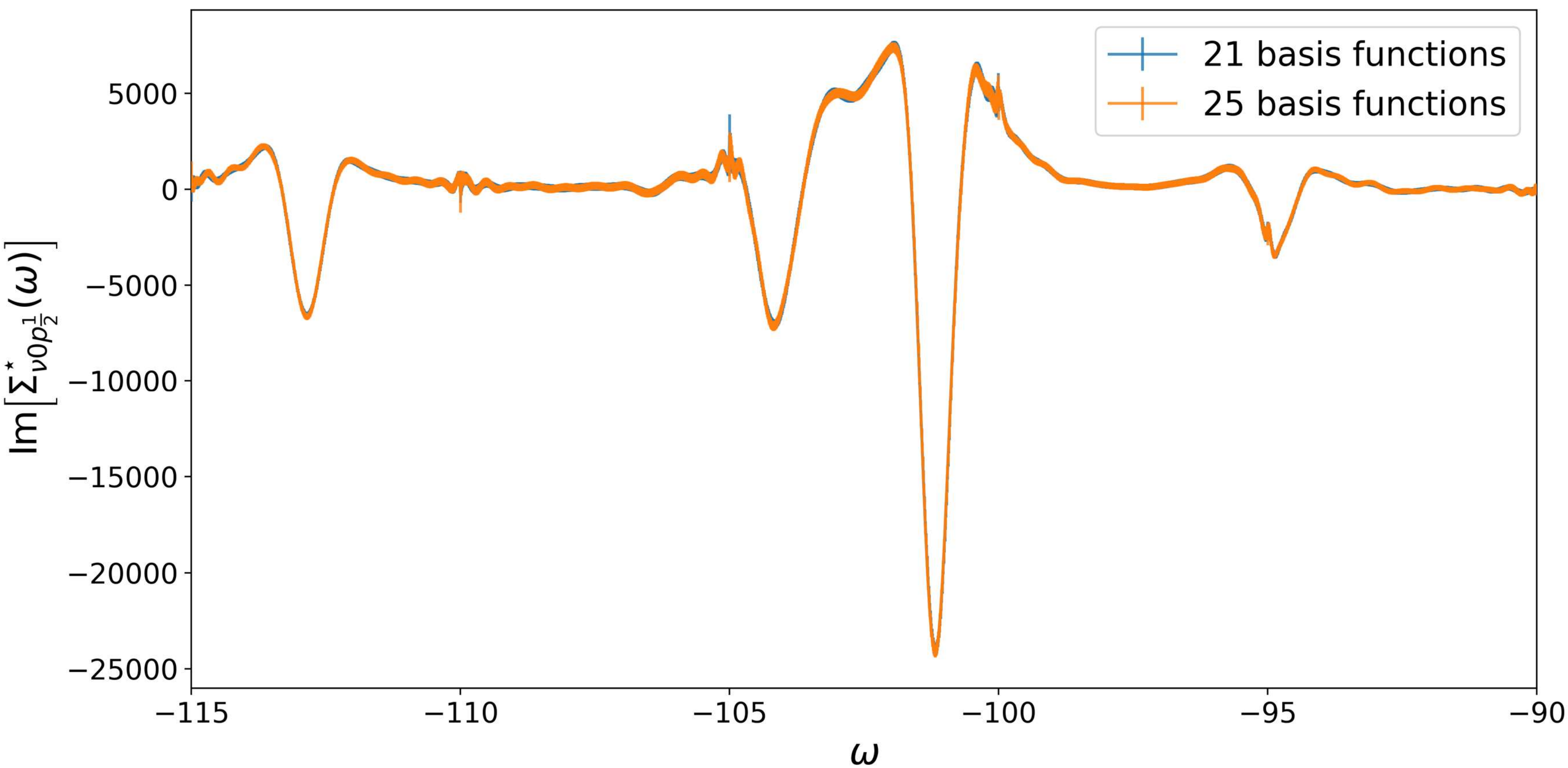
- Now we expand up to order $\sim 25$ with bins of size 5 MeV.
- Currently exploring higher orders and other basis functions. Maybe other polynomial basis (e.g. Chebyshev) have better performance.

# RICHARDSON MODEL: FINITE REGULATOR ERROR




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

# NUMBER OF BASIS FUNCTIONS



# HOW PERTURBATION THEORY BREAKS CAUSALITY

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

At third order, the terms that break causality have the form:

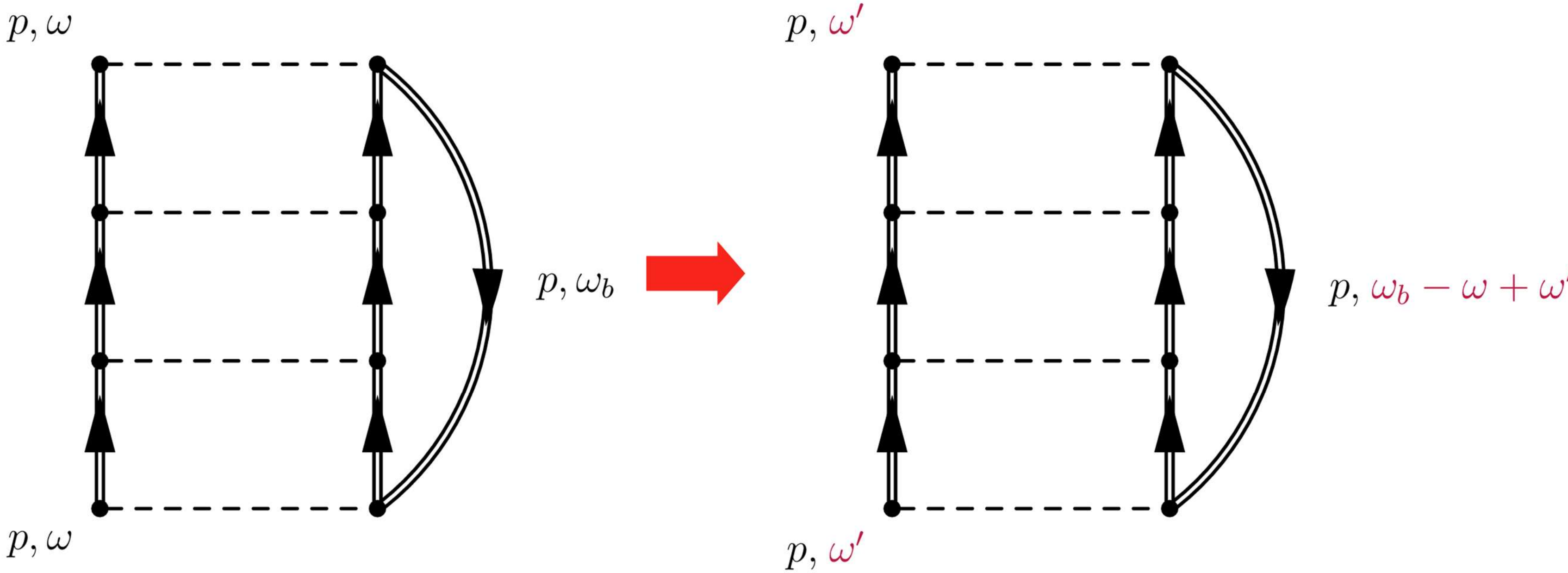
$$\left(M^{I}\right)^{\dagger}_{\alpha r}\frac{1}{\omega - E^{>}_{r} + i\eta} C^{I}_{r,r'}\frac{1}{\omega - E^{>}_{r'} + i\eta} M^{I}_{r',\beta}$$

ADC(n) builds the following expression from the PT results by matching terms

$$\left(M^{I}\right)^{\dagger}_{\alpha r}\frac{1}{\omega - [E^{>} + C^{I}]_{r,r'} + i\eta} M^{I}_{r',\beta}$$

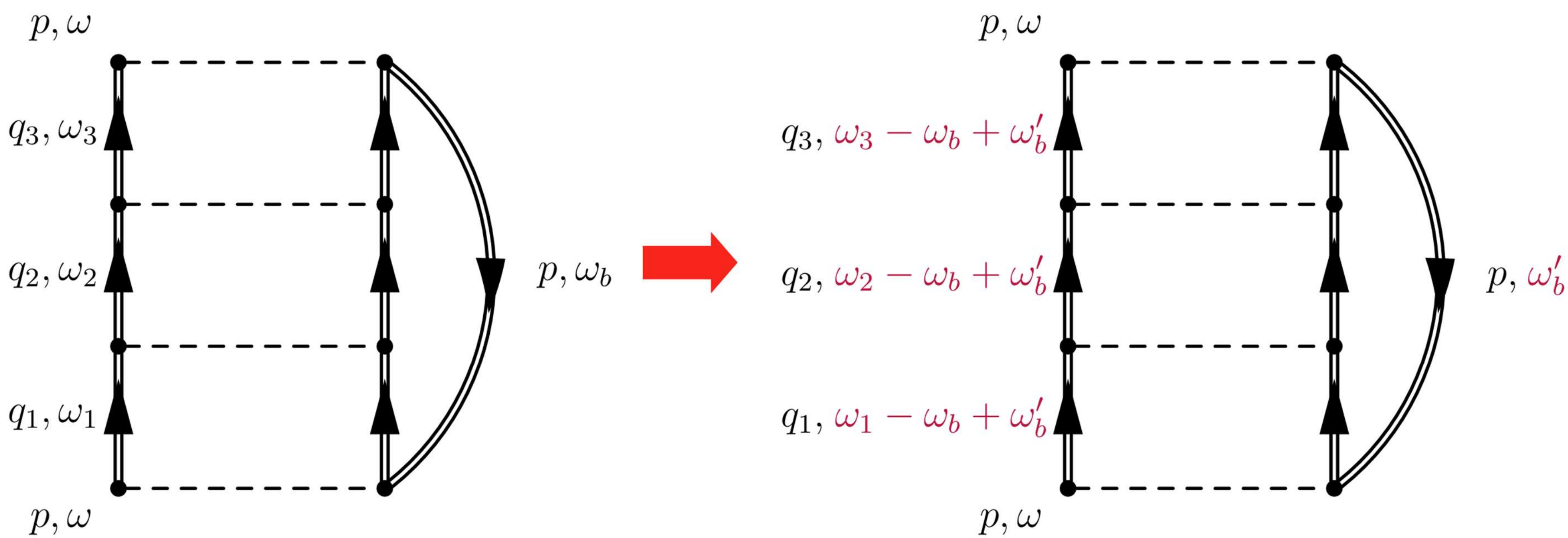
# UPDATES OF THE RICHARDSON MODEL

# CHANGE $\omega$



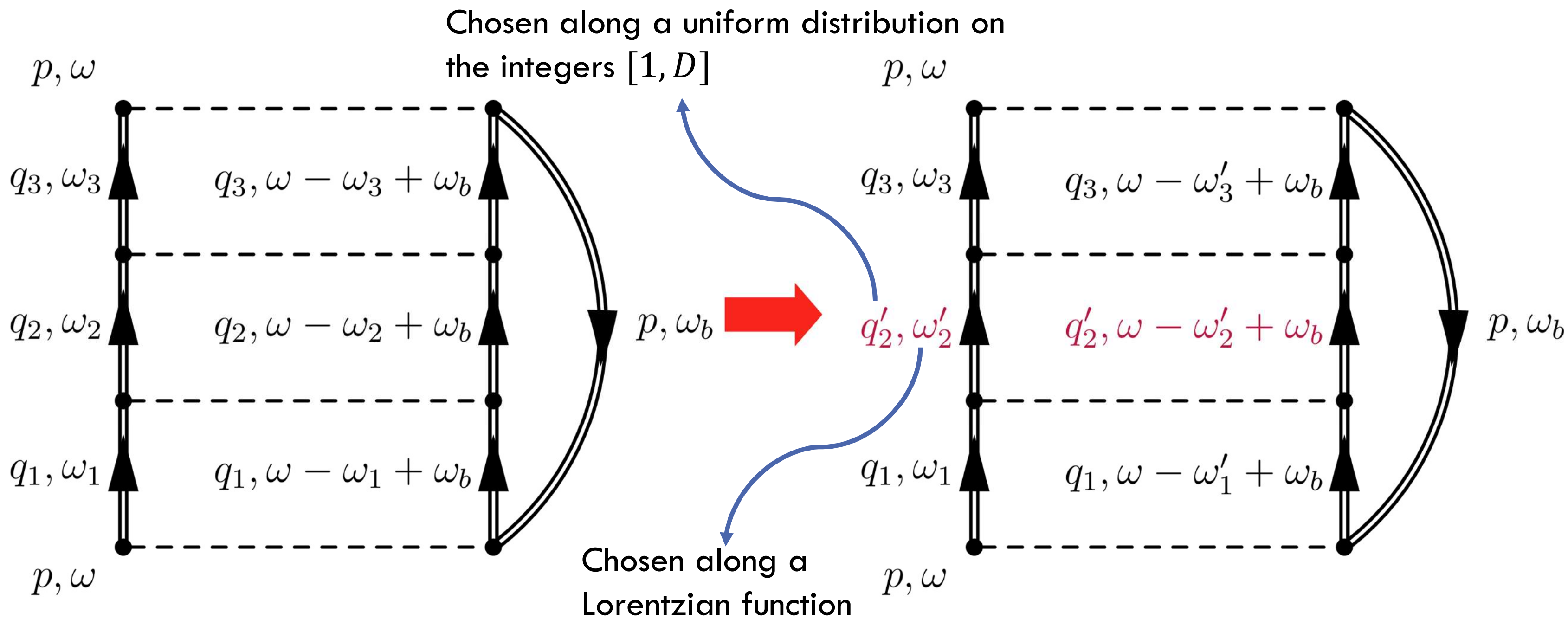

$$q_{C\omega} = \frac{|G_p(\omega_b - \omega + \omega')|}{|G_p(\omega_b)|}$$

# CHANGE INTERNAL FREQUENCIES



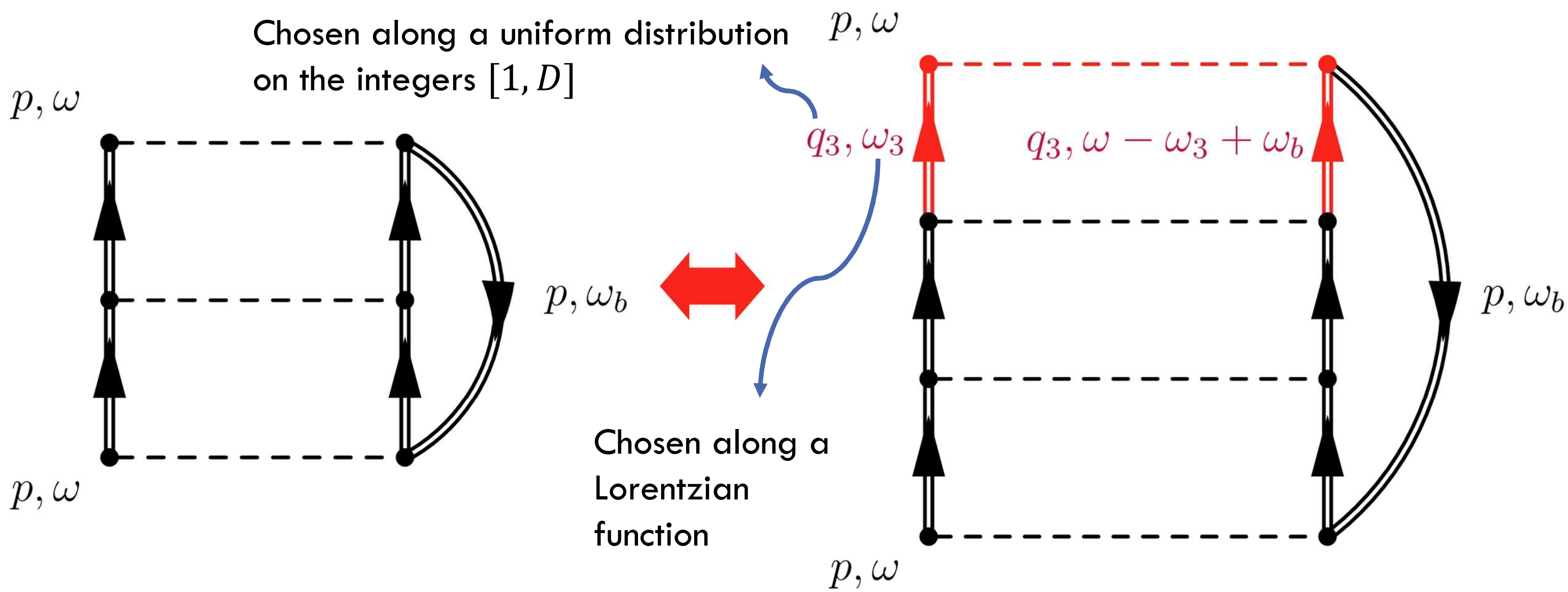

$$q_{\omega\ int} = \frac{L(\omega_b)}{L(\omega_b{}')} \frac{|G_p(\omega_b{}')|}{|G_p(\omega_b)|} \prod_{j=1}^{order} \frac{|G_{q_j}(\omega_j - \omega_b + \omega_b{}')|}{|G_{q_j}(\omega_j)|}$$

# CHANGE SP QUANTUM NUMBERS AND FREQUENCIES




$$q_{q,\omega} = \frac{L(\omega_2)}{L(\omega_2')} \frac{|G_{q_2'}(\omega_2') G_{q_2'}(\omega - \omega_2' + \omega_b)|}{|G_{q_2}(\omega_2) G_{q_2}(\omega - \omega_2 + \omega_b)|}$$

# ADD/REMOVE RUNG




$$q_{Add} = \frac{|g|}{4\pi} \frac{D}{L(\omega_3)} \left| G_{q_3}(\omega_3) G_{q_3}(\omega - \omega_3 + \omega_b) \right| \qquad q_{Rem} = \frac{1}{q_{Add}}$$