Diagrammatic Monte Carlo for Nuclear Systems

Stefano Brolli

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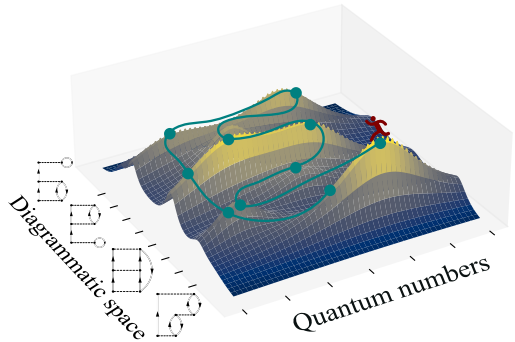
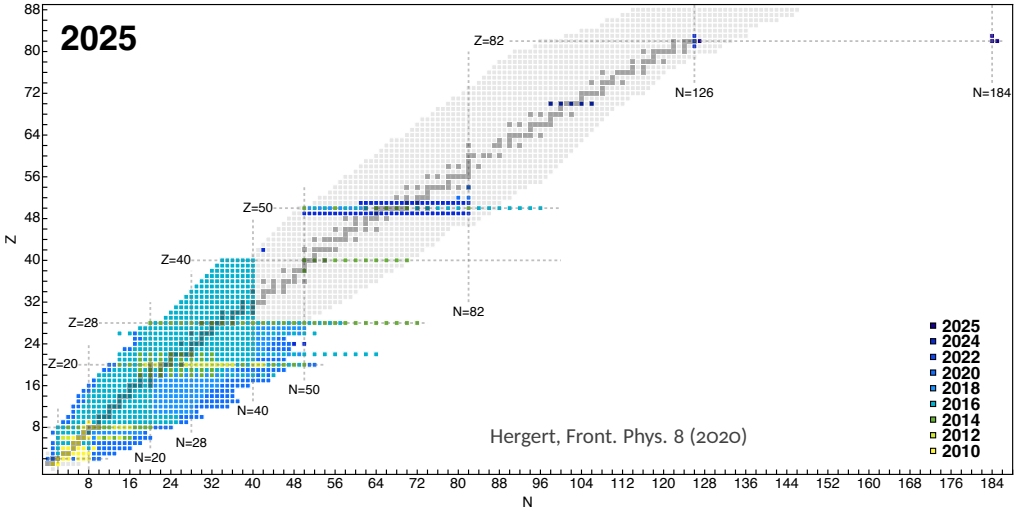


Ab Initio Structure Calculations



The Green's function

$$G_{\alpha\beta}(\omega) = \sum_n \frac{\langle \Psi_0^A | c_\alpha | \Psi_n^{A+1} \rangle \langle \Psi_n^{A+1} | c_\beta^\dagger | \Psi_0^A \rangle}{\omega - \left(E_n^{A+1} - E_0^A\right) + i\eta} + \sum_k \frac{\langle \Psi_0^A | c_\beta^\dagger | \Psi_k^{A-1} \rangle \langle \Psi_k^{A-1} | c_\alpha | \Psi_0^A \rangle}{\omega - \left(E_0^A - E_k^{A-1}\right) - i\eta}$$

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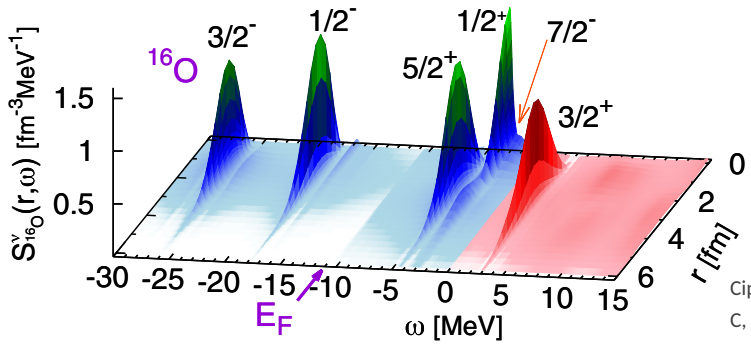
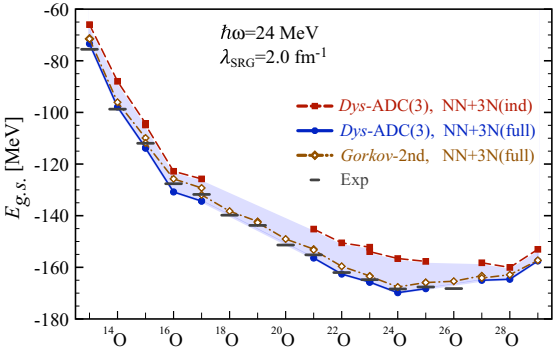
$$S_\nu^p(E, r) \propto \sum_n \left| \left\langle \Psi_n^{A+1} \middle| c_\nu^\dagger(r) \middle| \Psi_0^A \right\rangle \right|^2 \delta\left(E - (E_n^{A+1} - E_0^A)\right)$$



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

Structure Information



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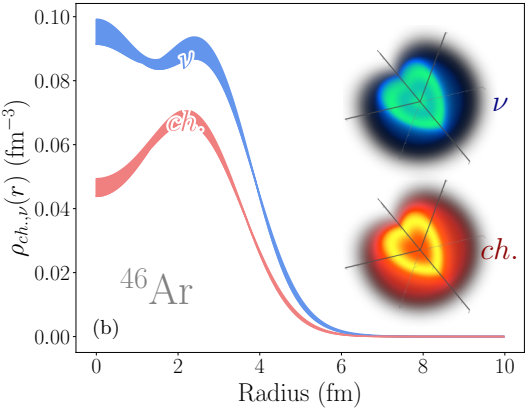

Brugnara, ..., Brolli et al., arXiv: 2506.23228v2 (2025)

Dyson equation

self-energy

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

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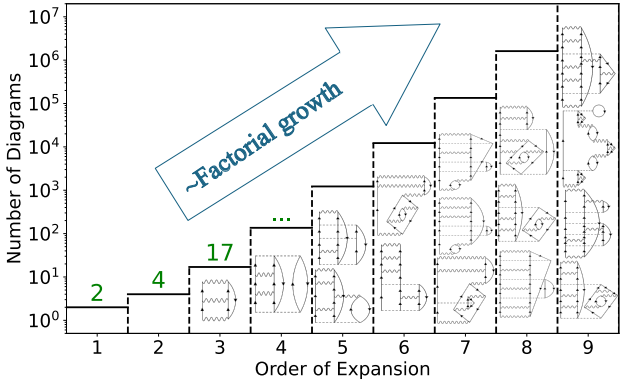
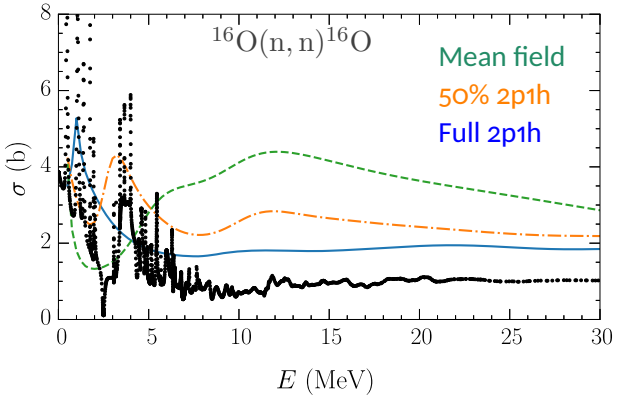


Brolli et al., Phys. Rev. Lett. 134, 182502 (2025)

Optical Potential

Capuzzi and Mahaux, Ann. Phys. 245, 147 (1996)

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



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

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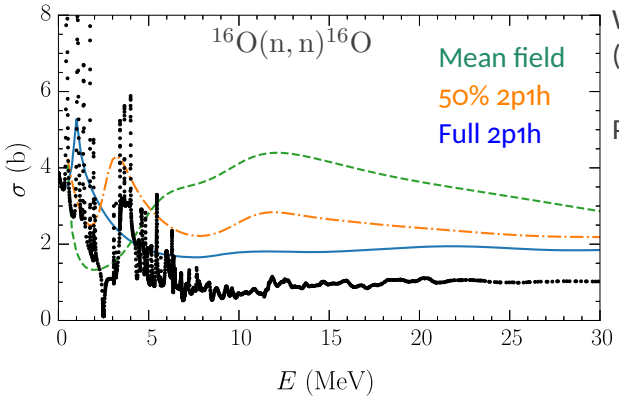


We do not include ISCs beyond 2p1h (diagrams of order $\gg 3$).

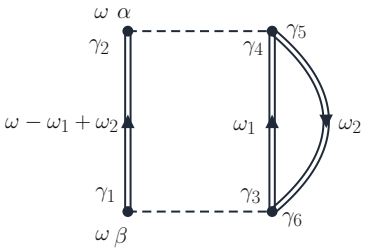
Progress towards high-orders:

- Drischler et al., arXiv:2603.24532 (2026)
- Drischler et al., Phys. Rev. Lett. 122, 042501 (2019)
- Arthuis et al., Comp. Phys. Comm. 240, 202 (2019)

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

Diagrammatic Monte Carlo

Prokof'ev et al., Phys. Rev. Lett. 81, 2514 (1998)



Topology

$$\mathcal{C} = \Big(\boxed{\mathcal{T}}, \{\omega_i\}, \{\gamma_i\}\Big)$$

$$\boxed{w_{\alpha\beta}(\omega, \mathcal{C}) = \frac{|\mathcal{D}_{\alpha\beta}(\omega, \mathcal{C})|}{Z_{\alpha\beta}}} \qquad Z_{\alpha\beta} = \int d\mathcal{C}\ |\mathcal{D}_{\alpha\beta}(\omega, \mathcal{C})|$$

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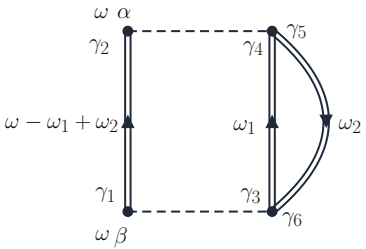

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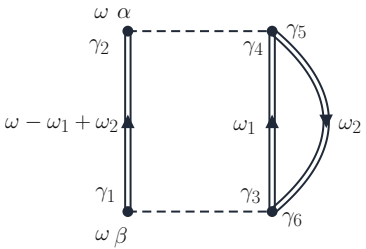

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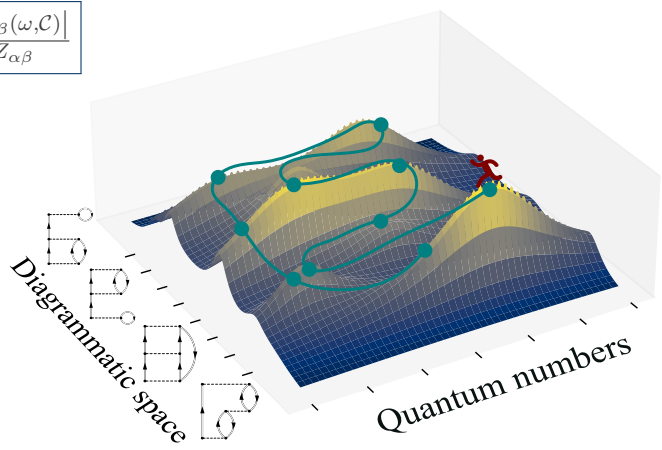
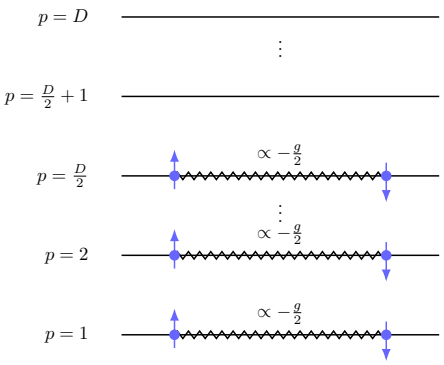
Sampling the diagrammatic space

$$w_{\alpha\beta}(\omega, \mathcal{C}) = \frac{|\mathcal{D}_{\alpha\beta}(\omega, \mathcal{C})|}{Z_{\alpha\beta}}$$



Richardson model

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



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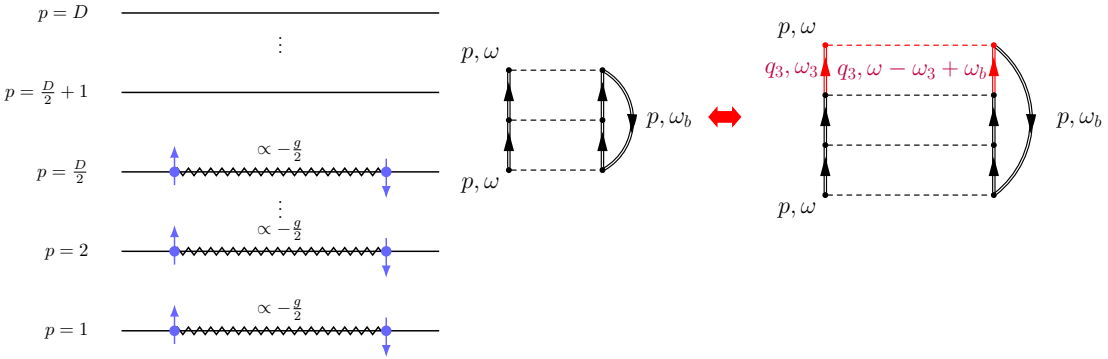
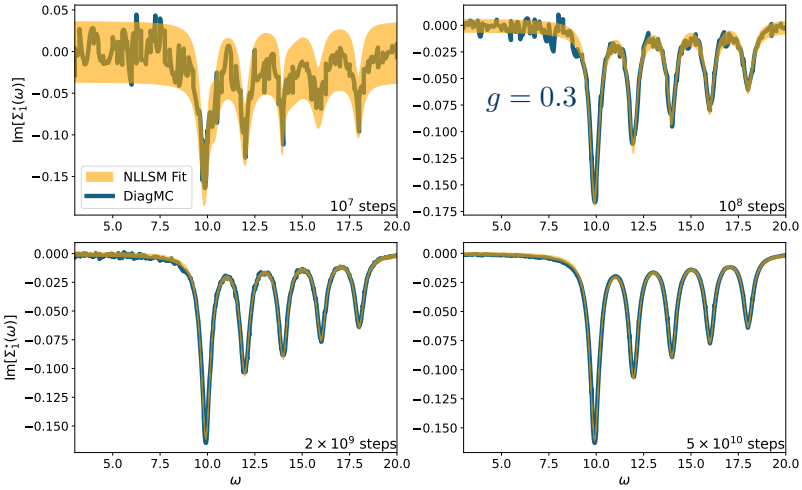


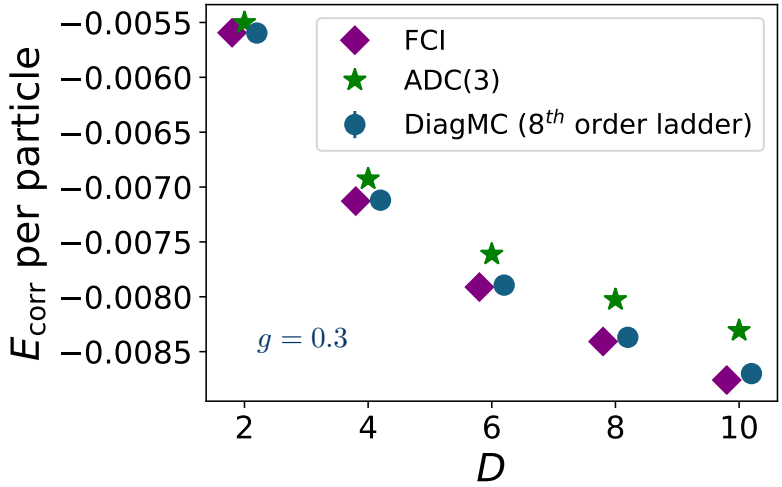
Richardson model: self-energy



Up to 8^{th} order, the self-energy converges smoothly.

Brolli, S. et al., Phys. Rev. Lett. 134, 182502 (2025)

Richardson model: ground state energy



DiagMC outperforms state-of-the-art SCGF truncations.

Brolli, S. et al., Phys. Rev. Lett. 134, 182502 (2025)

Time-Ordered Diagrammatic Monte Carlo (TO-DiagMC)

To perform a DiagMC simulation in a large model space with a realistic nuclear interaction—for us a chiral interaction—[1] we need

1. A different weight function to control the sign problem.

[1] This em dash is human generated.

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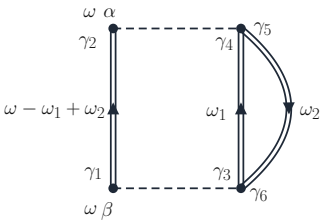
To perform a DiagMC simulation in a large model space with a realistic nuclear interaction—for us a chiral interaction—[1] we need

1. A different weight function to control the sign problem.
2. To reduce the sampling space.
3. A more efficient updating scheme that can
   - Sample all topologies, not just ladder ones.
   - Keep track of the conservation laws at each vertex.

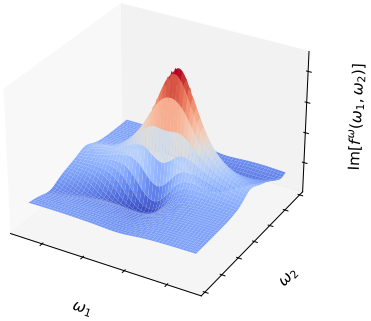
[1] This em dash is human generated.

The sign problem



The integrals in $\{\omega_i\}$ can suffer from severe cancellations.

$$\mathcal{D} \propto \int \{d\omega_i\} \frac{1}{\omega - \omega_1 + \omega_2 - \epsilon_1 + i\eta} \frac{1}{\omega_1 - \epsilon_2 + i\eta} \frac{1}{\omega_2 - \epsilon_3 + i\eta} = 0$$



Managing the sign problem and the regulator η

The residue theorem applied to Feynman diagrams gives Goldstone (time-ordered) diagrams.

$$\int \{d\omega_i\} \frac{1}{\omega - \omega_1 + \omega_2 - \epsilon_1 \pm i\eta} \frac{1}{\omega_1 - \epsilon_2 \pm i\eta} \frac{1}{\omega_2 - \epsilon_3 \pm i\eta} = 2\pi i \sum_k \mathrm{Res}(\mathrm{pole}_k).$$

The residue theorem gives more control of the regulator η:

- We run the simulations with $\eta \neq 0$ and take the limit $\eta \to 0^+$.

Time-ordered diagrammatic Monte Carlo

$$\Sigma^{\star}_{\alpha\beta}(\omega) = \int d\mathcal{C}\, \mathcal{D}_{\alpha\beta}(\omega, \mathcal{C})$$
$$= \sum_{\mathcal{T}\{i_l\}} \prod V_{\{i_l\}} \boxed{\int \{d\omega_r\} \prod \tilde{G}_{\{i_l\}}(\{\omega_r\})}$$
$$= \sum_{\mathcal{T}\{i_l\}} \prod V_{\{i_l\}} \boxed{\sum_T R^T_{\{i_l\}}}$$

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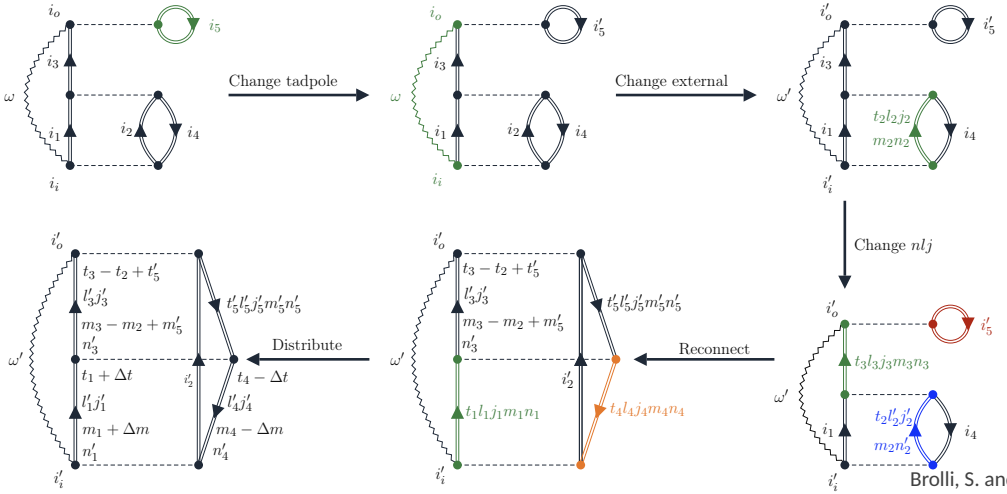
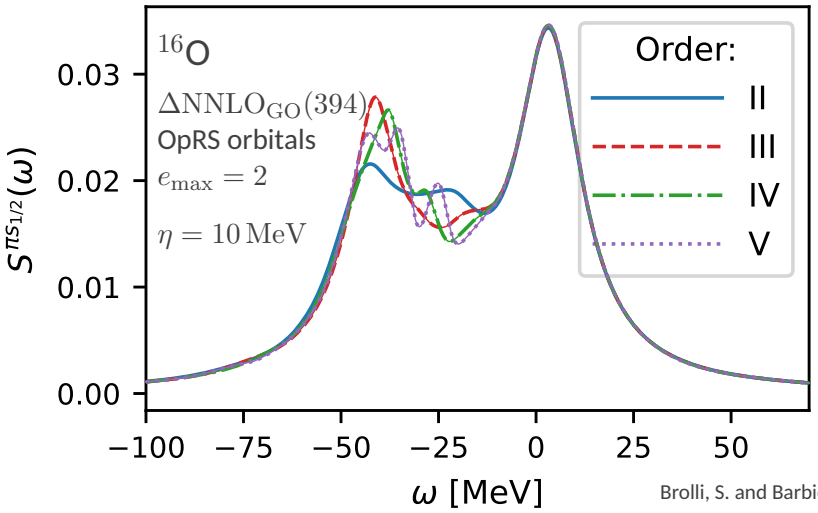
$$\Sigma^{\star}_{\alpha\beta}(\omega) = Z_{\alpha\beta} \lim_{N\to\infty} \frac{1}{N} \sum_{j=1}^{N} \frac{R^{T_j}_{\{i_l\}_j}}{p_{T_j^{\{i_l\}_j}}} \mathrm{sign}\left(\prod V_{\{i_l\}_j}\right) \qquad w_{k,\{i_l\},T} = \frac{\left|\prod V_{\{i_l\}}\right| \boxed{p_T^{\{i_l\}}}}{Z_{\alpha\beta}}$$

Updates



Brolli, S. and Barbieri, C.,
arXiv:2605.30527

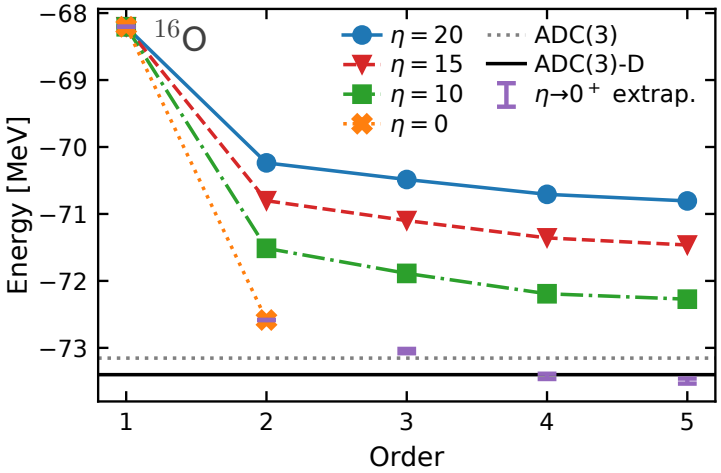
Spectral function



Fifth order calculations are possible.

Brolli, S. and Barbieri, C., arXiv:2605.30527

Ground state energy



The ground state energy is accurately reproduced by TO-DiagMC.

Brolli, S. and Barbieri, C., arXiv:2605.30527

Many ways to move forward!

- DiagMC can outperform state-of-the-art truncations of SCGF theory in simple models and small model spaces.

Many ways to move forward!

- DiagMC can outperform state-of-the-art truncations of SCGF theory in simple models and small model spaces.

- Larger model spaces require optimizing the weight distribution.
  - Pre-summing diagram blocks (?) [Van Houcke et al., Phys. Rev. B. 99, 035140 (2019)]
  - Using determinants (?) [Rossi, Phys. Rev. Lett. 119, 045701 (2017)]
  - Contracting some interaction indices on the fly (?)

Diagrammatic Monte Carlo for Nuclear Systems

Thank you for listening!
Any questions?

Backup slides

Determining $\mathcal{Z}_{\alpha\beta}$

$$\Sigma^{(n)}_{\alpha\beta} = \mathcal{Z}_{\alpha\beta} \lim_{N\to\infty} \frac{1}{N} \sum_j B^n(\omega_j) e^{i\arg\left[\mathcal{D}_{\alpha\beta}(\omega,\mathcal{C}_j)\right]}$$

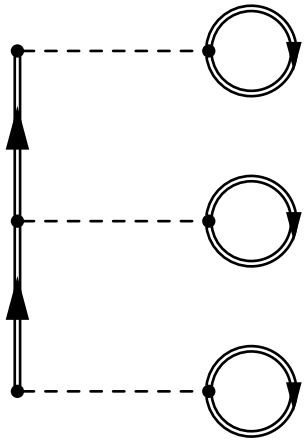
$\mathcal{Z}_{\alpha\beta} = \int_{\omega_{\min}}^{\omega_{\max}} d\omega \int d\mathcal{C} \; |\mathcal{D}_{\alpha\beta}(\omega,\mathcal{C})|$ is not known but can be estimated.

If the weight of a subset of the diagrams $\mathcal{S}_N$ ($\mathcal{Z}^N_{\alpha\beta}$) is known, we can estimate $\mathcal{Z}_{\alpha\beta}$ knowing how many times $\mathcal{S}_N$ is visited ($\mathcal{N}$).

$$\lim_{N\to\infty} \frac{\mathcal{N}}{N} = \frac{\mathcal{Z}^N_{\alpha\beta}}{\mathcal{Z}_{\alpha\beta}}.$$

Sign-problem-free by construction!

Choice of $\mathcal{S}_N$

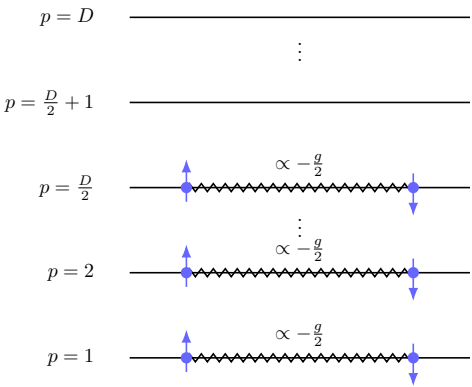


- At order ν, we choose the ν-tadpoles diagram as the only member of $\mathcal{S}_N$.
- The calculation of $\mathcal{Z}^N_{\alpha\beta}$ scales very favorably with the order and $e_{\max}$ ($\propto N_{sp}^{7/3} + \nu N_{sp}^2$).

Brolli, S. and Barbieri, C., arXiv:2605.30527

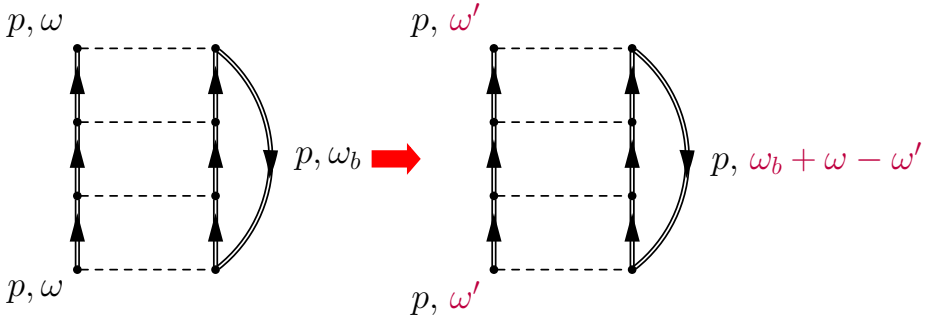
Brolli et al., Phys. Rev. Lett. 134, 182502 (2025)

Updates of the Richardson model



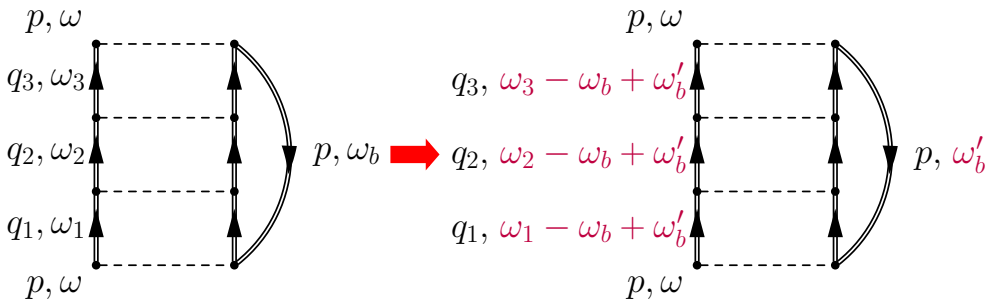
Brolli et al., Phys. Rev. Lett. 134, 182502 (2025)

Change of ω



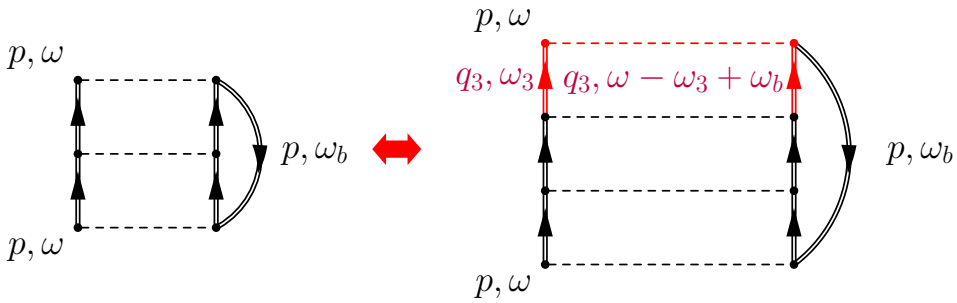
$$q_\omega = \left| \frac{G_p(\omega_b + \omega - \omega')}{G_p(\omega)} \right|$$

Change of the internal frequencies



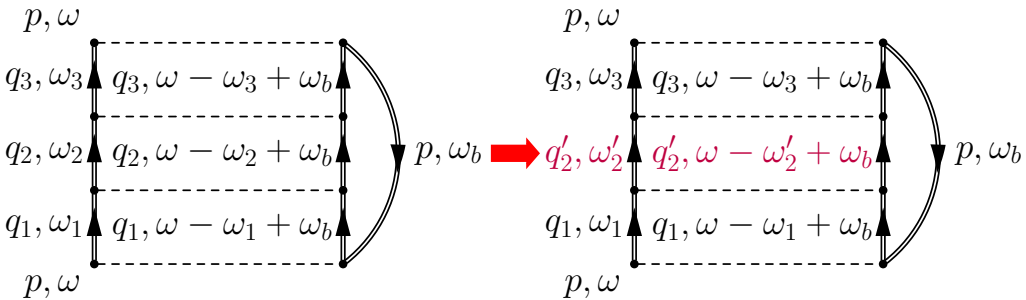
$$q_{\omega\, int} = \frac{L(\omega_b)}{L(\omega'_b)} \left| \frac{G_p(\omega'_b)}{G_p(\omega_b)} \right| \prod_{j=1}^{\nu-1} \frac{\left| G_{q_j}(\omega_j - \omega_b + \omega'_b) \right|}{\left| G_{q_j}(\omega_j) \right|}$$

Add / Remove rung



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

Change of single particle quantum numbers and frequencies



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

Optimized reference state (OpRS) orbitals

$$G_{\alpha\beta}(\omega) = \sum_n \frac{\langle \Psi_0^A | c_\alpha | \Psi_n^{A+1} \rangle \langle \Psi_n^{A+1} | c_\beta^\dagger | \Psi_0^A \rangle}{\omega - \left(E_n^{A+1} - E_0^A \right) + i\eta} + \sum_k \frac{\langle \Psi_0^A | c_\beta^\dagger | \Psi_k^{A-1} \rangle \langle \Psi_k^{A-1} | c_\alpha | \Psi_0^A \rangle}{\omega - \left(E_0^A - E_k^{A-1} \right) - i\eta}$$

$$M_{\alpha\beta}^{(p)} = \sum_n \frac{\langle \Psi_0^A | c_\alpha | \Psi_n^{A+1} \rangle \langle \Psi_n^{A+1} | c_\beta^\dagger | \Psi_0^A \rangle}{\left[E_F - \left(E_n^{A+1} - E_0^A \right) \right]^p} + \sum_k \frac{\langle \Psi_0^A | c_\beta^\dagger | \Psi_k^{A-1} \rangle \langle \Psi_k^{A-1} | c_\alpha | \Psi_0^A \rangle}{\left[E_F - \left(E_0^A - E_k^{A-1} \right) \right]^p}$$

$$M^{\mathrm{OpRS}(p)}_{\alpha\beta} = M^{(p)}_{\alpha\beta} \qquad p = 0, 1$$

$$\rightarrow \quad G^{\mathrm{OpRS}}_{\alpha\beta}(\omega) = \sum_n \frac{(\tilde{\mathcal{X}}_\alpha^n)^* \tilde{\mathcal{X}}_\beta^n}{\omega - \tilde{\varepsilon}_n^+ + i\eta} + \sum_k \frac{\tilde{\mathcal{Y}}_\alpha^k (\tilde{\mathcal{Y}}_\beta^k)^*}{\omega - \tilde{\varepsilon}_k^- - i\eta} \qquad \text{Mean field propagator}$$

Perturbative series of the self-energy

$$\Sigma^{\star}(\omega) = \Sigma^{(\infty)} + M^{\dagger}\frac{1}{\omega - E^{>} - C + i\eta}M + N\frac{1}{\omega - E^{<} - D - i\eta}N^{\dagger}$$

The perturbation theory expansion breaks this structure starting from the third order

$$\Sigma_p^{\star II}(\omega) = M^{I\dagger}\frac{1}{\omega - E^{>} + i\eta}M^{I}$$

$$\begin{aligned}\Sigma_p^{\star III}(\omega) = {} & M^{I\dagger}\frac{1}{\omega - E^{>} + i\eta}M^{II} + M^{II\dagger}\frac{1}{\omega - E^{>} + i\eta}M^{I} \\ & + M^{I\dagger}\frac{1}{\omega - E^{>} + i\eta}C\frac{1}{\omega - E^{>} + i\eta}M^{I}\end{aligned}$$

Dyson matrix

In SCGF theory, the ADC(n) approximation calculates directly the matrices M, N, C, and D.

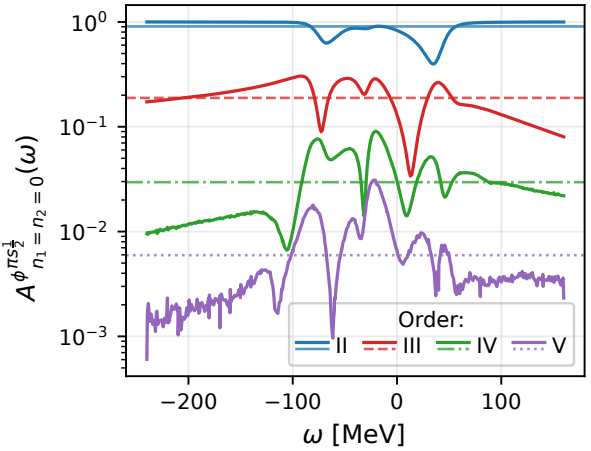
$$\Sigma^\star(\omega) = \Sigma^{(\infty)} + M^\dagger \frac{1}{\omega - E^> - C + i\eta} M + N \frac{1}{\omega - E^< - D - i\eta} N^\dagger$$

The Dyson equation $G = G^{(0)} + G^{(0)}\Sigma^\star G$ can be recast into

$$\begin{pmatrix} T + \Sigma^{(\infty)} & M^\dagger & N^\dagger \\ M & E^> + C & 0 \\ N & 0 & E^< + D \end{pmatrix} \begin{pmatrix} \mathcal{Z}^{(i)} \\ \mathcal{W}^{(i)} \\ \mathcal{V}^{(i)} \end{pmatrix} = \epsilon_i \begin{pmatrix} \mathcal{Z}^{(i)} \\ \mathcal{W}^{(i)} \\ \mathcal{V}^{(i)} \end{pmatrix}$$

$$\mathcal{Z}_\alpha^{(i)} = \begin{cases} \langle \Psi_i^{A+1} | a_\alpha^\dagger | \Psi_0^A \rangle & i < F \\ \\ \langle \Psi_i^{A-1} | a_\alpha | \Psi_0^A \rangle & i > F \end{cases}$$

Sign problem in TO-DiagMC



$$A^{\phi^{tlj}}_{i_o i_i}(\omega_r^k) = \frac{\left(\left|\langle\sigma^{tlj}\rangle\right|\right)_{kri_o i_i}}{\left(\langle|\sigma^{tlj}|\rangle\right)_{kri_o i_i}}.$$

σ is the quantity that is sampled in the Markov chain.