Diagrammatic Monte Carlo and Emulating Many-Body Green's Functions

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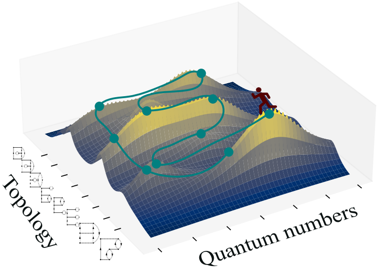
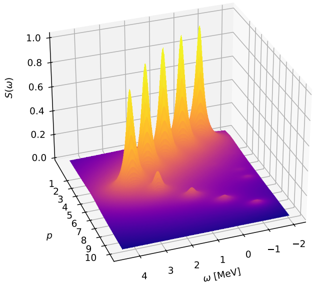
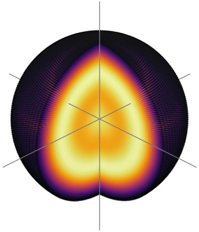
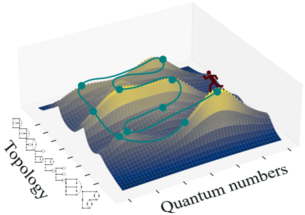




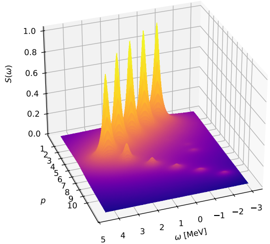
Outline

1. **An overview of *ab initio* many-body methods and challenges**
   - Structure
   - Reactions





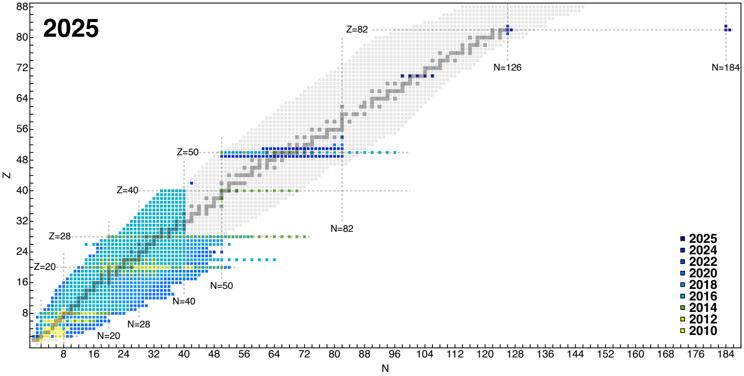
2. **Diagrammatic Monte Carlo**
   - Principles
   - Richardson Pairing Model
   - Chiral Potentials



3. **Emulating the Green's Function**
   - Principles
   - Richardson Pairing Model

Ab Initio Structure Calculations

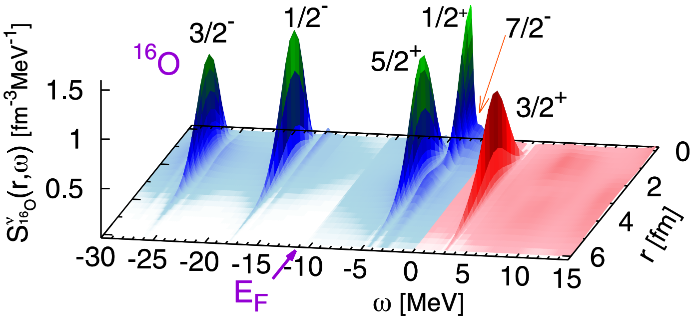
- Medium-light mass nuclei are accurately described.
- Many-body methods agree on ground-state properties.
- Main uncertainty arises from the Hamiltonian.
- Current focus: heavy and deformed nuclei.



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

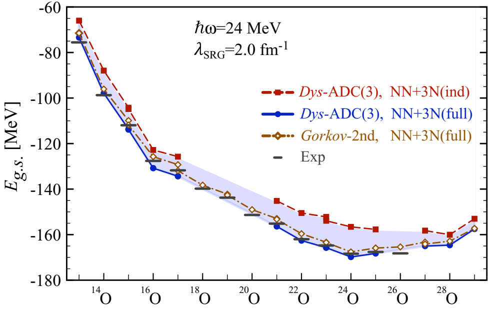
Self-Consistent Green's Function

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

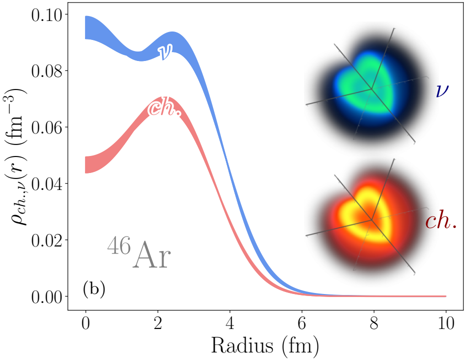


Cipollone et al., Phys. Rev. C, 92, 014306 (2015)

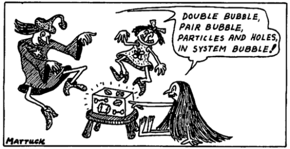
Structure Information



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



Brolli, B.Sc. Thesis, and Brugnara, ..., Brolli et al., arXiv: 2506.23228v2 (2025)

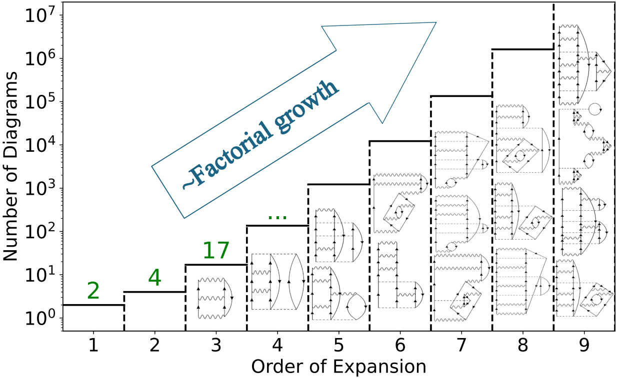


Mattuck, A Guide to Feynman Diagrams in the Many-Body Problem (1992)

Dyson Equation

self-energy

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

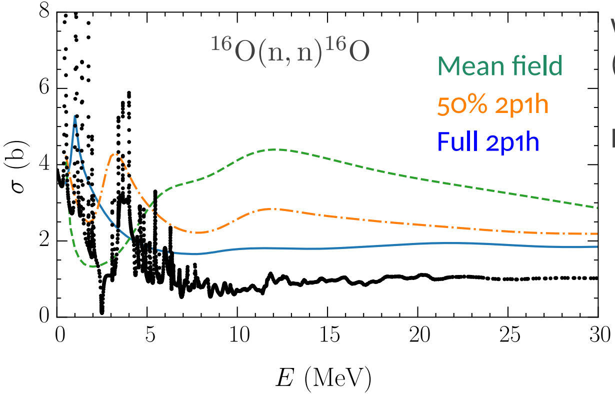


Brolli et al., Phys. Rev. Lett. 134, 182502 (2025)

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)

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

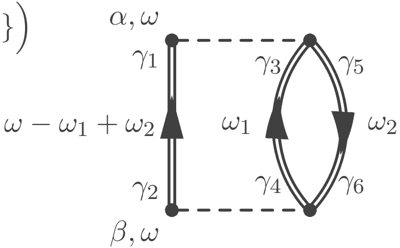
Progress towards high-orders:

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

Diagrammatic Monte Carlo

Topology

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



$$\Sigma^{\star}_{\alpha\beta}(\omega) = \int d\mathcal{C}\, \mathcal{D}_{\alpha\beta}(\omega, \mathcal{C}) = \int d\mathcal{C}\ |\mathcal{D}_{\alpha\beta}(\omega, \mathcal{C})|\, e^{i\arg\left[\mathcal{D}_{\alpha\beta}(\omega,\mathcal{C})\right]}$$

Legendre polynomials

$$\Sigma^{(n)}_{\alpha\beta} = \int_{\omega_{min}}^{\omega_{max}} d\omega \int d\mathcal{C} \boxed{B^n(\omega)} |\mathcal{D}_{\alpha\beta}(\omega, \mathcal{C})|\, e^{i\arg\left[\mathcal{D}_{\alpha\beta}(\omega,\mathcal{C})\right]}$$

Diagrammatic Monte Carlo

$$\Sigma_{\alpha\beta}^{(n)} = Z_{\alpha\beta} \int_{\omega_{min}}^{\omega_{max}} d\omega \int d\mathcal{C}\, B^n(\omega) \frac{|\mathcal{D}_{\alpha\beta}(\omega, \mathcal{C})|}{Z_{\alpha\beta}} e^{i\arg[\mathcal{D}_{\alpha\beta}(\omega,\mathcal{C})]}$$

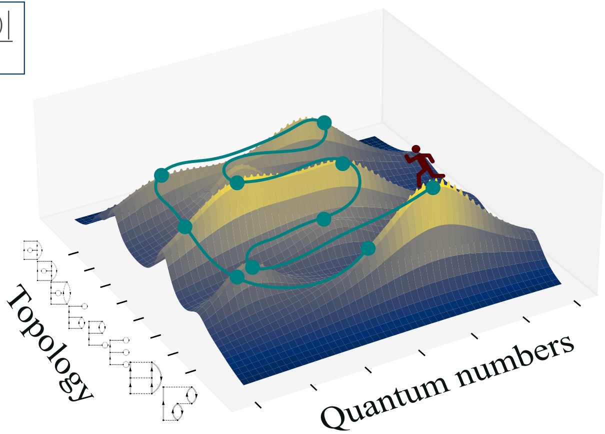
$$= Z_{\alpha\beta} \lim_{N\to\infty} \frac{1}{N} \sum_{j=1}^{N} B^n(\omega_j) e^{i\arg[\mathcal{D}_{\alpha\beta}(\omega_j,\mathcal{C}_j)]}$$

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

$$Z_{\alpha\beta} = \int_{\omega_{min}}^{\omega_{max}} d\omega \int d\mathcal{C}\, |\mathcal{D}_{\alpha\beta}(\omega, \mathcal{C})|$$

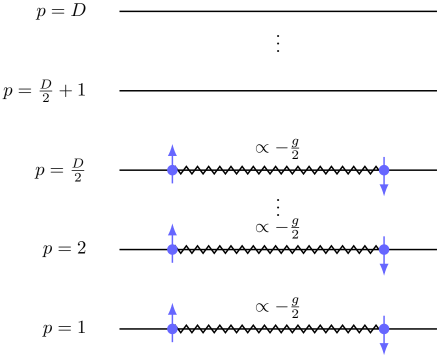
Sampling the diagrammatic space

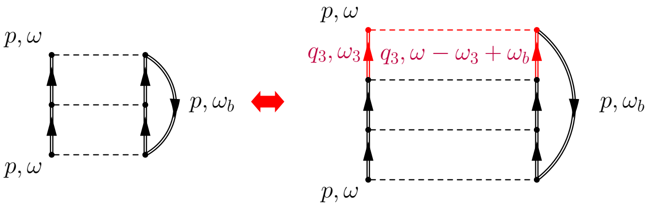
$$w_{\alpha\beta}(\omega, \mathcal{C}) = \frac{|\mathcal{D}_{\alpha\beta}(\omega,\mathcal{C})|}{Z_{\alpha\beta}}$$



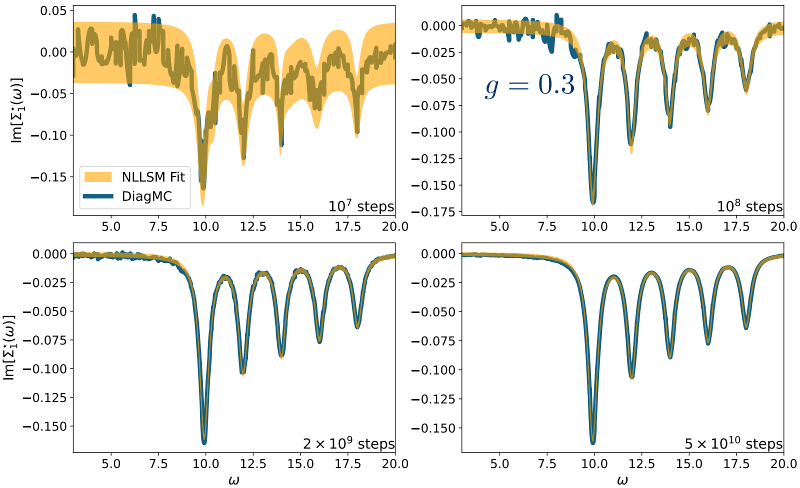
Richardson model

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





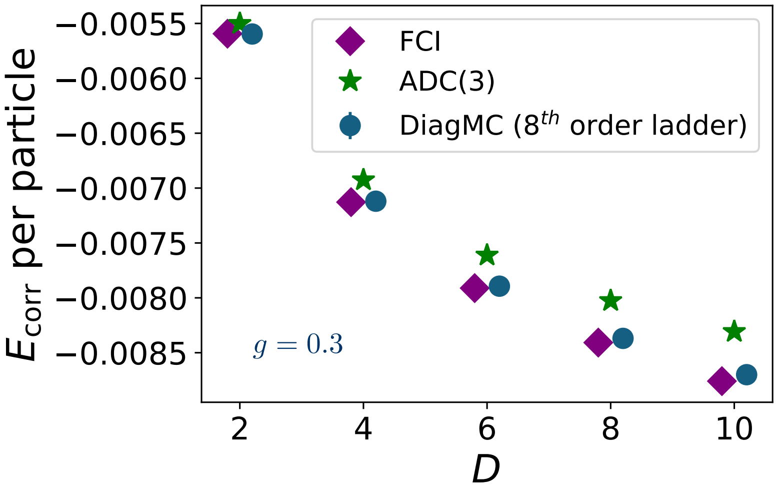
Richardson model: self-energy



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

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

Richardson model: ground state energy



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

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

Chiral potentials

To perform a DiagMC simulation in a large model space with a chiral interactions, 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.

Time-ordered diagrammatic Monte Carlo

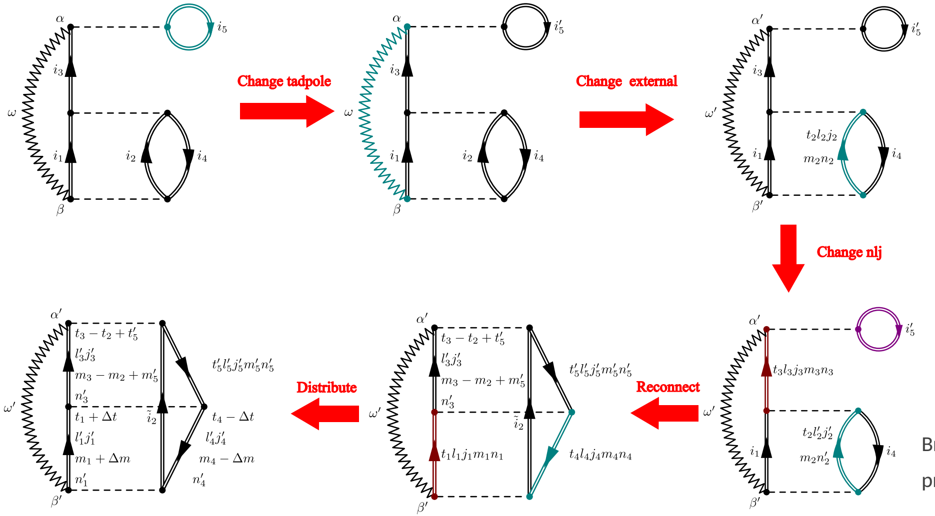
$$\Sigma^{(n)}_{\alpha\beta} = \int_{\omega_{min}}^{\omega_{max}} d\omega \int d\mathcal{C}\, B^n(\omega)\mathcal{D}_{\alpha\beta}(\omega, \mathcal{C})$$

$$\Sigma^{(n)}_{\alpha\beta} = \sum_k W_k B^n(\omega_k) \sum_{\mathcal{T}\{i_l\}} \prod V_{\{i_l\}} \boxed{\int \{d\omega_r\} \prod \tilde{G}_{\{i_l\}}(\{\omega_r\})}$$

$$= \sum_k W_k B^n(\omega_k) \sum_{\mathcal{T}\{i_l\}} \prod V_{\{i_l\}} \boxed{\textstyle\sum_T R^T_{\{i_l\}}}$$

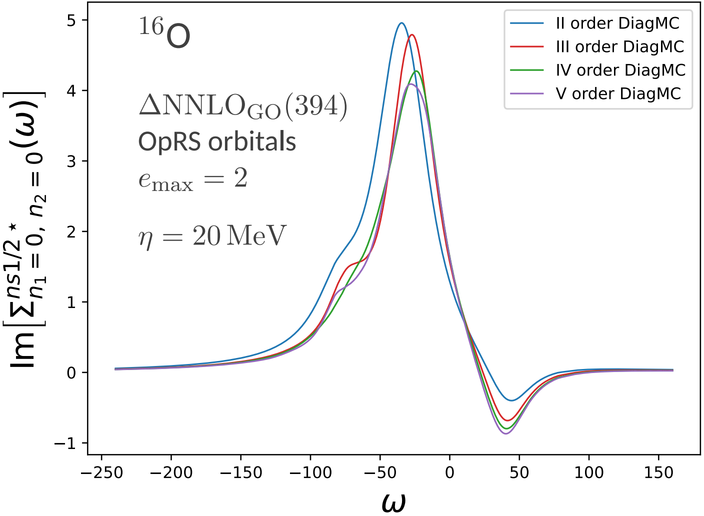
$$\Sigma^{(n)}_{\alpha\beta} = \lim_{N\to\infty} \frac{Z_{\alpha\beta}}{N} \sum_{j=1}^{N} B^n(\omega_j) \frac{R^{T_j}_{\{i_l\}_j}}{p_{T_j}^{\{i_l\}_j}} \mathrm{sign}\left(\prod V_{\{i_l\}_j}\right) \qquad w_{k,\{i_l\},T} = \frac{W_k \left|\prod V_{\{i_l\}}\right| p_T^{\{i_l\}}}{Z_{\alpha\beta}}$$

Updates

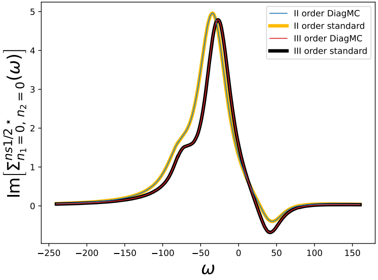


Brolli et al., In preparation.

Self-energy

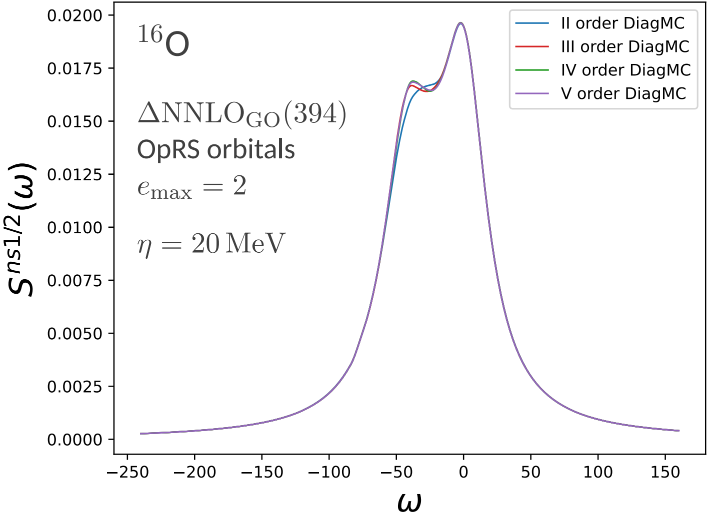


Fifth order calculations are now possible.



Brolli et al., In preparation.

Spectral function



Fifth order calculations are now possible.

Brolli et al., In preparation.

Outlook

- DiagMC can outperform state-of-the-art many-body truncations 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)]
  - Contracting some interaction indices on the fly (?)
  - Use a different basis B^n (?)

Many ways to move forward!

Emulating the Green's Function

1. Uncertainty quantification of nuclear spectroscopic properties.
2. Novel strategies for constraining nuclear interactions.
3. Extrapolation to regimes where the perturbative expansion breaks down.

Our approach:

- The ground state: (from eigenvector continuation theory)

  $|\Psi_0^A(g)\rangle \approx \sum_{k=1}^{N} v_k \, |\Psi_0^A(g_k)\rangle.$

- Excited states:

  $|\Psi_n^{A+1}(g)\rangle \approx \sum_{k\alpha} A_{k\alpha}^{n} c_\alpha^\dagger \, |\Psi_0^A(g_k)\rangle$

Emulating the Green's Function

$$\sum_{k\alpha} \langle \Psi_0^A(g_j) | c_\beta H(g) c_\alpha^\dagger | \Psi_0^A(g_k) \rangle \, A_{k\alpha}^n = E_n^{A+1} \sum_{k\alpha} \langle \Psi_0^A(g_j) | c_\beta c_\alpha^\dagger | \Psi_0^A(g_k) \rangle \, A_{k\alpha}^n$$

Linear in g. $$\sum_{k\alpha} \boxed{\mathcal{M}_{j\beta,k\alpha}(g)} A_{k\alpha}^n = E_n^{A+1} \sum_{k\alpha} \boxed{\mathcal{N}_{j\beta,k\alpha}} A_{k\alpha}^n$$ Does not depend on g.

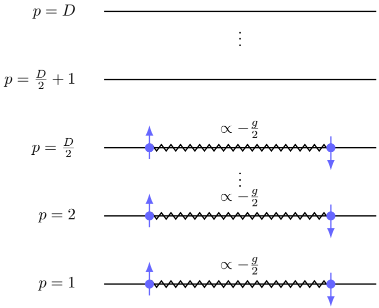
$$\langle \Psi_n^{A+1}(g) | c_\beta^\dagger | \Psi_0^A(g) \rangle = \sum_{jk\alpha} v_j \mathcal{N}_{j\beta,k\alpha} A_{k\alpha}^n \qquad \epsilon_n^+ = E_n^{A+1} - E_0^A$$

Similarly can be done for the hole part of the Green's function.

Back to the Richardson Model

$$\sum_{k\alpha} \mathcal{M}_{j\beta,k\alpha}(g) A^n_{k\alpha} = E^{A+1}_n \sum_{k\alpha} \mathcal{N}_{j\beta,k\alpha} A^n_{k\alpha}$$

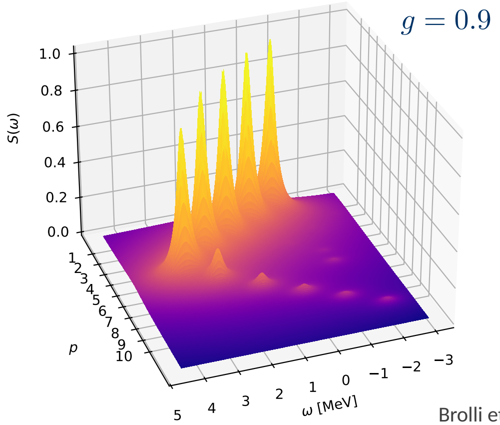
$$\langle \Psi^{A+1}_n(g) | c^\dagger_\beta | \Psi^A_0(g) \rangle = \sum_{jk\alpha} v_j \mathcal{N}_{j\beta,k\alpha} A^n_{k\alpha} \qquad \epsilon^+_n = E^{A+1}_n - E^A_0$$



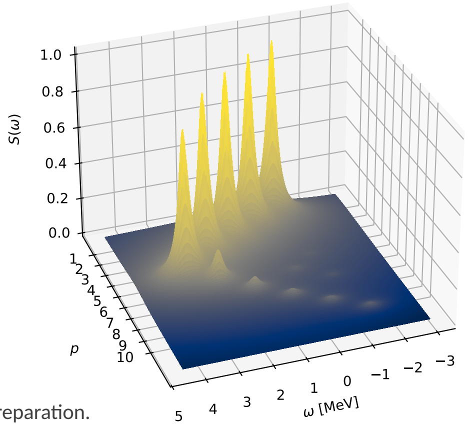
- The Green's function is diagonal in the level $p \rightarrow$ One pair $\left(\mathcal{M}^{(p)}, \mathcal{N}^{(p)}\right)$ for each level.
- We calculate the $\left(\mathcal{M}^{(p)}, \mathcal{N}^{(p)}\right)$ matrices from five "training points" $\rightarrow 5 \times 5$ matrices.
- We focus on the set $g_T = -0.1, 0.1, 0.3, 0.5, 0.7$.

Spectral function of the Richardson model

Emulator:

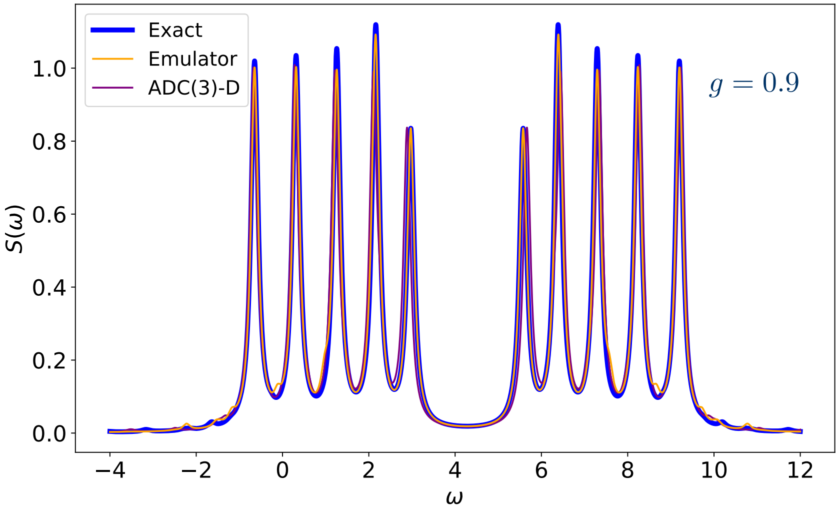


Exact:



Brolli et al., In preparation.

Spectral function of the Richardson model

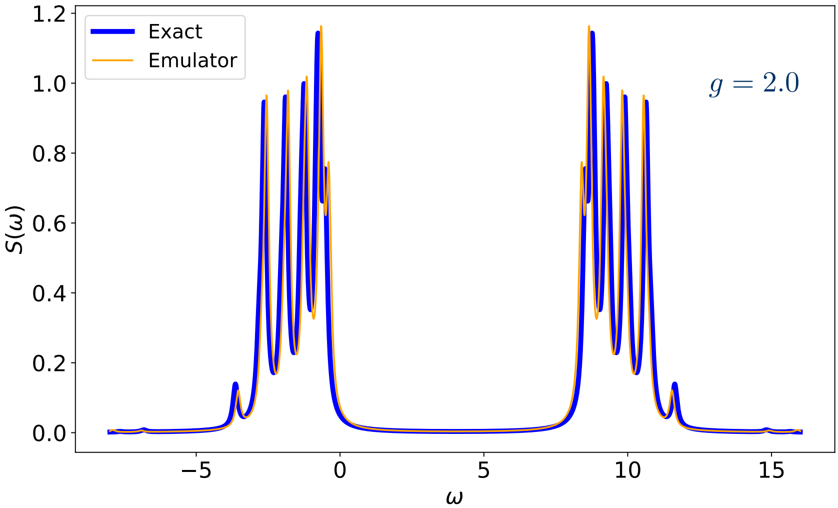


$\mathcal{L}_{\text{emul}} = 0.007$

$\mathcal{L}_{\text{exact}} = 0.04$

Brolli et al., In preparation.

Extrapolation of the spectral function



$\mathcal{L}_{\mathrm{emul}} = 0.07$

Brolli et al., In preparation.

Outlook

- We can see $\mathcal{M}$ and $\mathcal{N}$ as the primary matrices of a Parametric Matrix Model (PMM).
  Cook et al., Nat. Commun. 16, 5929 (2025)

- The PMM framework avoids $|\Psi_0^A\rangle$, and we can train the emulator on spectroscopic data from Green's function calculations.

In collaboration with Alberto (Chalmers University of Technology)

- Uncertainty quantification of the spectroscopic properties of medium- and heavy-mass nuclei.

Diagrammatic Monte Carlo and Emulating Many-Body Green’s Functions

Thank you for listening!

Any questions?

Backup slides

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

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

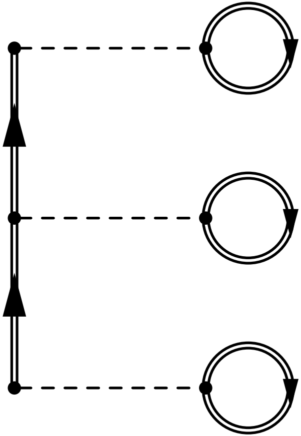
$\mathcal{Z}_{\alpha\beta} = \int_{\omega_{\min}}^{\omega_{\max}} d\omega \int d\mathcal{C}\ |\mathcal{D}_{\alpha\beta}(\omega,\mathcal{C})|$ is not known but can be estimated.

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 $\mathcal{S}_N$

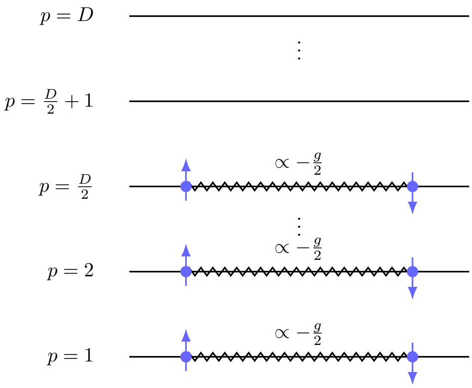


- At order ν, we choose the ν-tadpoles diagram as the only member of $\mathcal{S}_N$.
- The calculation of $\mathcal{Z}^N_{\alpha\beta}$ scales very favorably with the order and $e_{\max}$ ($\propto N_{sp}^{7/3} + \nu N_{sp}^2$).

Brolli et al., In preparation.

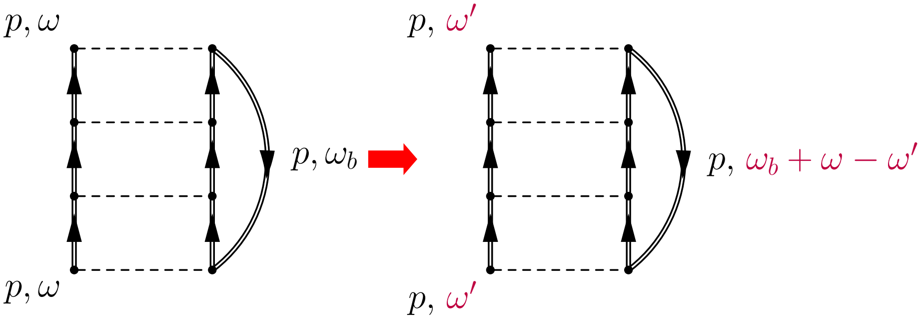
Brolli et al., Phys. Rev. Lett. 134, 182502 (2025)

Updates of the Richardson model



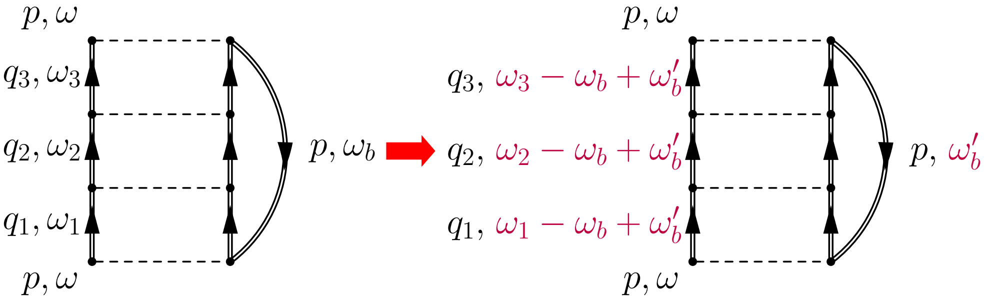
Brolli et al., Phys. Rev. Lett. 134, 182502 (2025)

Change of ω



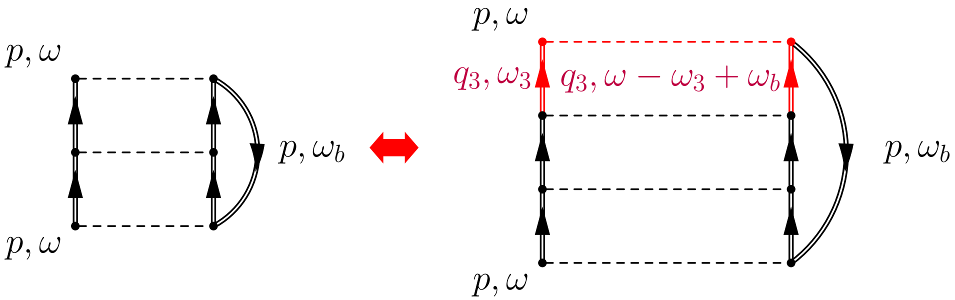
$$q_\omega = \left| \frac{G_p(\omega_b + \omega - \omega')}{G_p(\omega)} \right|$$

Change of the internal frequencies



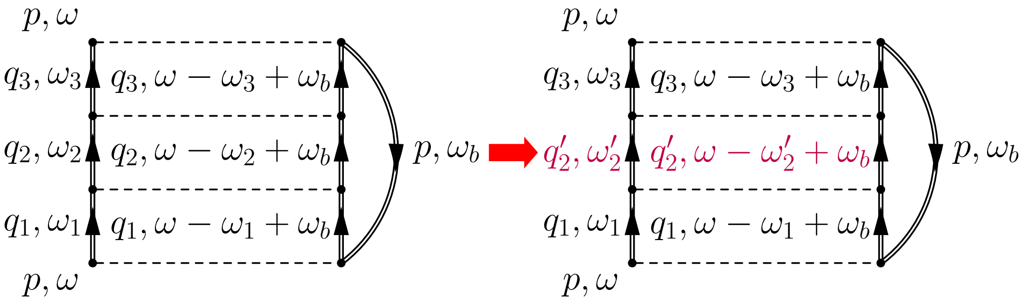
$$q_{\omega\, int} = \frac{L(\omega_b)}{L(\omega_b')} \left| \frac{G_p(\omega_b')}{G_p(\omega_b)} \right| \prod_{j=1}^{\nu-1} \frac{|G_{q_j}(\omega_j - \omega_b + \omega_b')|}{|G_{q_j}(\omega_j)|}$$

Add / Remove rung



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

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

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

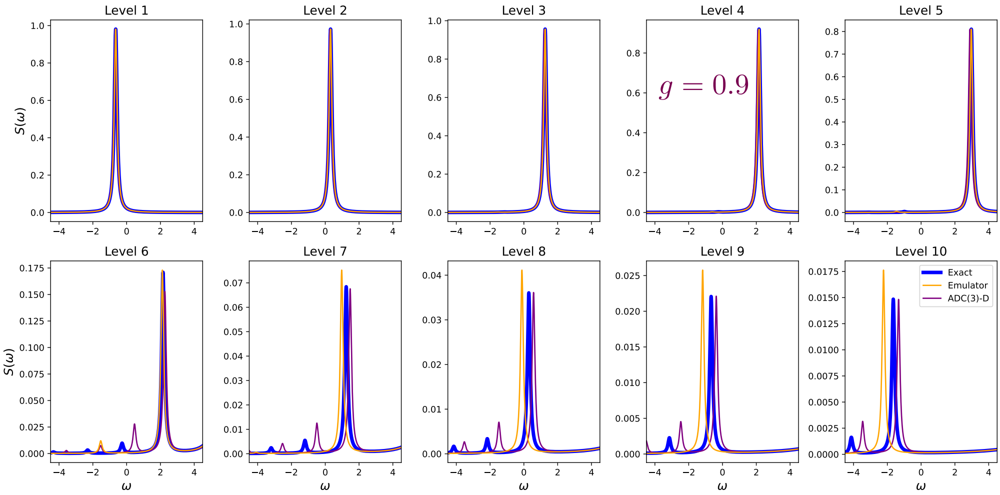
$$M_{\alpha\beta}^{(p)} = \sum_n \frac{\langle \Psi_0^A | c_\alpha | \Psi_n^{A+1} \rangle \langle \Psi_n^{A+1} | c_\beta^\dagger | \Psi_0^A \rangle}{\left[E_F - \left(E_n^{A+1} - E_0^A\right)\right]^p} + \sum_k \frac{\langle \Psi_0^A | c_\beta^\dagger | \Psi_k^{A-1} \rangle \langle \Psi_k^{A-1} | c_\alpha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

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

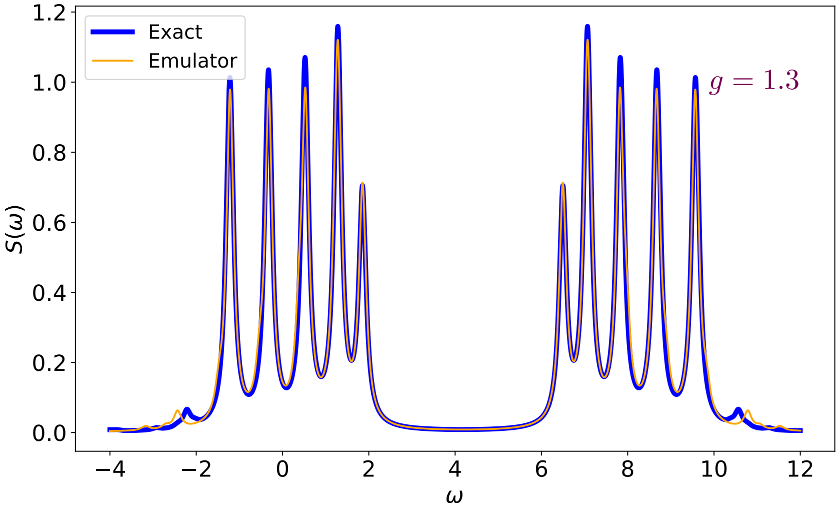
$$\rightarrow \quad G_{\alpha\beta}^{\mathrm{OpRS}}(\omega) = \sum_n \frac{(\tilde{\mathcal{X}}_\alpha^n)^* \tilde{\mathcal{X}}_\beta^n}{\omega - \tilde{\varepsilon}_n^+ + i\eta} + \sum_k \frac{\tilde{\mathcal{Y}}_\alpha^k (\tilde{\mathcal{Y}}_\beta^k)^*}{\omega - \tilde{\varepsilon}_k^- - i\eta}$$

Mean field propagator

Spectral function of the Richardson model per partial wave



Spectral function of the Richardson model for $g = 1.3$



$\mathcal{L}_{\mathrm{emul}} = 0.01$

Brolli et al., In preparation.