Diagrammatic Monte Carlo for Atomic Nuclei

Towards a consistent approach for nuclear structure and reactions: microscopic optical potentials

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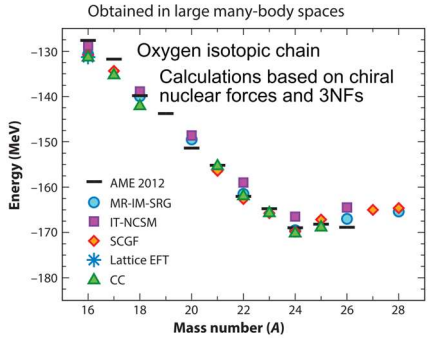
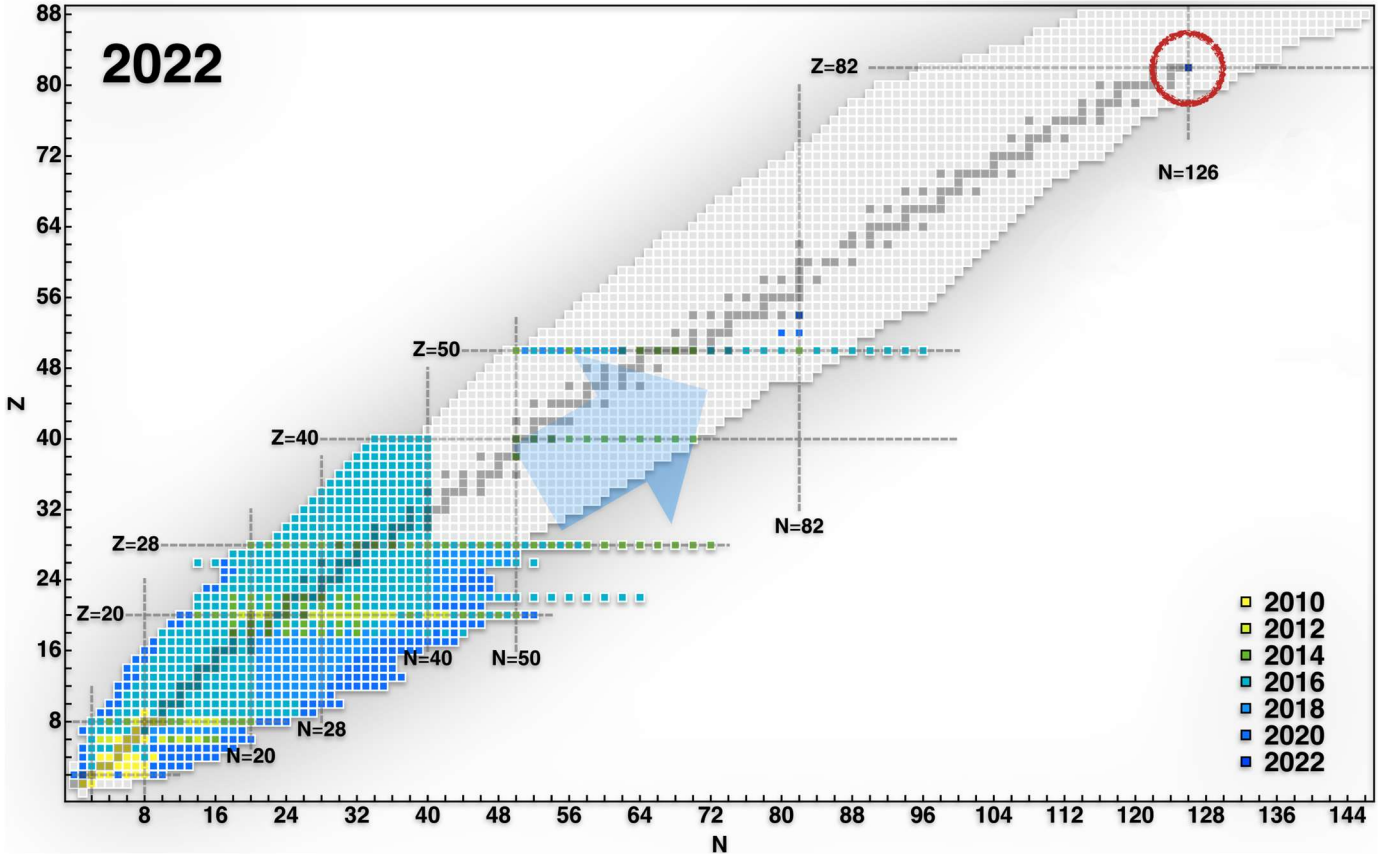
Ab initio structure calculations

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



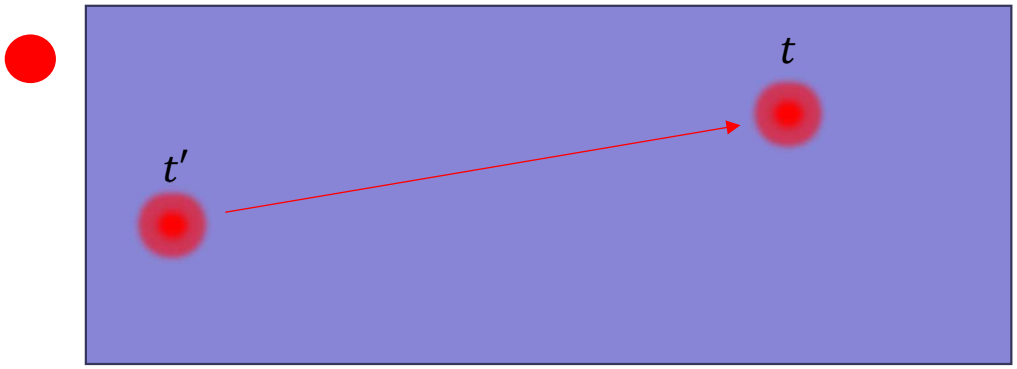
Hebeler et al., Annu. Rev. Nucl. Part. Sci. (2015)



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

The Green's function

The Green's function describes the propagation of a particle (hole) in the system.



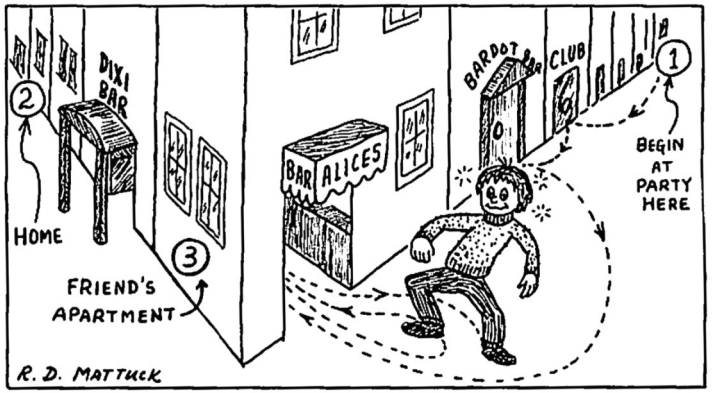


Fig. 1.1 *Propagation of Drunken Man*

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

Spectral function

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

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

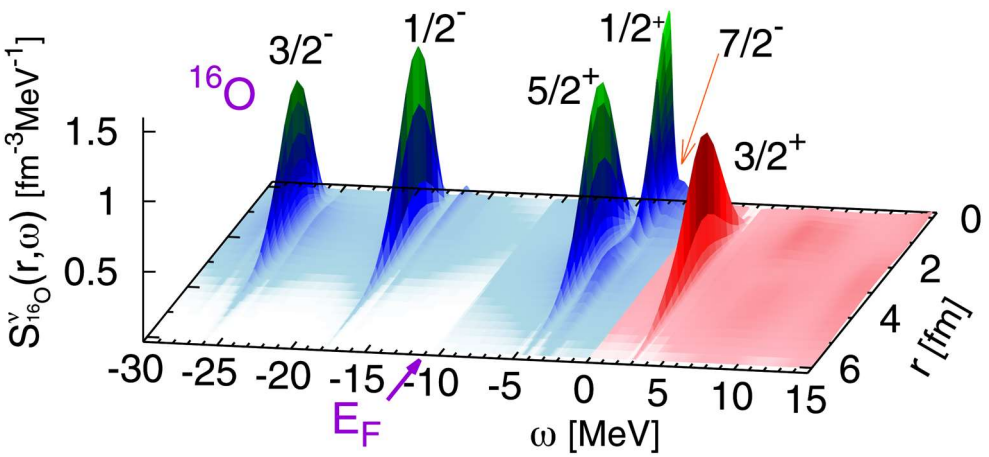
$$\varepsilon_n^+ = E_n^{A+1} - E_0^A \qquad \varepsilon_k^- = E_0^A - E_k^{A-1}$$

The Green's function contains the full one-particle addition and removal spectroscopy

$$S(\omega) = \sum_n SF_n^+ \, \delta(\omega - \varepsilon_n^+) + \sum_k SF_k^- \, \delta(\omega - \varepsilon_k^-)$$

Probability of adding a nucleon to the single-particle orbit of energy ε_n^+.

Probability of removing a nucleon to the single-particle orbit of energy ε_k^-.



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

Nuclear structure

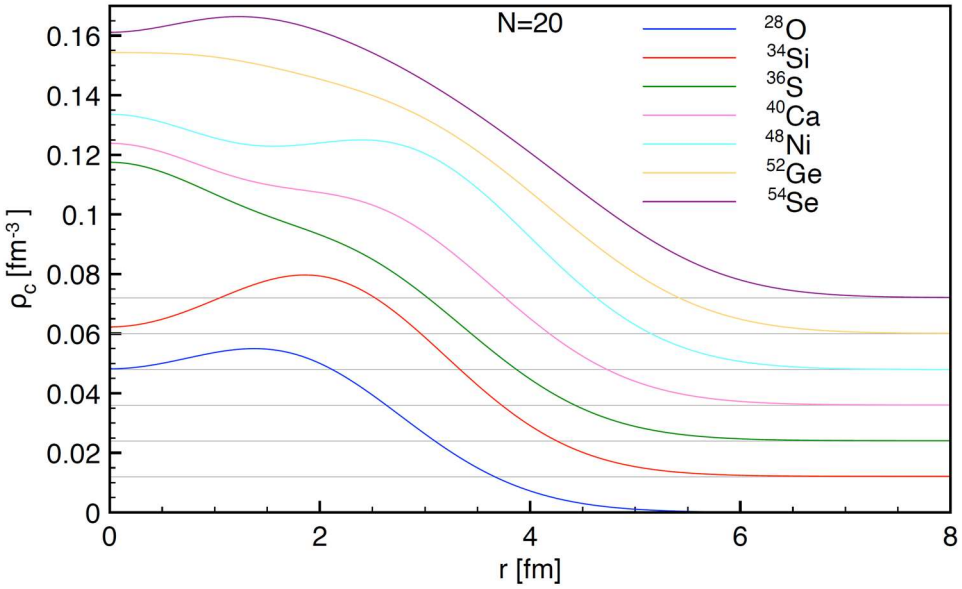
$$G_{\alpha\beta}(\omega) = \sum_n \frac{(X_\alpha^n)^* X_\beta^n}{\omega - \varepsilon_n^+ + i\eta} + \sum_k \frac{Y_\alpha^k \left(Y_\beta^k\right)^*}{\omega - \varepsilon_k^- - i\eta}$$

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

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

Structure information:

- All one-body observables
  (e.g. charge and point-matter densities and radii).
- Ground state energy.
- Single-particle energies and spectroscopic factors.



SB, Bachelor's thesis (2020)

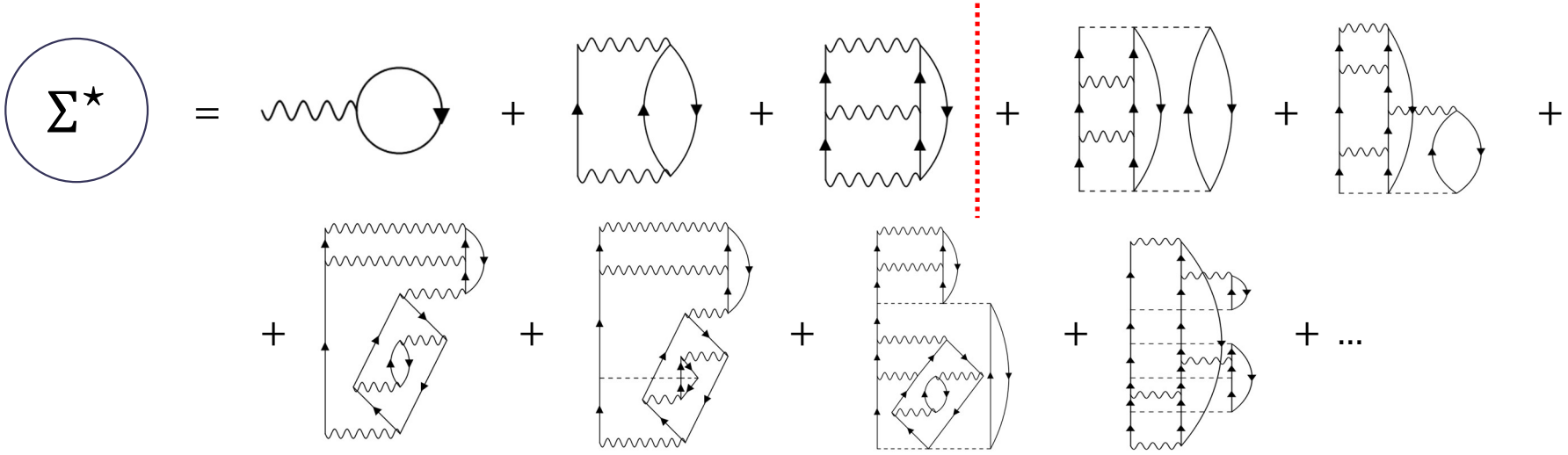
Dyson equation

The Green's function is the exact solution of the Dyson equation

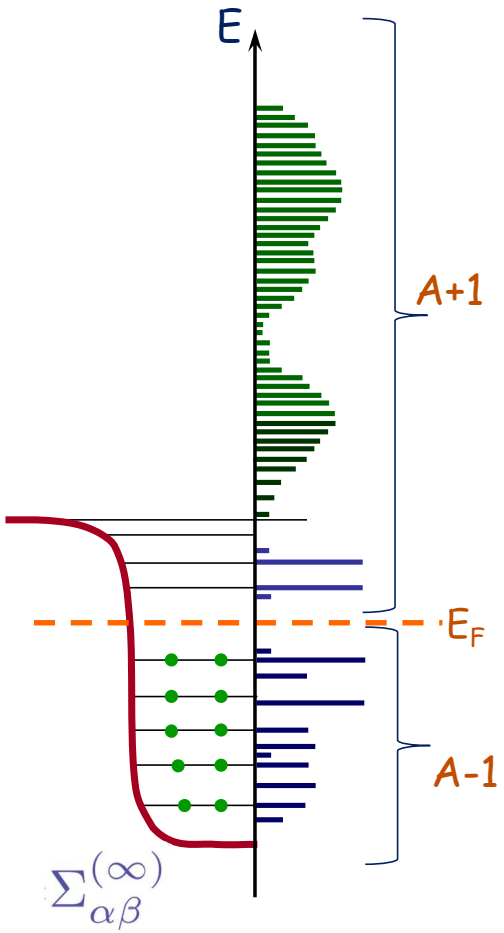
$$G_{\alpha\beta}(\omega) = G^{(0)}_{\alpha\beta}(\omega) + G^{(0)}_{\alpha\gamma}(\omega)\Sigma^{\star}_{\gamma\delta}(\omega)G_{\delta\beta}(\omega)$$

Unperturbed propagator

Irreducible self-energy, the central element of the theory



Microscopic optical potential



The Feshbach formalism projects on the space of ground state + a particle flying off.

The self-energy is an extension of the Feshbach optical potential that includes both holes and particles.

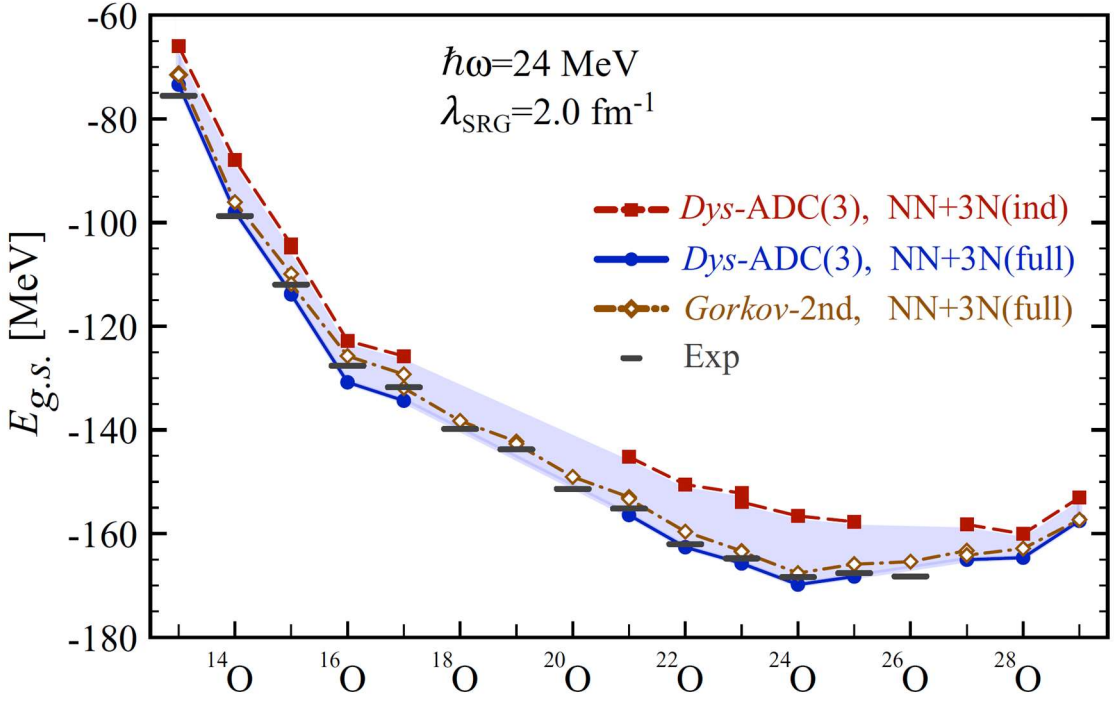
Complex, non-local, energy-dependent optical potential

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

Dyson equation

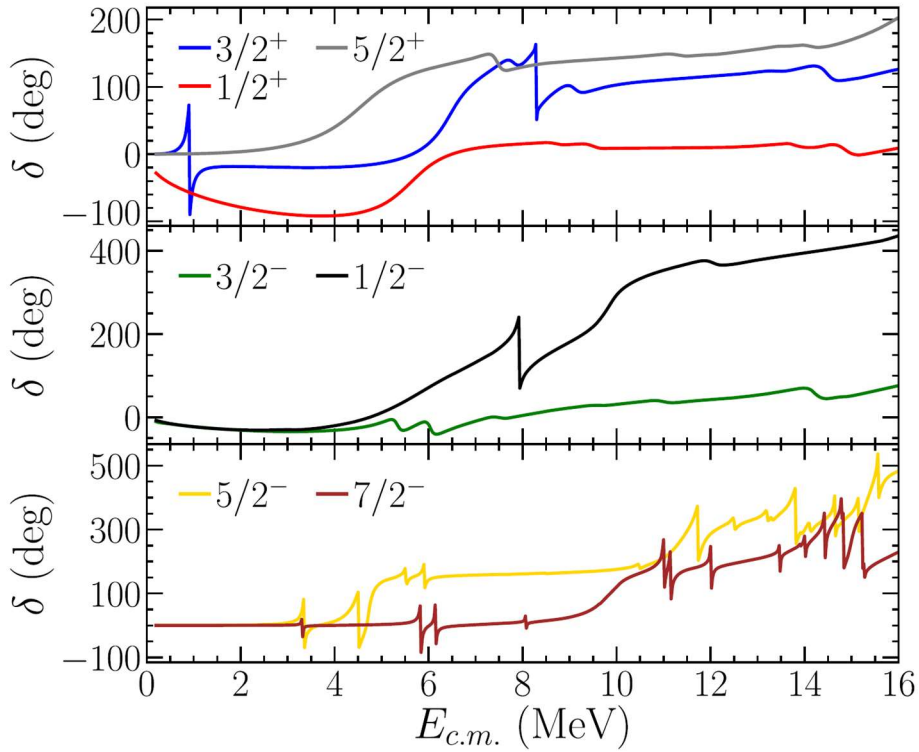
Structure AND Reactions

The Green's function naturally contains both structure and reaction information



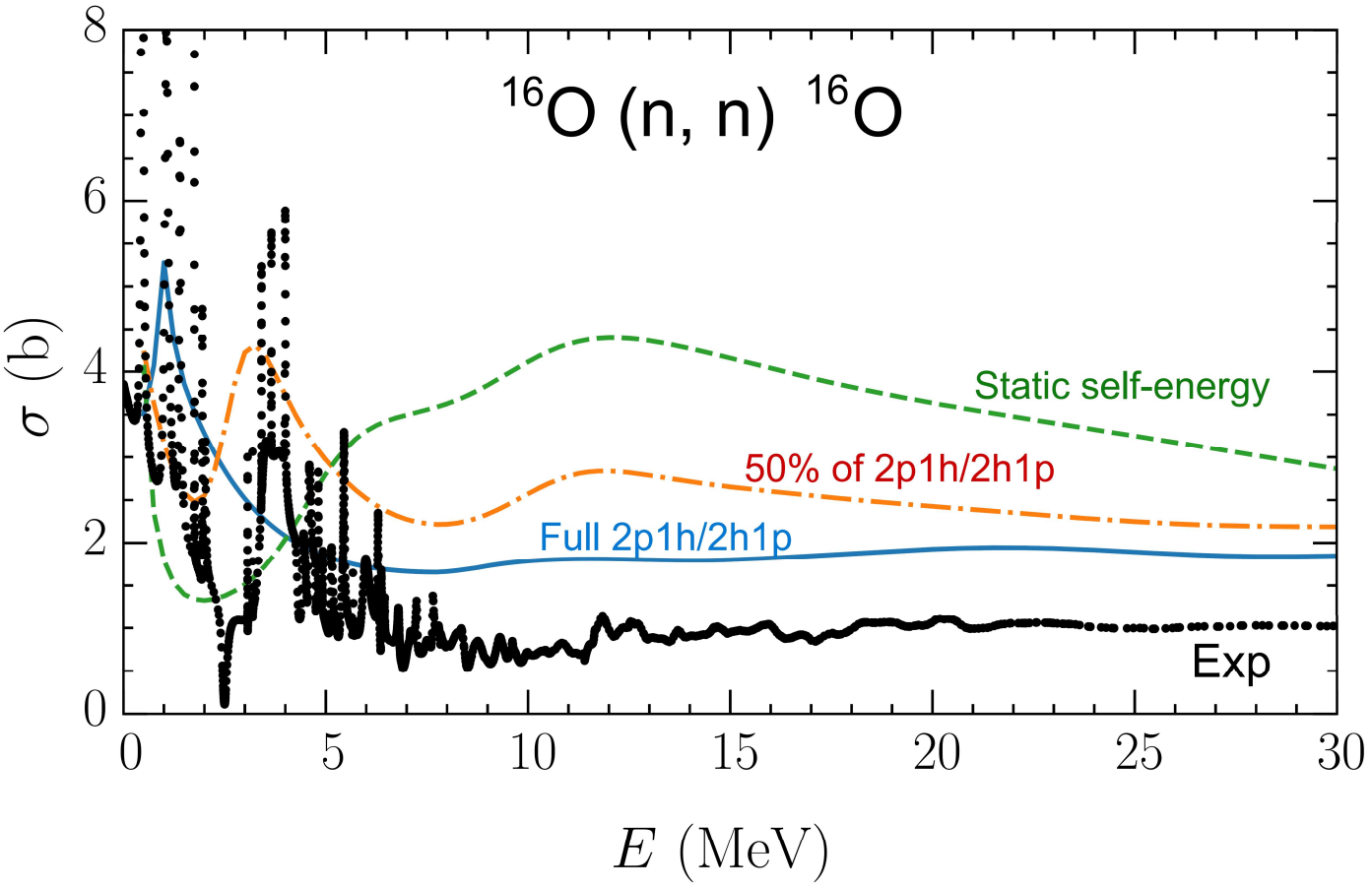
Cipollone et al., Phys. Rev. C, 92, 014306 (2015)

$^{16}O(n,n)^{16}O$ phase shifts



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

Status of reactions

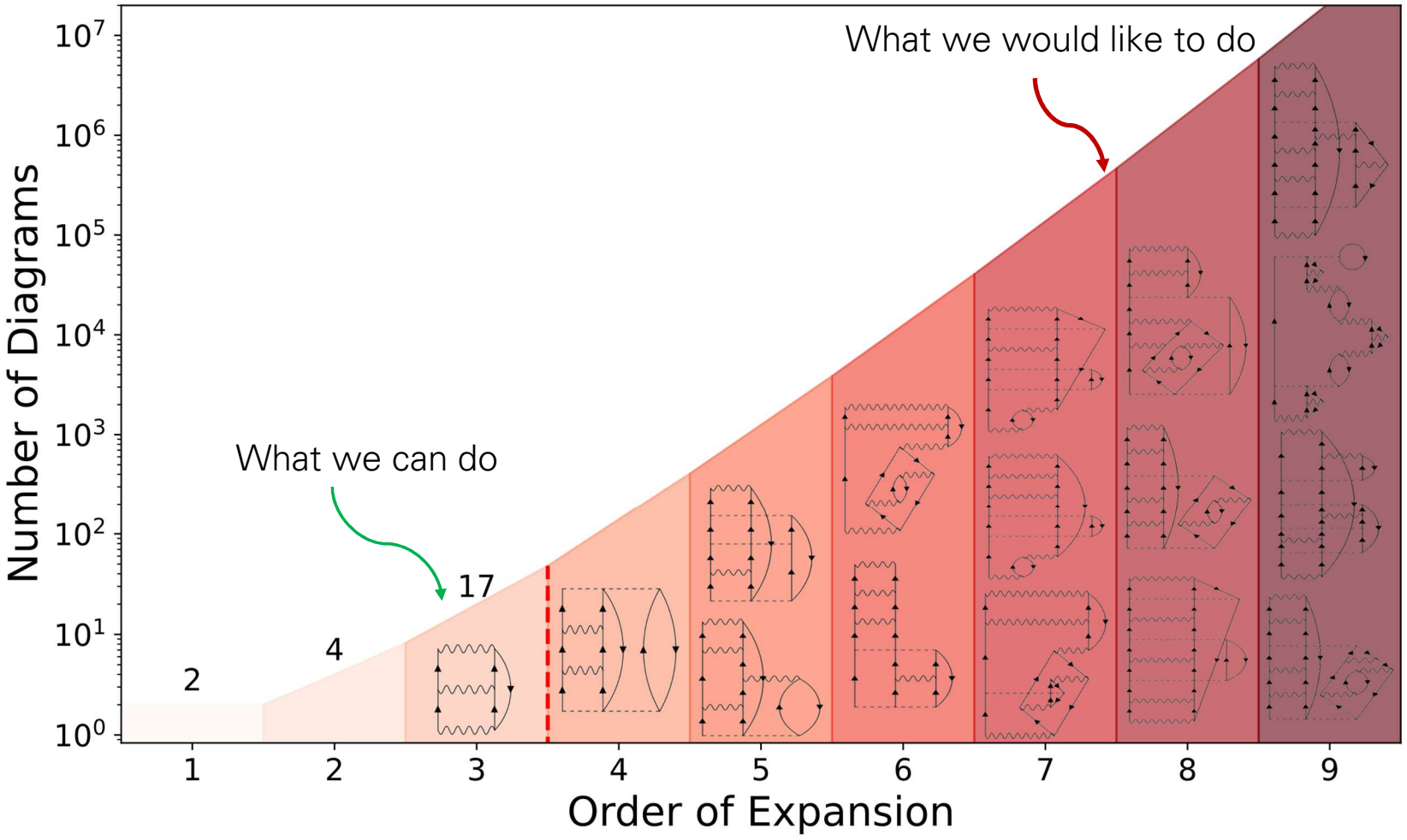


Idini et al., Phys. Rev. Lett., 123, 092501 (2019)

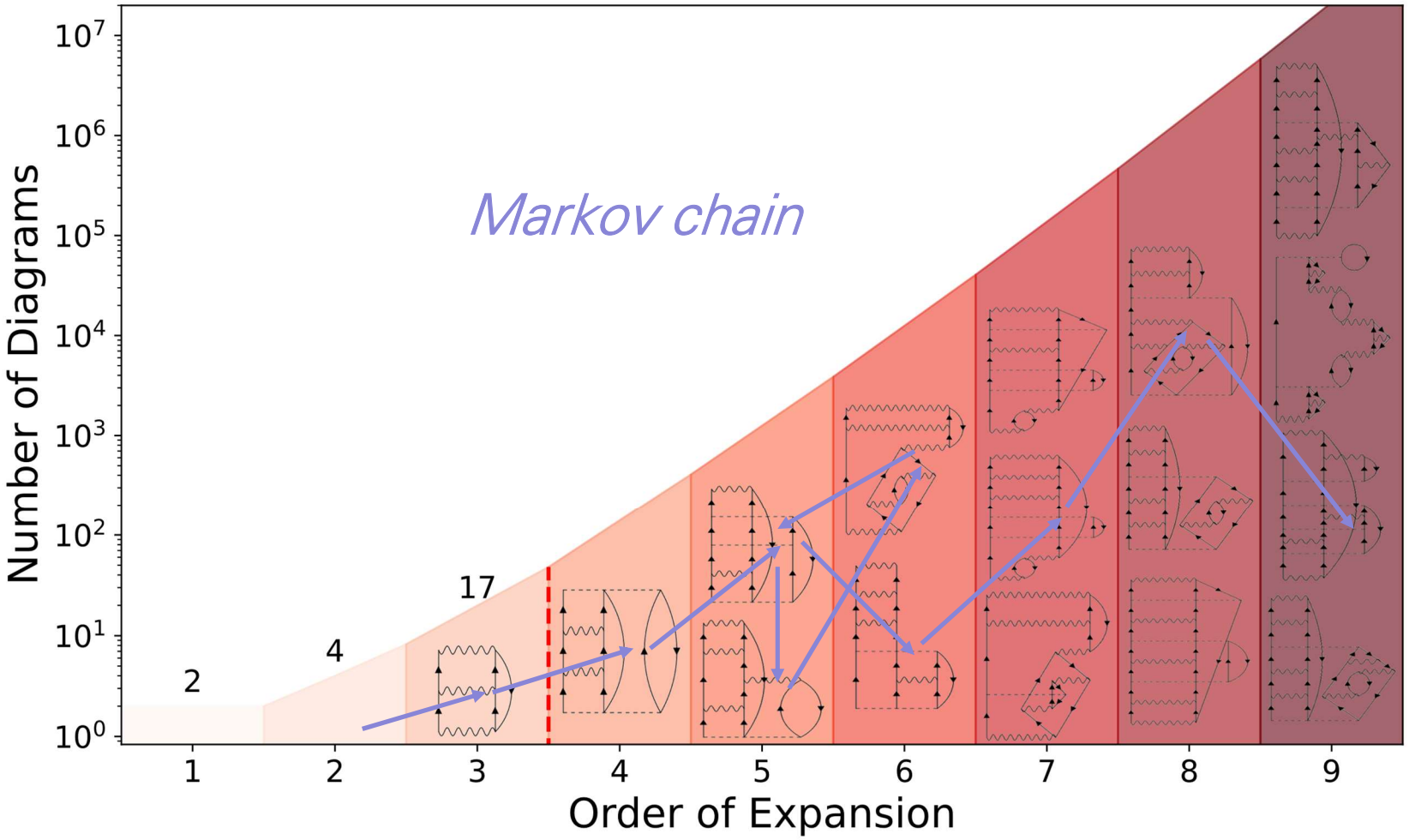
- We do not include ISCs beyond $2p1h$.
- $3p2h$ (and beyond) configurations have an important absorption contribution.
- As a result the cross section is overestimated.
- We need to include high order diagrams ($\gg 3$).
- Diagrams at order 4 are already computationally unreachable.

What we have

What we want



Diagrammatic Monte Carlo sampling



Diagrammatic Monte Carlo

Diagrammatic Monte Carlo (diagMC) has been developed in the context of condensed matter physics.

- It proved to be a reliable way to include contributions from high order Feynman diagrams in solid state systems[1].
- Designed for infinite systems in the finite temperature regime.

It has never been applied in nuclear physics systems, and it needs to be adapted to

- Handle discrete-level system at zero-temperature.
- Much more challenging *ab initio* nuclear interactions.
- DiagMC samples perturbation theory contributions, but the causality principle needs to be implemented non-perturbatively (Lehmann representation).

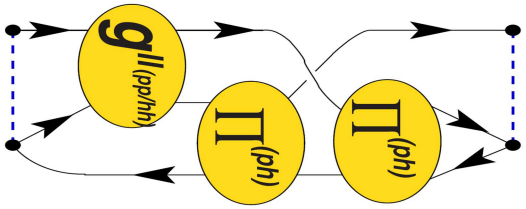
1. DiagMC included diagrams up to order 9 for the unitary Fermi gas, see K. Van Houcke et al., Phys. Rev. B., 99, 035140 (2019)

Lehmann representation of the self-energy

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



The Lehmann representation encapsulates the causality principle.

$ADC(n)$ truncations were developed with the aim of preserving the Lehmann representation.

State-of-the-art $ADC(3)$ only retains $2p1h$ intermediate state configurations (ISCs).

Nuclear structure

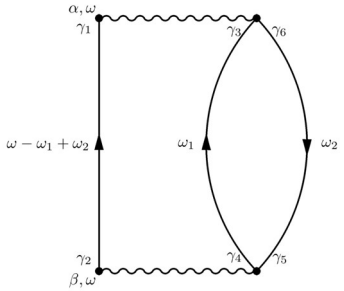
Reactions

A bit of mathematical machinery (just a bit, I promise)

We can project the self-energy on a basis $B_n(\omega)$ (for us orthonormalized Legendre polynomials over a range $[\omega_{min}, \omega_{Max}]$).

DiagMC simulates this overlap

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



Diagrams of the self-energy expansion

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

Topology

Internal single-particle quantum numbers

Internal frequencies

Normalization factor

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

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

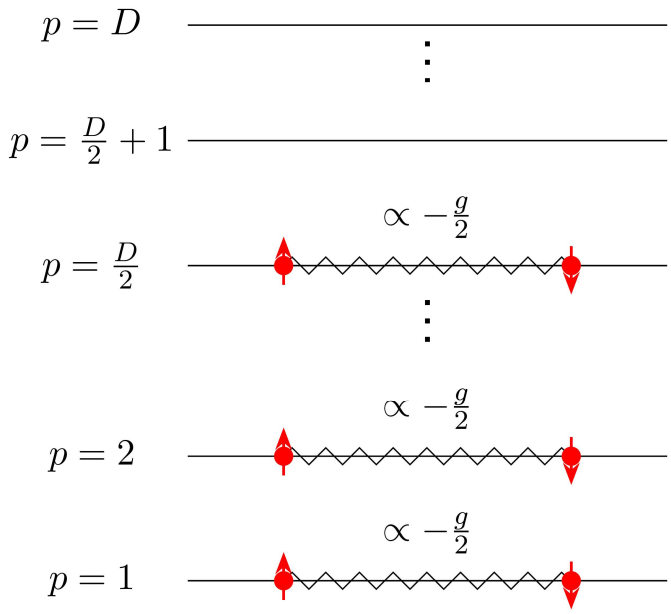
$w_{\alpha\beta}(\omega, C)$, probability distribution function

Proof of principle: Richardson pairing model

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

Energy level — Spin (up or down)

- D equally spaced energy levels.
- Particles of opposite spin on the same energy level interact with a constant interaction.
- We consider a half-filling situation of ${}^{D}/_{2}$ pairs of nucleons (D is even).
- Simple but challenging due to a pure pairing interaction (we'll see that $ADC(3)$ does not do well for this model).
- Exactly solvable: it has been used to benchmark many-body methods[1].



1. M. Hjorth-Jensen et al., An Advanced Course in Computational Nuclear Physics, Springer (2017)

Sampling diagrams

- The self-energy expansion of the Richardson model is dominated by the ladder diagrams.
- We adopt the self-consistent formalism – the self-energy is expressed as a function of G.
- To sample diagrams, we build a Markov chain with carefully tuned Metropolis-Hastings update ratios designed to reproduce the PDF $w_{\alpha\beta}(\omega, C)$.
- The Markov chain "moves" thanks to four possible updates

  1. *Change ω*
  2. *Change internal frequencies*
  3. *Change sp quantum numbers and frequencies*
  4. *Add/Remove Rung*

- After the diagMC simulation, we fit the imaginary part of the self-energy as a function of Lorenzians to enforce the causality principle (i.e. the Lehmann representation).
- This is allowed only within the convergence radius of the self-energy expansion. The extension to non-perturbative regimes ($g \gg 1$) is a work in progress...

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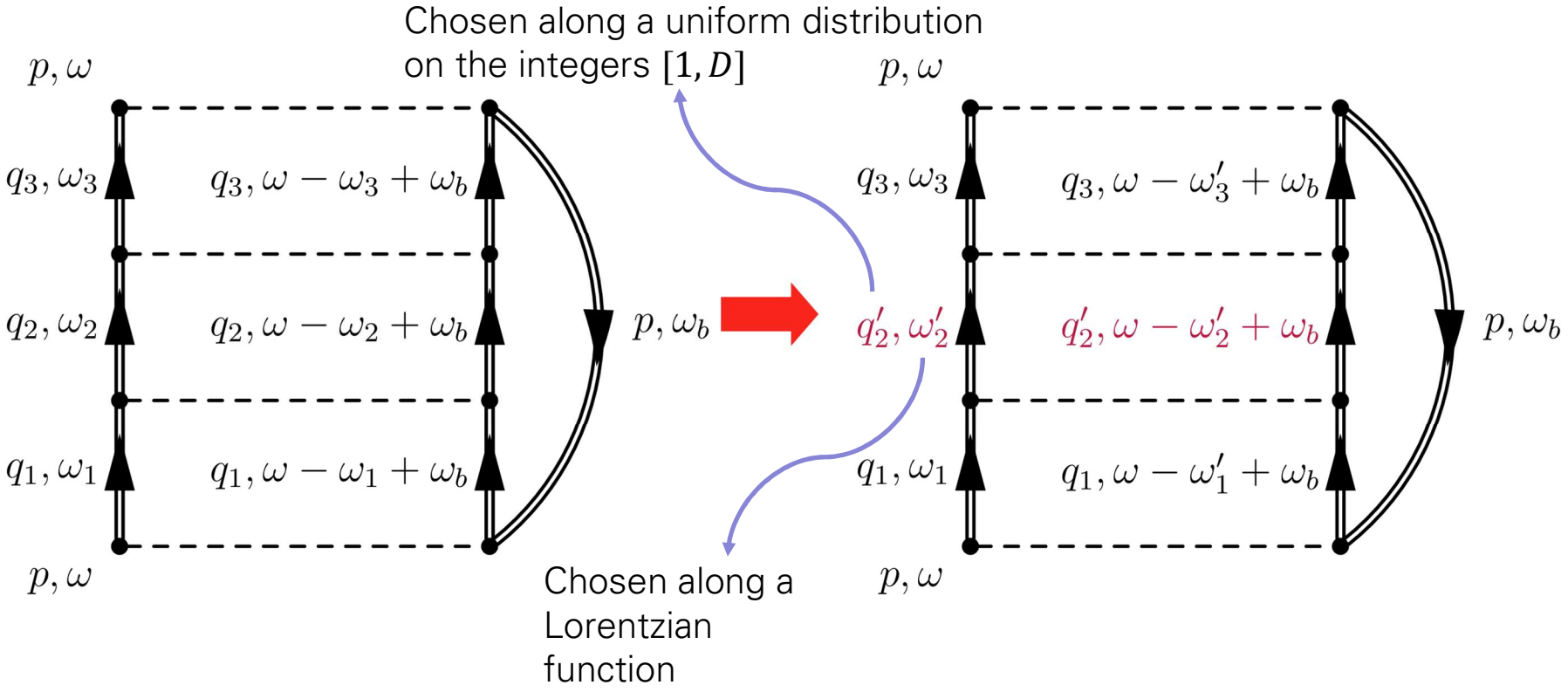
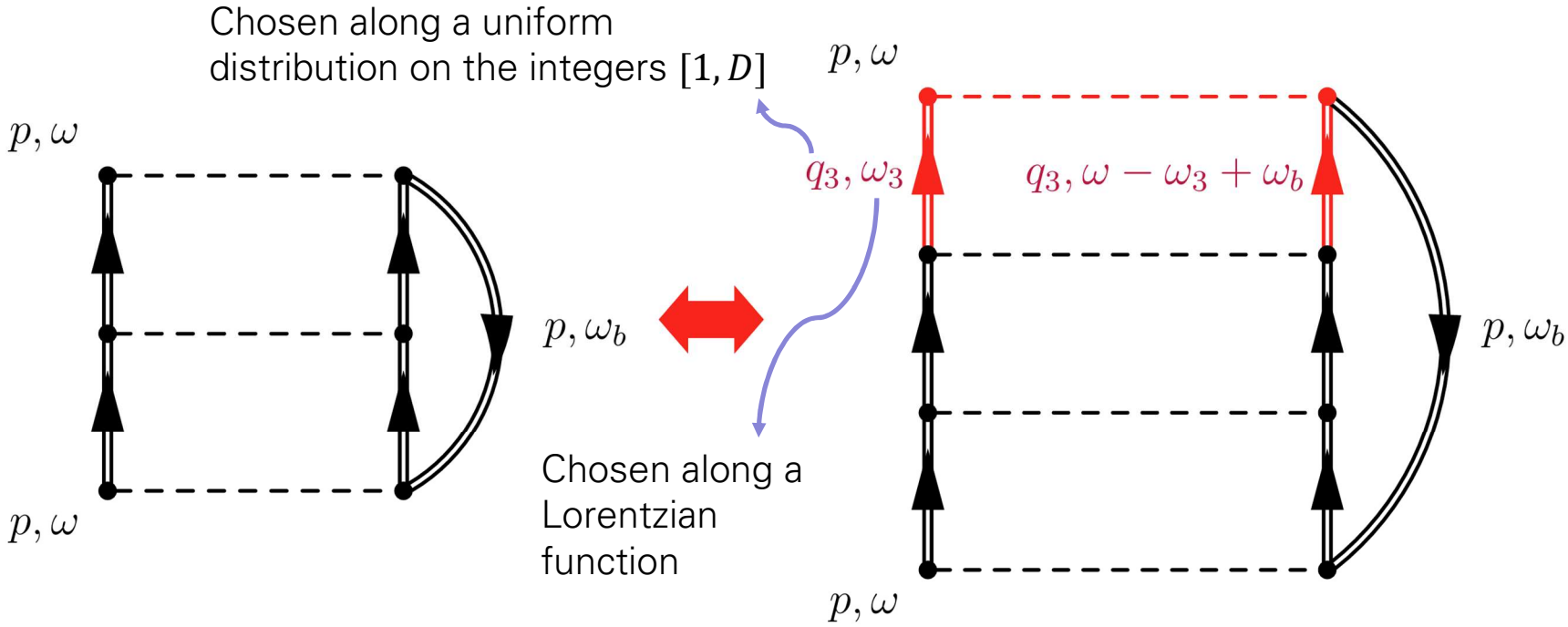
Change sp quantum numbers and frequencies



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

Add/Remove rung



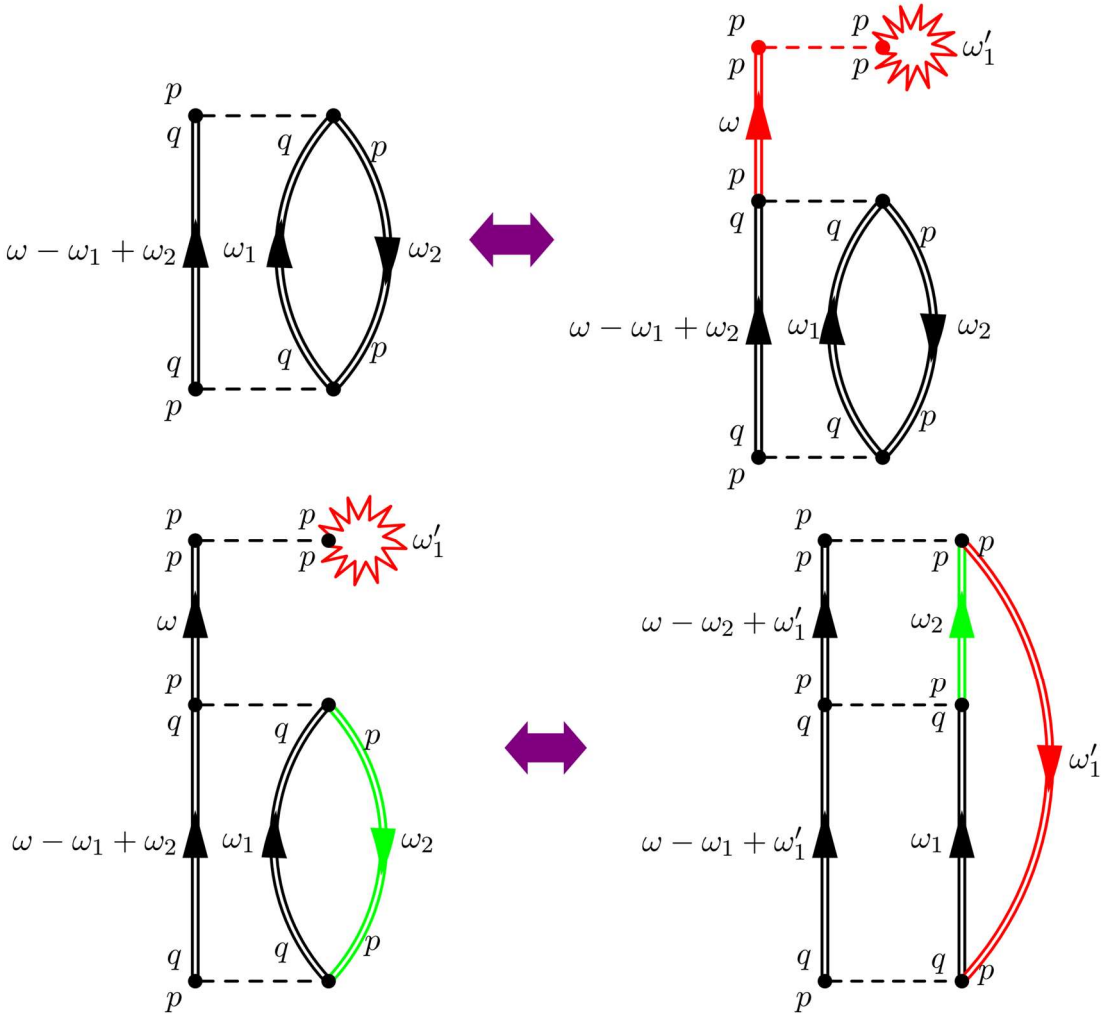
$$q_{Add} = \frac{|g|}{4\pi} \frac{D}{L(\omega_3)} \left| G_{q_3}(\omega_3) G_{q_3}(\omega - \omega_3 + \omega_b) \right| \qquad q_{Rem} = \frac{1}{q_{Add}}$$

Is this the only possible way to sample diagrams?

NO. It might not even be the best way.

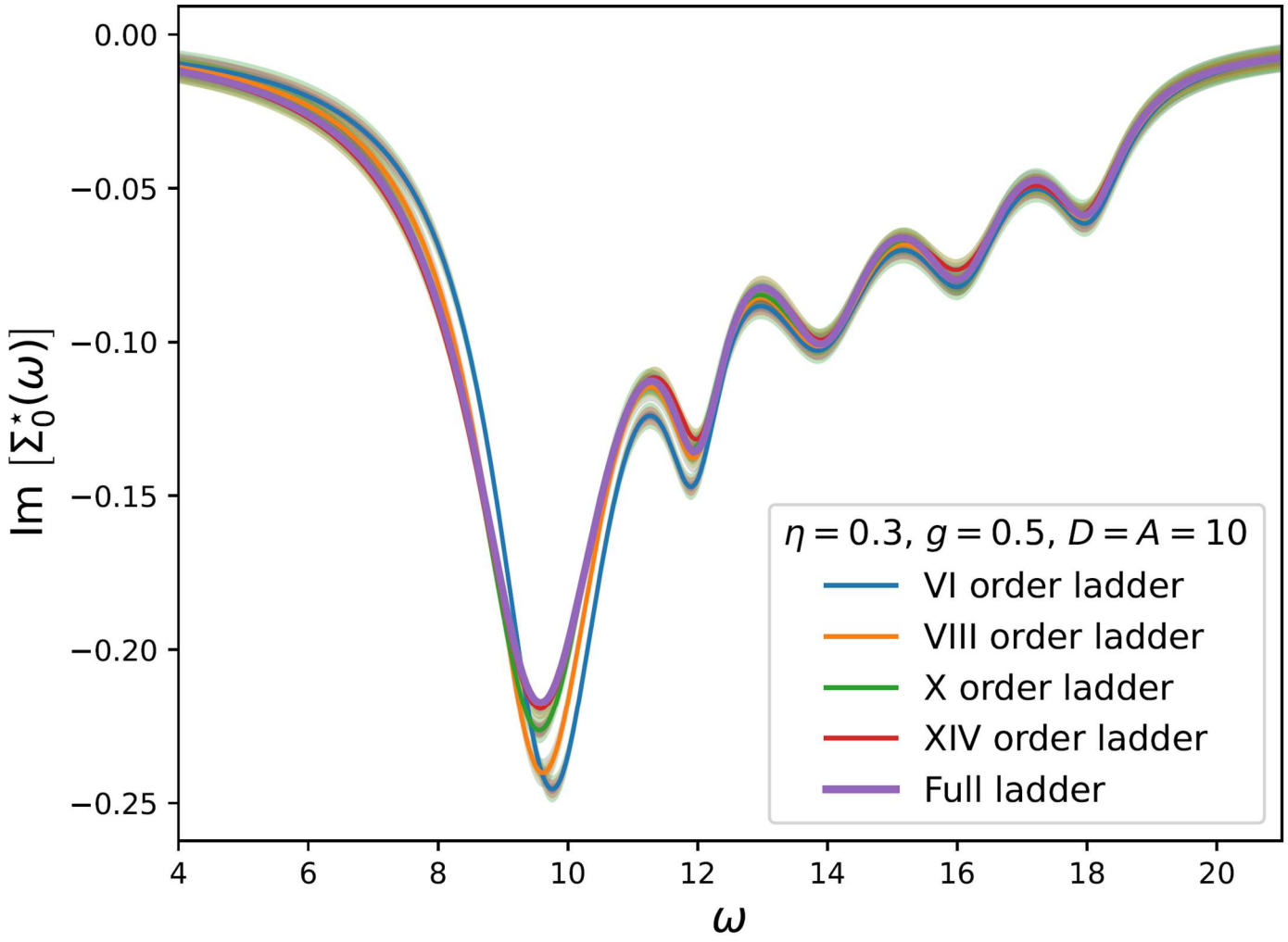
There were other attempts

We chose the current one through trial and error.



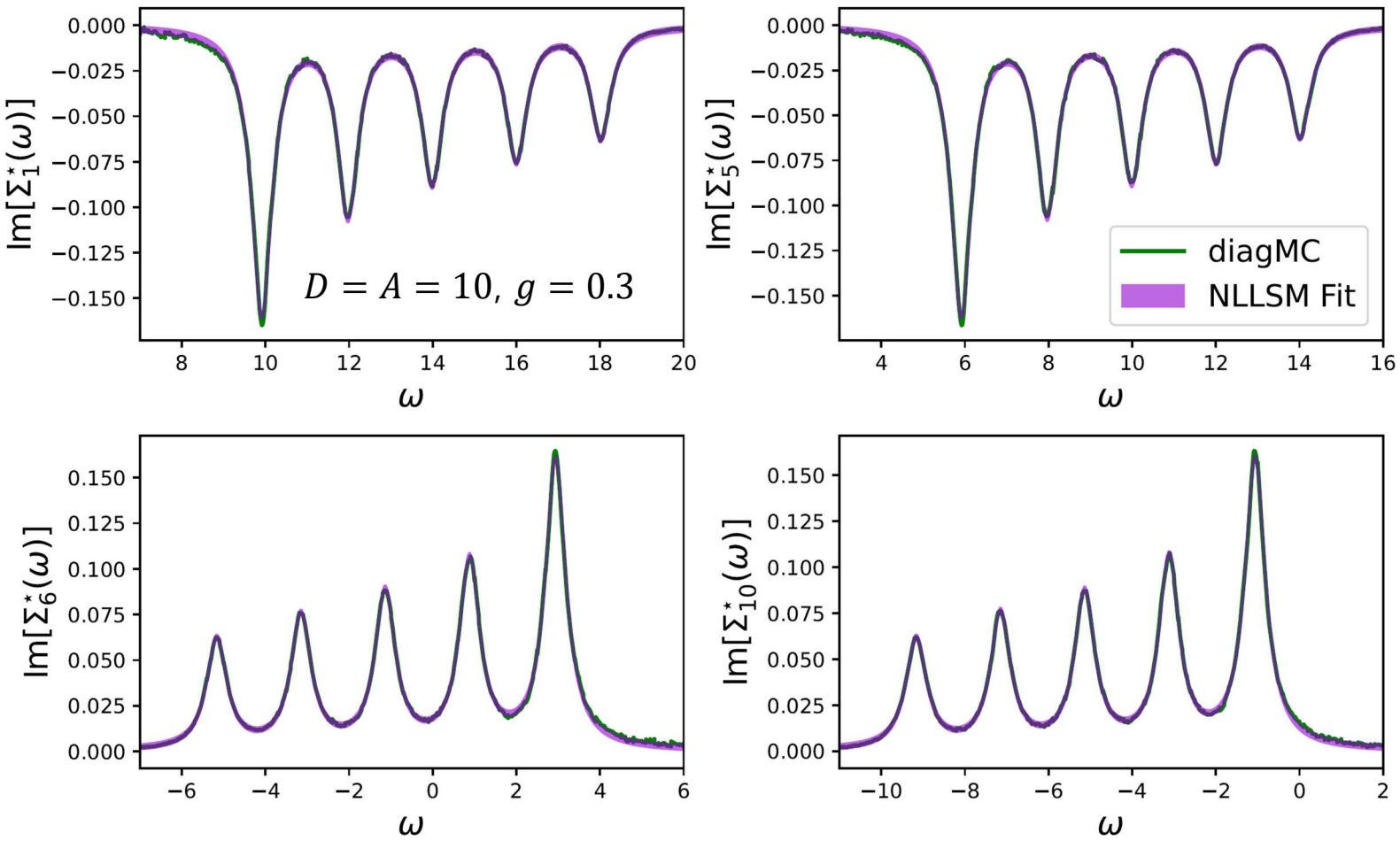
Some results

Sampling at very high orders



SB, Barbieri, Vigezzi, to be published

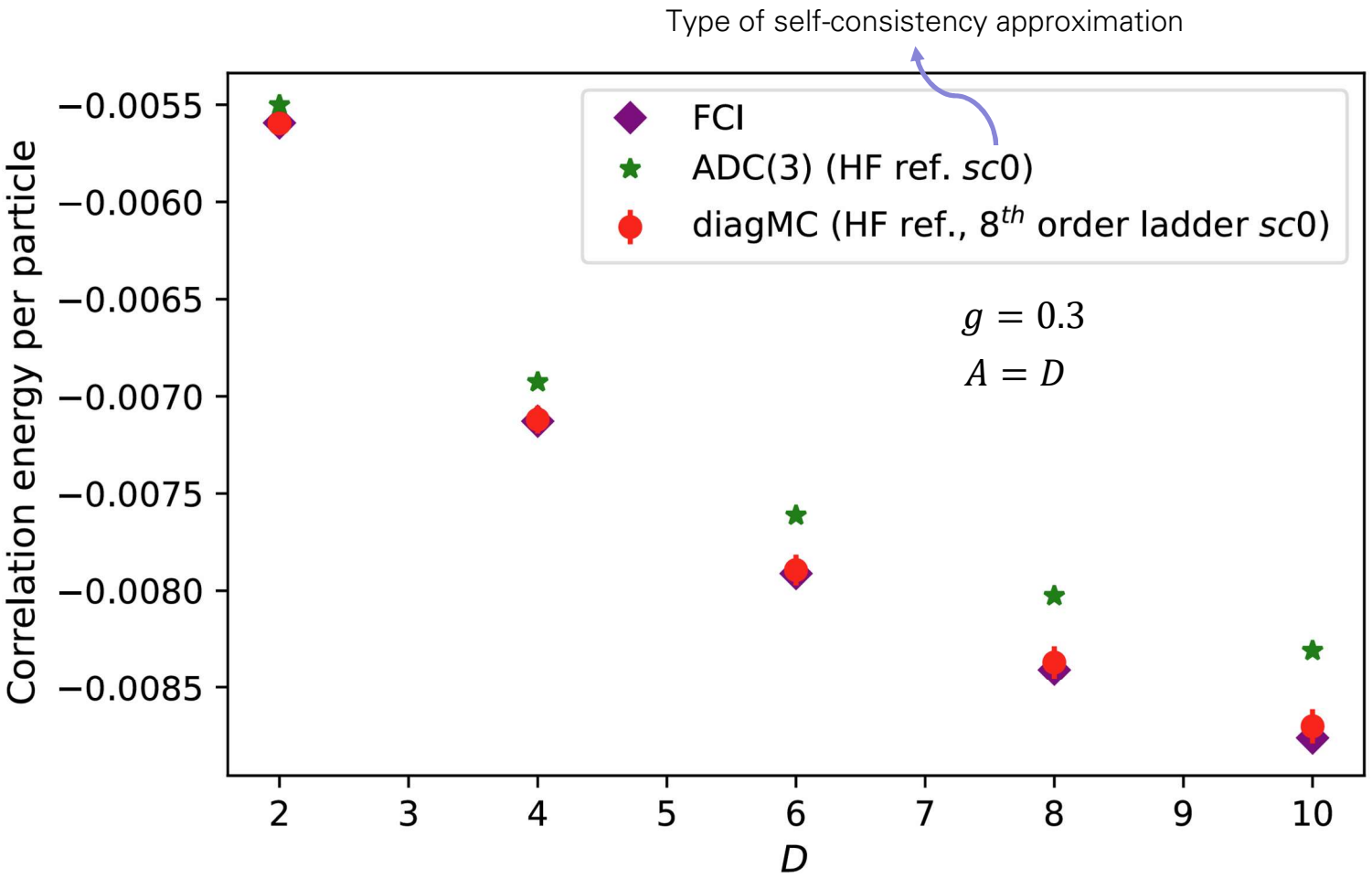
Results of the self-energy simulation



8^{th}-order ladder self-energy simulation (HF ref.).

SB, Barbieri, Vigezzi, to be published

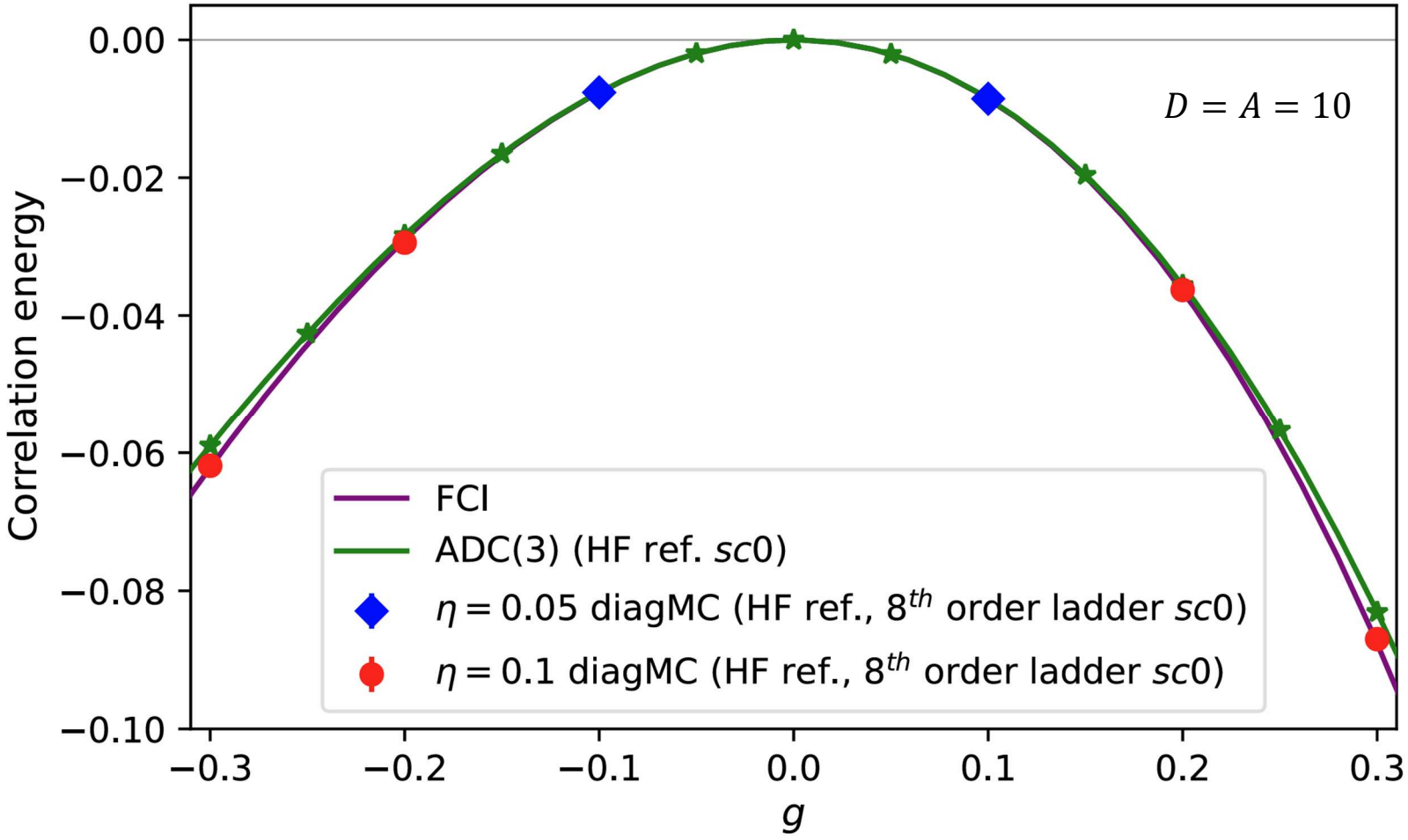
Benchmarking with FCI and ADC(3)



diagMC does much better than ADC(3)!!

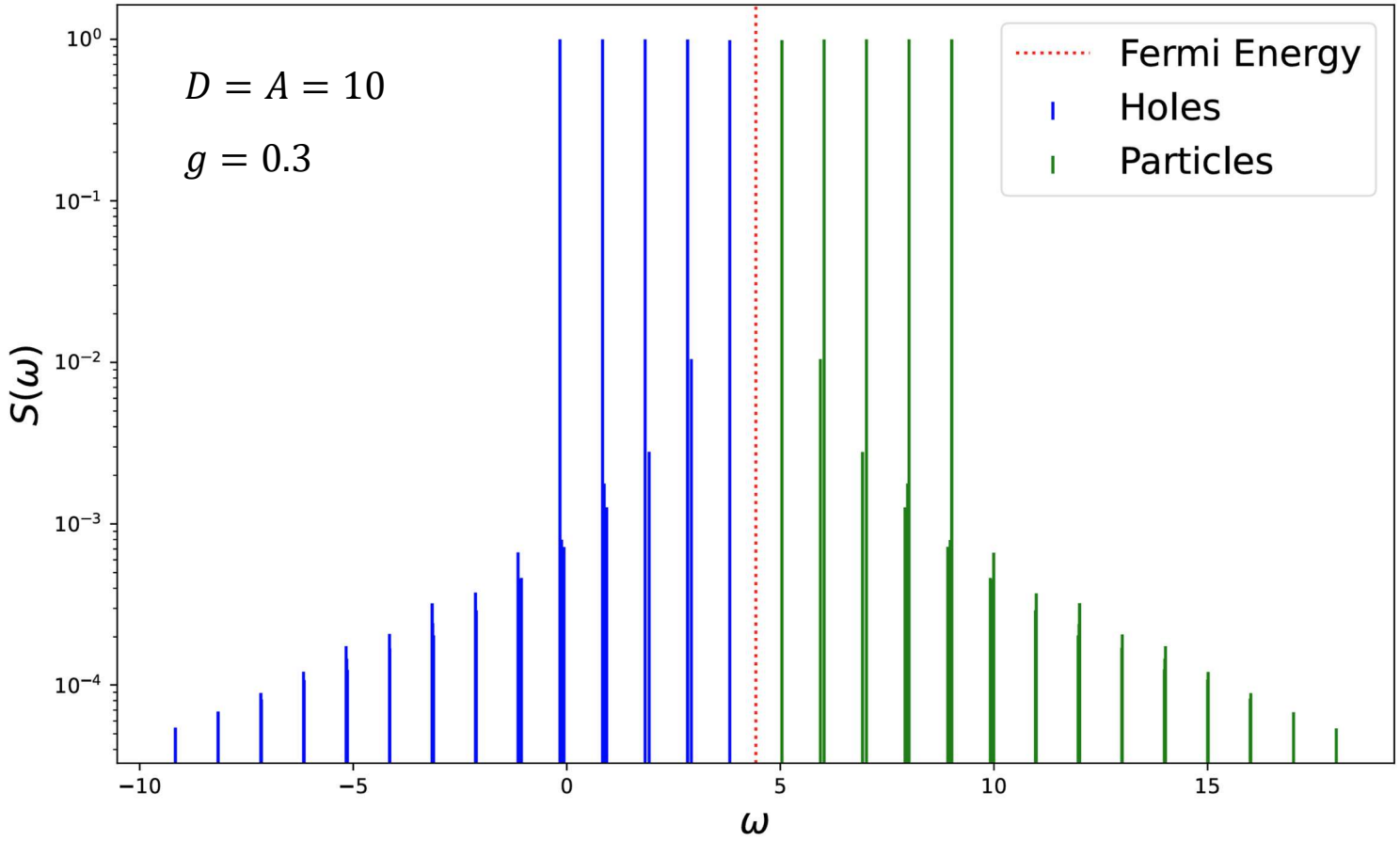
SB, Barbieri, Vigezzi, to be published

Benchmarking with FCI and ADC(3) (2)



SB, Barbieri, Vigezzi, to be published

Spectral function and fragmentation



The model is weakly fragmented and highly symmetric (as expected from particle-hole symmetry).

SB, Barbieri, Vigezzi, to be published

Towards *ab initio* 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).
- We are in the early stages, however…

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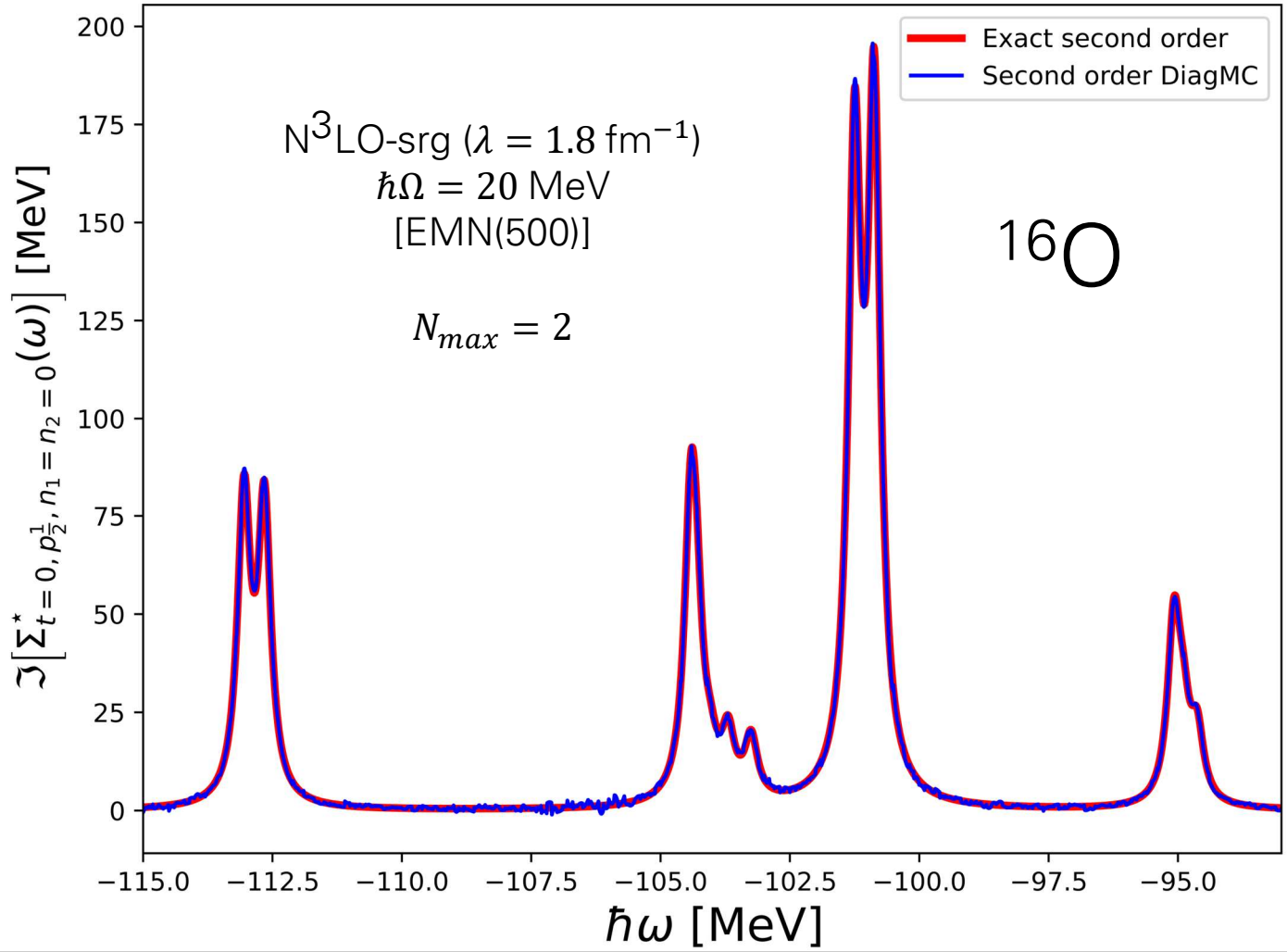
DiagMC calculation of a second order self-energy



SB, Barbieri, Vigezzi, to be published

Outlook & An important comment

- Move to large model spaces
- Better way to retain causality
- Higher order calculations

I only spoke of the Green's function but DiagMC can be used in any expansion that involves diagrams (CC, MBPT, …)

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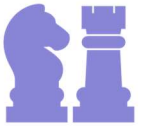
THANK YOU!!



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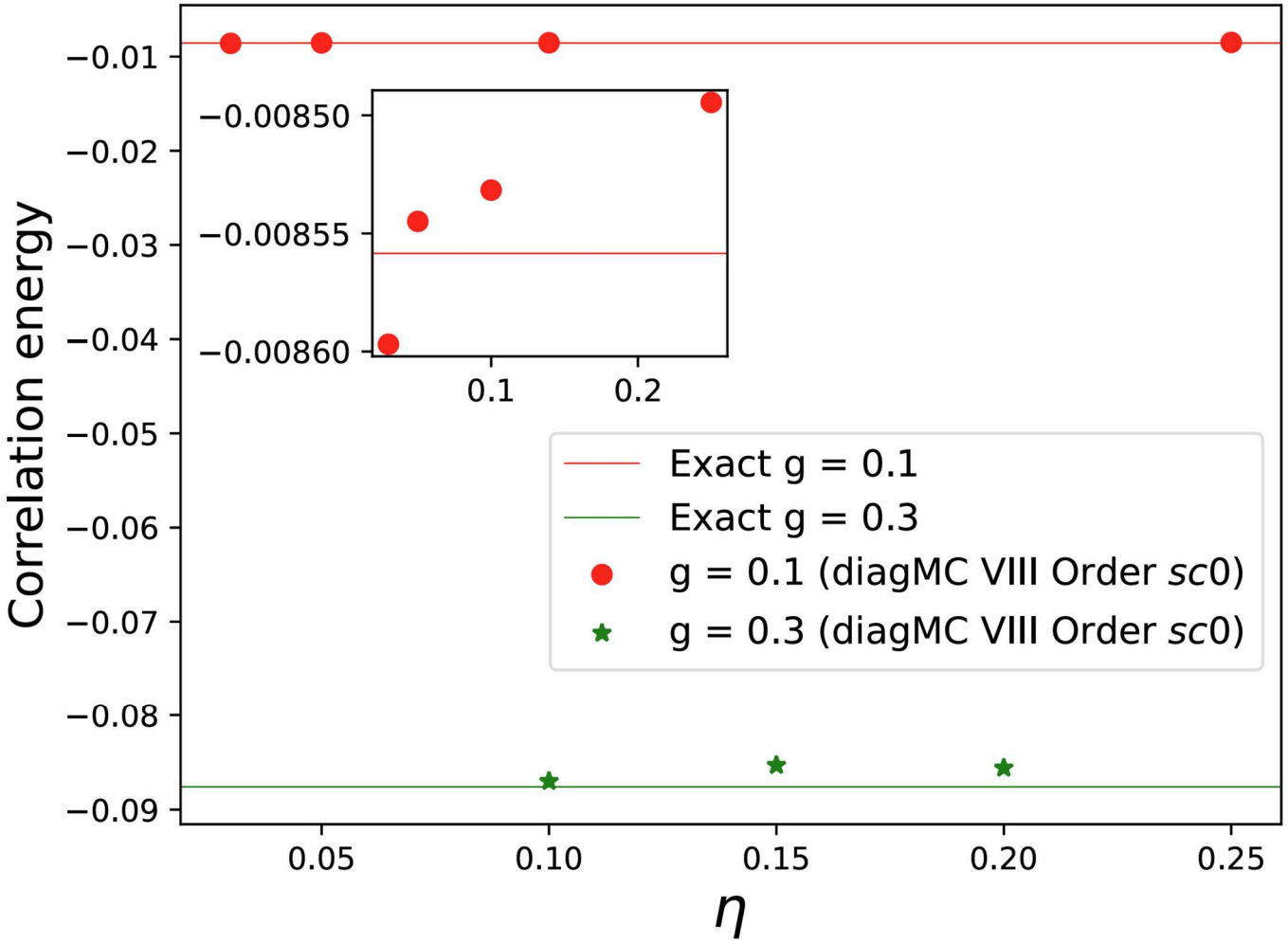
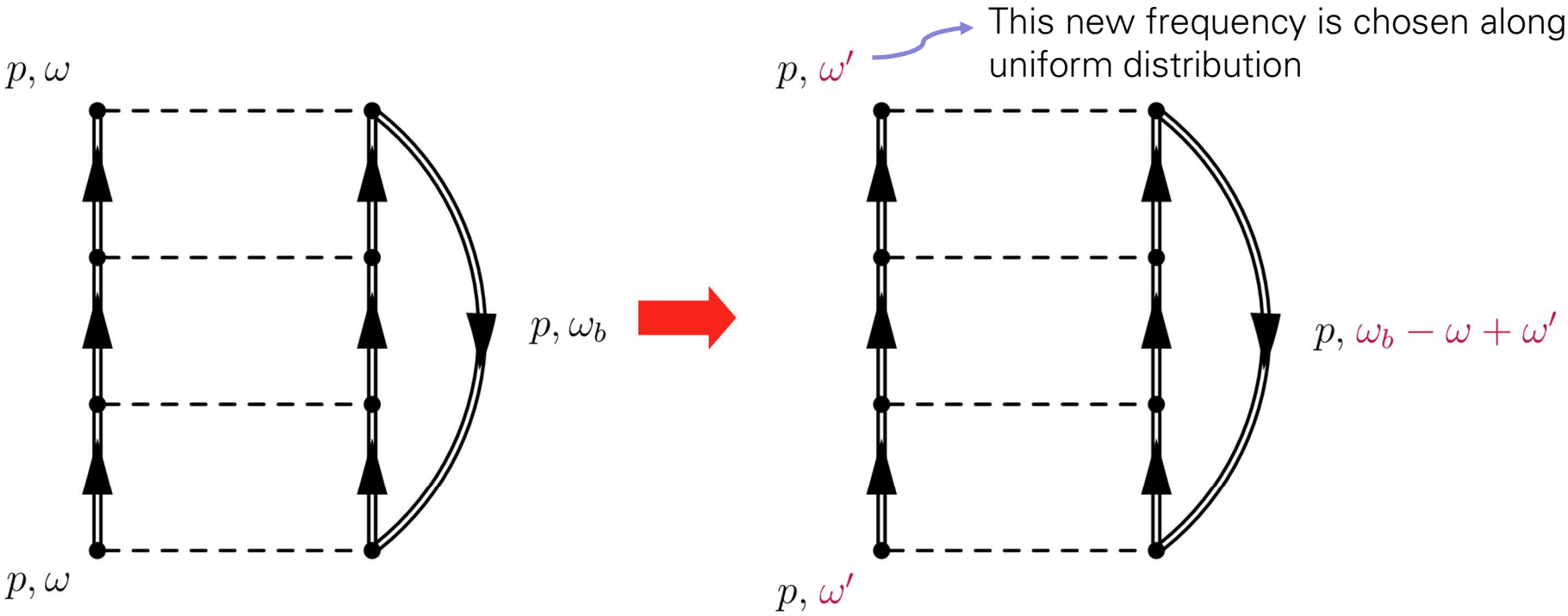
Error evaluation



The error due to a finite η dominates.

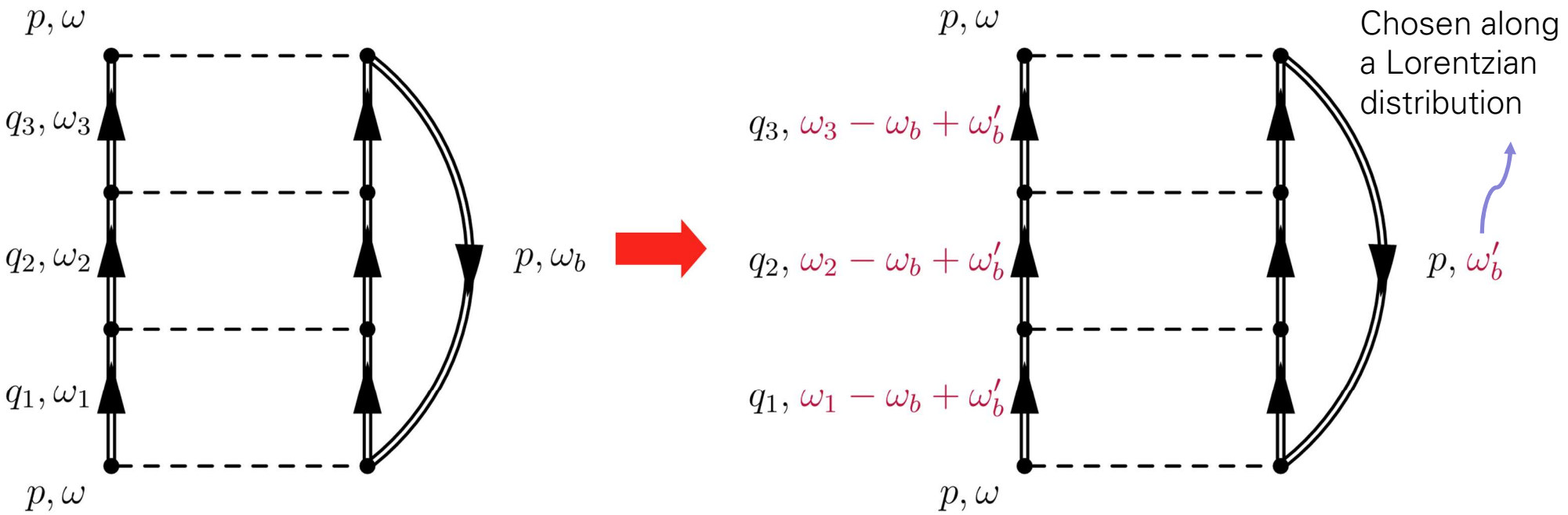
We checked this by propagating the error on the parameters of the fit with a Monte Carlo simulation.

Change ω



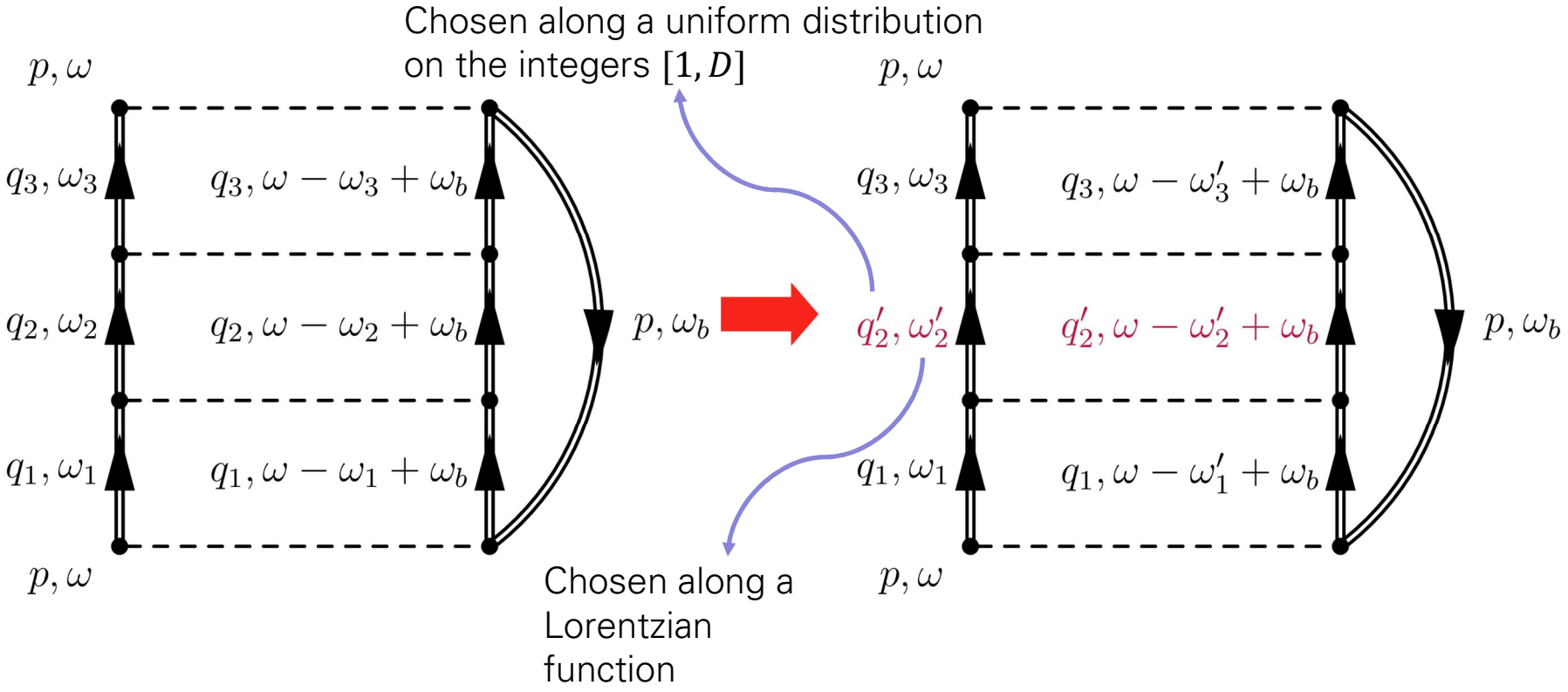
$$q_{C\omega} = \frac{|G_p(\omega_b - \omega + \omega')|}{|G_p(\omega_b)|}$$

Change internal frequencies



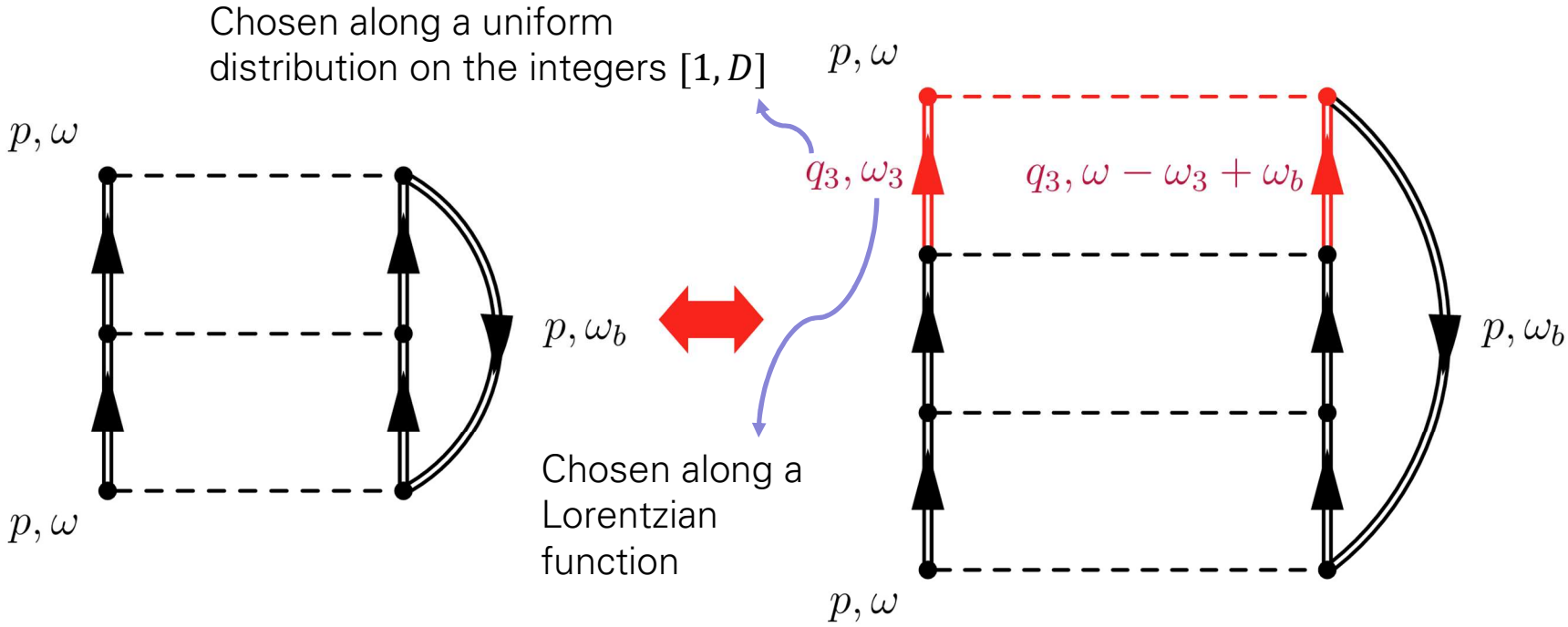
$$q_{\omega\ int} = \frac{L(\omega_b)}{L(\omega_b{}')} \frac{|G_p(\omega_b{}')|}{|G_p(\omega_b)|} \prod_{j=1}^{order-1} \frac{|G_{q_j}(\omega_j - \omega_b + \omega_b{}')|}{|G_{q_j}(\omega_j)|}$$

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



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

Dealing with $Z_{\alpha\beta}$

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

Normalization factor of the PDF of Feynman $Z_{\alpha\beta} = \int d\omega \int dC \, |D_{\alpha\beta}(\omega)|$ (i.e. their "weight").

- $Z_{\alpha\beta}$ is not known, however it can be estimated.
- If the weight of a subset S_N of diagrams (called normalization sector) is known, we can use the number of times S_N is visited ($\mathcal{N}$) to compute the normalization factor.

$$Z_{N\,\alpha\beta} = \int d\omega \int_{\mathcal{T}\in S_N} dC \, |D_{\alpha\beta}(\omega)| \qquad \lim_{N\to\infty} \frac{\mathcal{N}}{N} = \frac{Z_{N\,\alpha\beta}}{Z_{\alpha\beta}}$$

We arrive at the fundamental equation of DiagMC

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

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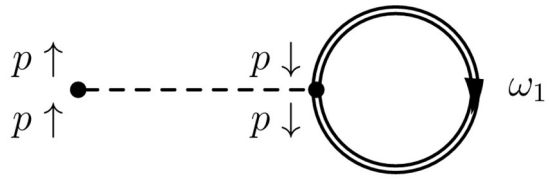
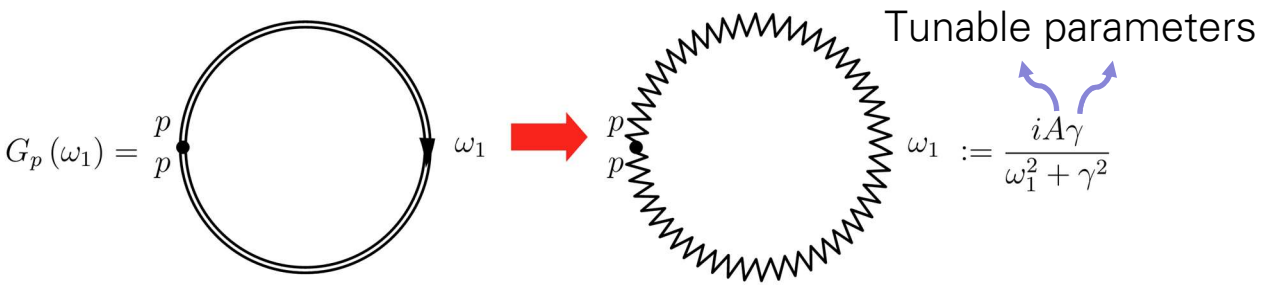
Normalization sector pt. 1/2

- We computed the tadpole diagram (i.e. the first order or Hartree-Fock) diagram *before* the simulation.



- We replace the self-closing propagator with an unphysical one (and exclude it from the self-energy expansion).



- This is needed because the HF diagram diverges without a convergence factor (difficult to handle numerically!).

Normalization sector pt. 2/2

- The weight of the normalization sector becomes $Z_N = \frac{|g|}{4} A(\omega_{Max} - \omega_{min})$.
- The result of the simulation is the dynamic (ω-dependent) self energy. To obtain the total one we simply combine the dynamic self-energy with the previously calculated Hartree-Fock diagram.