Open-shell medium-mass nuclei from ab-initio Green's function calculations

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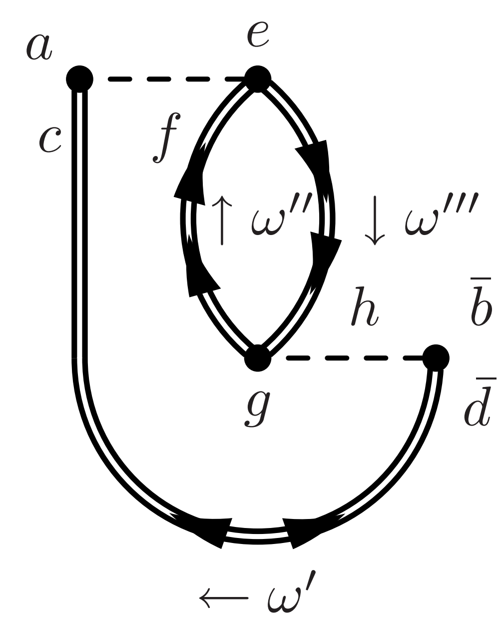


Based on:

VS, Duguet, Barbieri, PRC 84 064317 (2011)

"The Extreme Matter Physics of Nuclei:
From Universal Properties to Neutron-rich Extremes"

EMMI Program, GSI, 9 May 2012

Towards a unified description of nuclei

Ab-initio Green's functions

✤ How to extend to open-shell?

➟ this talk

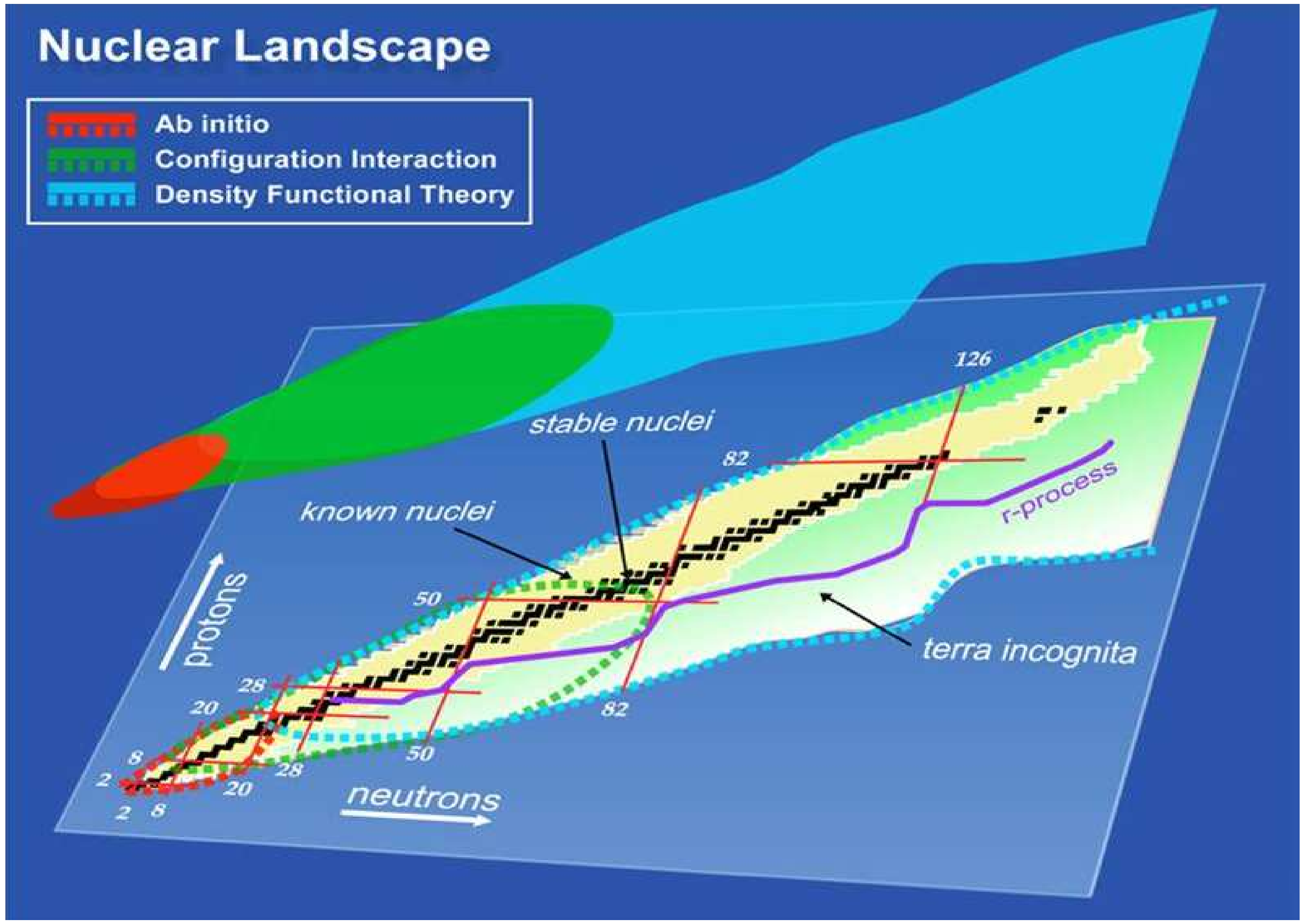
✤ How to link with EDF?

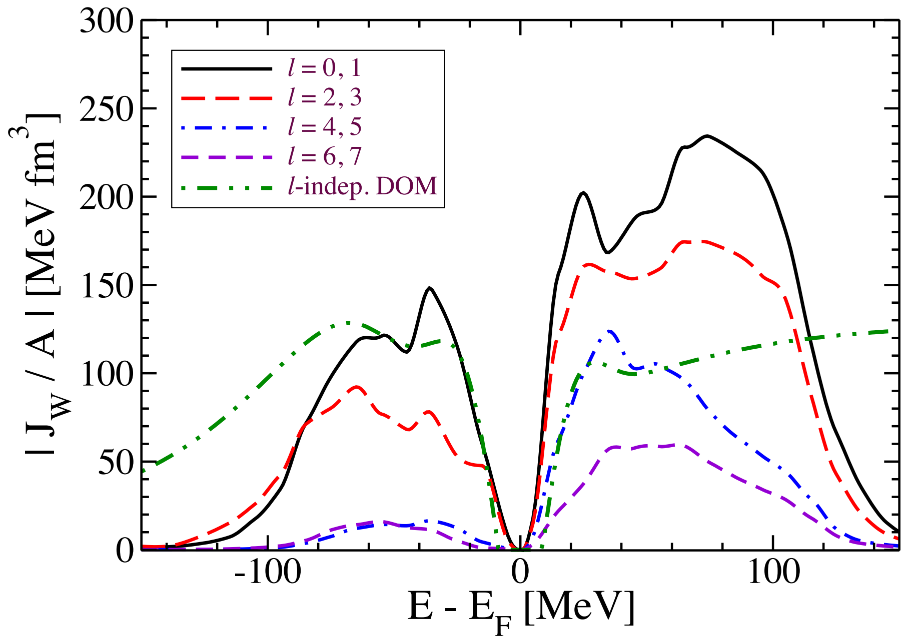
➟ link to DME

✤ How to calculate reactions?

➟ TD-GF [Rios *et al.* 2011]

➟ link to DOM





[Waldecker, Barbieri, Dickhoff 2011]

State-of-the-art ab-initio nuclear structure theory

✷ Methods for an ab-initio description of medium-mass nuclei

(1) Self-consistent Dyson-Green's function [Barbieri, Dickhoff, ...]

(2) Coupled-cluster [Dean, Hagen, Hjorth-Jensen, Papenbrock, ...]

(3) In-medium similarity renormalization group [Tsukiyama, Bogner, Schwenk, ...]

→ Similar level of accuracy

→ But limited to to doubly-closed-shell ± 1 and ± 2 nuclei

✷ Truly open-shell nuclei

(a) Multi-reference methods: IMSRG + CI, MR-CC, microscopic VS-SM

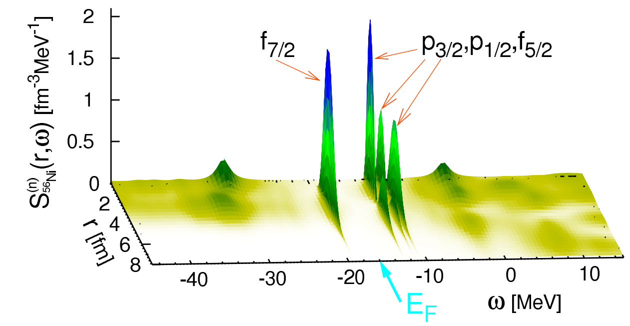
(b) Single-reference methods: explicit account of pairing mandatory

→ Dyson-Green's functions ⟶ Gorkov-Green's functions

Dyson Green's functions

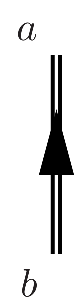
- ✺ Spectral function

$$S_a^-(\omega) \equiv \sum_k \left| \langle \psi_k^{N-1} | a_a | \psi_0^N \rangle \right|^2 \delta(\omega - (E_0^N - E_k^{N-1})) = \frac{1}{\pi} \, \mathrm{Im} \, G_{aa}(\omega)$$



- ✺ Green's function

$$\boxed{i \, G_{ab}(t,t') \equiv \langle \Psi_0^N | T \left\{ a_a(t) a_b^\dagger(t') \right\} | \Psi_0^N \rangle} \quad \equiv$$



- ➟ N-particle ground state
- ➟ One nucleon addition and removal (N±1 systems)

- ✺ Dyson equation

$$\boxed{G_{ab}(\omega) = G_{ab}^{(0)}(\omega) + \sum_{cd} G_{ac}^{(0)}(\omega) \, \Sigma_{cd}^\star(\omega) \, G_{db}(\omega)}$$

Solution breaks down when pairing instabilities appear

Going open-shell: Gorkov ansatz

✳ Formulate the expansion scheme around a Bogoliubov vacuum

→ Zeroth order already incorporates pairing

✳ Auxiliary many-body state $|\Psi_0\rangle \equiv \sum_N^{\text{even}} c_N \, |\psi_0^N\rangle$

→ Mixes various particle numbers

→ Introduce a “grand-canonical” potential $\Omega = H - \mu N$

⇒ $|\Psi_0\rangle$ minimizes $\Omega_0 = \langle \Psi_0 | \Omega | \Psi_0 \rangle$

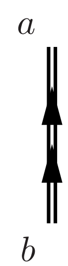
under the constraint $N = \langle \Psi_0 | N | \Psi_0 \rangle$

⇒ $\Omega_0 = \sum_{N'} |c_{N'}|^2 \Omega_0^{N'} \approx E_0^N - \mu N$

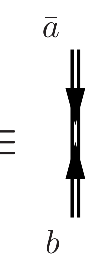
Gorkov Green's functions and equations

✺ Set of 4 Green's functions

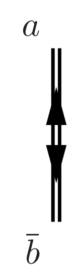
$$i\, G^{11}_{ab}(t,t') \equiv \langle \Psi_0 | T \left\{ a_a(t) a^\dagger_b(t') \right\} | \Psi_0 \rangle \quad \equiv$$



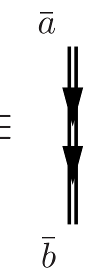
$$i\, G^{21}_{ab}(t,t') \equiv \langle \Psi_0 | T \left\{ \bar{a}^\dagger_a(t) a^\dagger_b(t') \right\} | \Psi_0 \rangle \quad \equiv$$



$$i\, G^{12}_{ab}(t,t') \equiv \langle \Psi_0 | T \left\{ a_a(t) \bar{a}_b(t') \right\} | \Psi_0 \rangle \quad \equiv$$



$$i\, G^{22}_{ab}(t,t') \equiv \langle \Psi_0 | T \left\{ \bar{a}^\dagger_a(t) \bar{a}_b(t') \right\} | \Psi_0 \rangle \quad \equiv$$



[Gorkov 1958]

$$\mathbf{G}_{ab}(\omega) = \mathbf{G}^{(0)}_{ab}(\omega) + \sum_{cd} \mathbf{G}^{(0)}_{ac}(\omega)\, \mathbf{\Sigma}^\star_{cd}(\omega)\, \mathbf{G}_{db}(\omega)$$

Gorkov equations

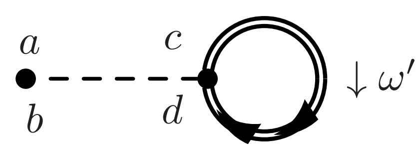
$$\mathbf{\Sigma}^\star_{ab}(\omega) \equiv \begin{pmatrix} \Sigma^{\star\,11}_{ab}(\omega) & \Sigma^{\star\,12}_{ab}(\omega) \\ \Sigma^{\star\,21}_{ab}(\omega) & \Sigma^{\star\,22}_{ab}(\omega) \end{pmatrix}$$

$$\mathbf{\Sigma}^\star_{ab}(\omega) \equiv \mathbf{\Sigma}_{ab}(\omega) - \mathbf{U}_{ab}$$

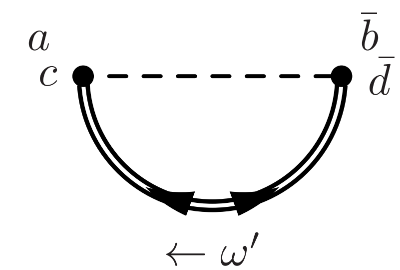
1st & 2nd order diagrams and eigenvalue problem

✺ 1st order ➟ energy-independent self-energy

$\Sigma^{11\,(1)}_{ab} =$

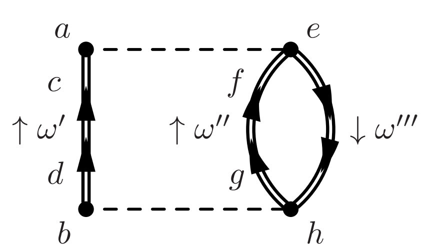


$\Sigma^{12\,(1)}_{ab} =$



✺ 2nd order ➟ energy-dependent self-energy

$\Sigma^{11\,(2)}_{ab}(\omega) =$



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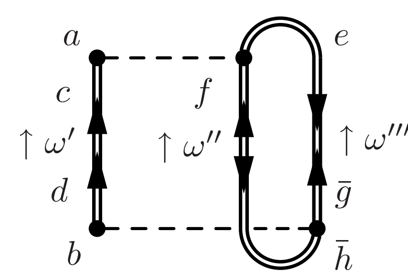
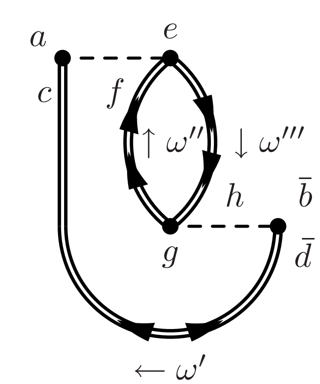


$\Sigma^{12\,(2)}_{ab}(\omega) =$



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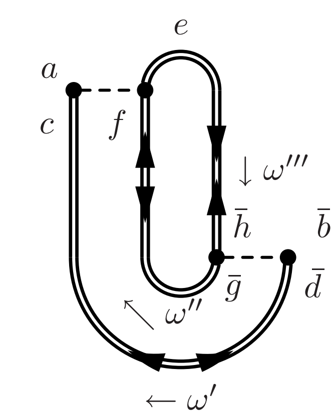


✺ Gorkov equations ⟶ eigenvalue problem

$$\boxed{\sum_b \begin{pmatrix} t_{ab} - \mu_{ab} + \Sigma^{11}_{ab}(\omega) & \Sigma^{12}_{ab}(\omega) \\ \Sigma^{21}_{ab}(\omega) & -t_{ab} + \mu_{ab} + \Sigma^{22}_{ab}(\omega) \end{pmatrix}\Bigg|_{\omega_k} \begin{pmatrix} \mathcal{U}^k_b \\ \mathcal{V}^k_b \end{pmatrix} = \omega_k \begin{pmatrix} \mathcal{U}^k_a \\ \mathcal{V}^k_a \end{pmatrix}}$$

$$\mathcal{U}^{k*}_a \equiv \langle \Psi_k | \bar{a}^\dagger_a | \Psi_0 \rangle$$
$$\mathcal{V}^{k*}_a \equiv \langle \Psi_k | a_a | \Psi_0 \rangle$$

Gorkov equations

$$\sum_b \begin{pmatrix} t_{ab} - \mu_{ab} + \Sigma^{11}_{ab}(\omega) & \Sigma^{12}_{ab}(\omega) \\ \Sigma^{21}_{ab}(\omega) & -t_{ab} + \mu_{ab} + \Sigma^{22}_{ab}(\omega) \end{pmatrix}\Bigg|_{\omega_k} \begin{pmatrix} \mathcal{U}^k_b \\ \mathcal{V}^k_b \end{pmatrix} = \omega_k \begin{pmatrix} \mathcal{U}^k_a \\ \mathcal{V}^k_a \end{pmatrix}$$

$$\Downarrow$$

$$\boxed{\begin{pmatrix} T - \mu + \Lambda & \tilde{h} & \mathcal{C} & -\mathcal{D}^\dagger \\ \tilde{h}^\dagger & -T + \mu - \Lambda & -\mathcal{D}^\dagger & \mathcal{C} \\ \mathcal{C}^\dagger & -\mathcal{D} & E & 0 \\ -\mathcal{D} & \mathcal{C}^\dagger & 0 & -E \end{pmatrix} \begin{pmatrix} \mathcal{U}^k \\ \mathcal{V}^k \\ \mathcal{W}_k \\ \mathcal{Z}_k \end{pmatrix} = \omega_k \begin{pmatrix} \mathcal{U}^k \\ \mathcal{V}^k \\ \mathcal{W}_k \\ \mathcal{Z}_k \end{pmatrix}}$$

Energy *independent* eigenvalue problem

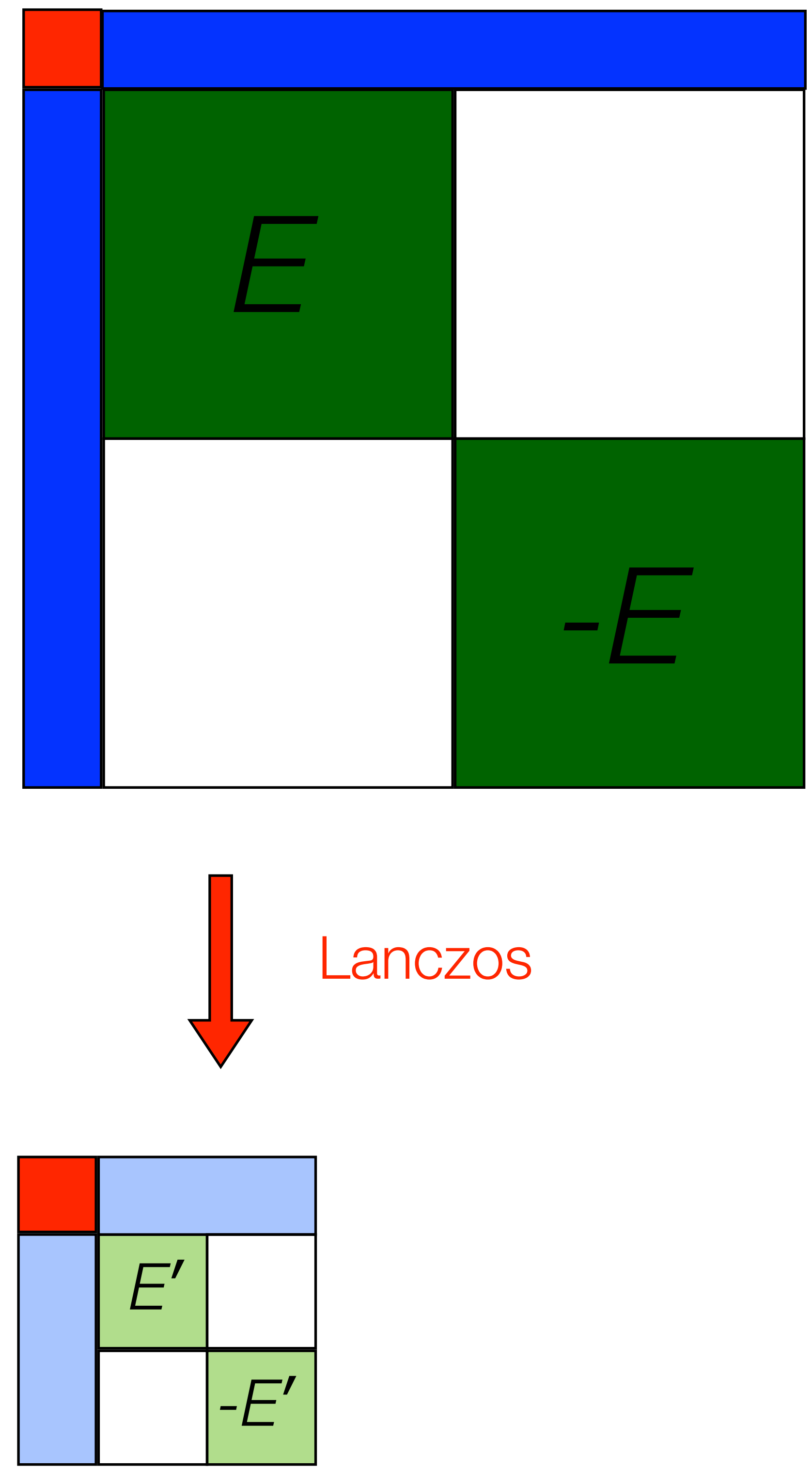
with the normalization condition $\sum_a \left[\left|\mathcal{U}^k_a\right|^2 + \left|\mathcal{V}^k_a\right|^2 \right] + \sum_{k_1 k_2 k_3} \left[\left|\mathcal{W}^{k_1 k_2 k_3}_k\right|^2 + \left|\mathcal{Z}^{k_1 k_2 k_3}_k\right|^2 \right] = 1$

How do we select the poles?

We do not...

➟ Lanczos projection of Gorkov matrix

$$\begin{pmatrix} T-\mu+\Lambda & \tilde{h} & \mathcal{C} & -\mathcal{D}^\dagger \\ \tilde{h}^\dagger & -T+\mu-\Lambda & -\mathcal{D}^\dagger & \mathcal{C} \\ \mathcal{C}^\dagger & -\mathcal{D} & E & 0 \\ -\mathcal{D} & \mathcal{C}^\dagger & 0 & -E \end{pmatrix} \begin{pmatrix} \mathcal{U}^k \\ \mathcal{V}^k \\ \mathcal{W}_k \\ \mathcal{Z}_k \end{pmatrix} = \omega_k \begin{pmatrix} \mathcal{U}^k \\ \mathcal{V}^k \\ \mathcal{W}_k \\ \mathcal{Z}_k \end{pmatrix}$$

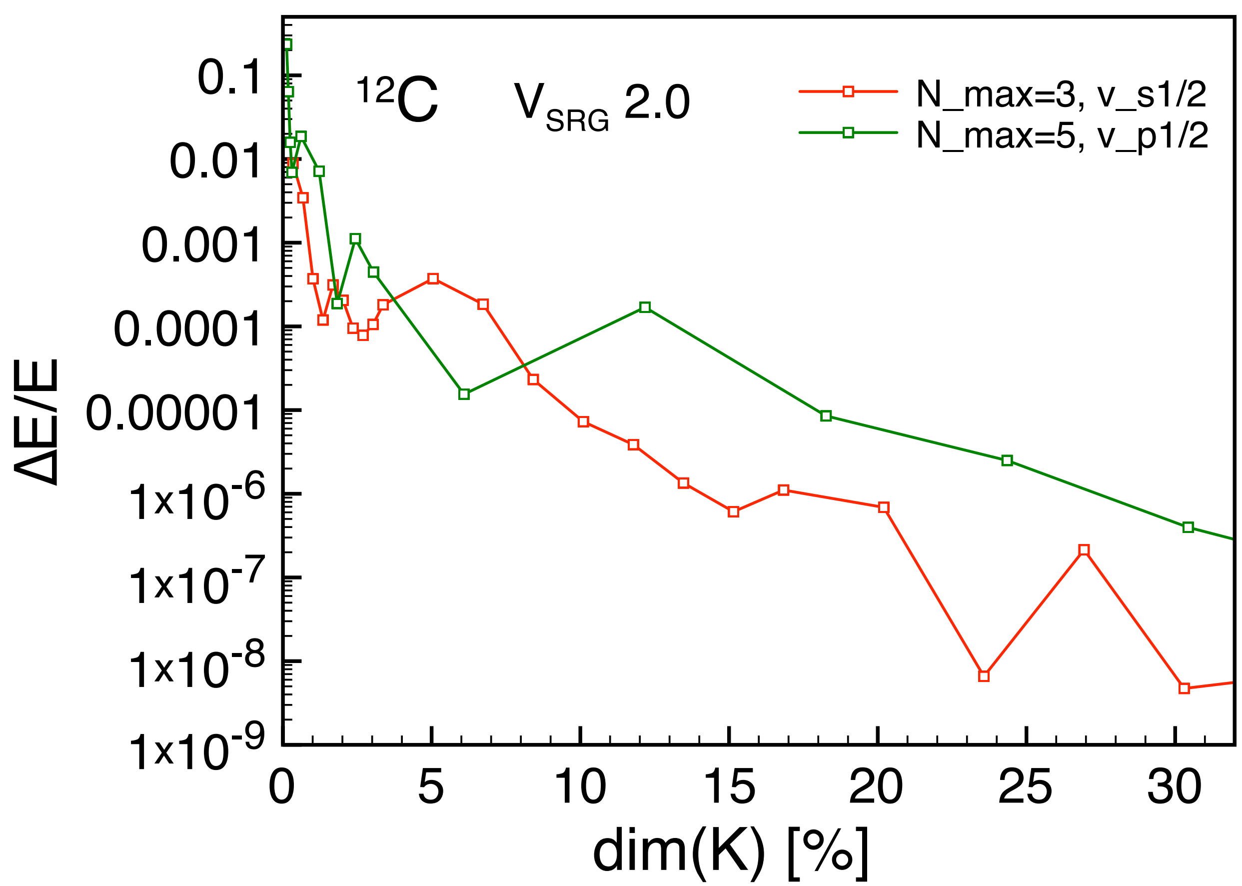


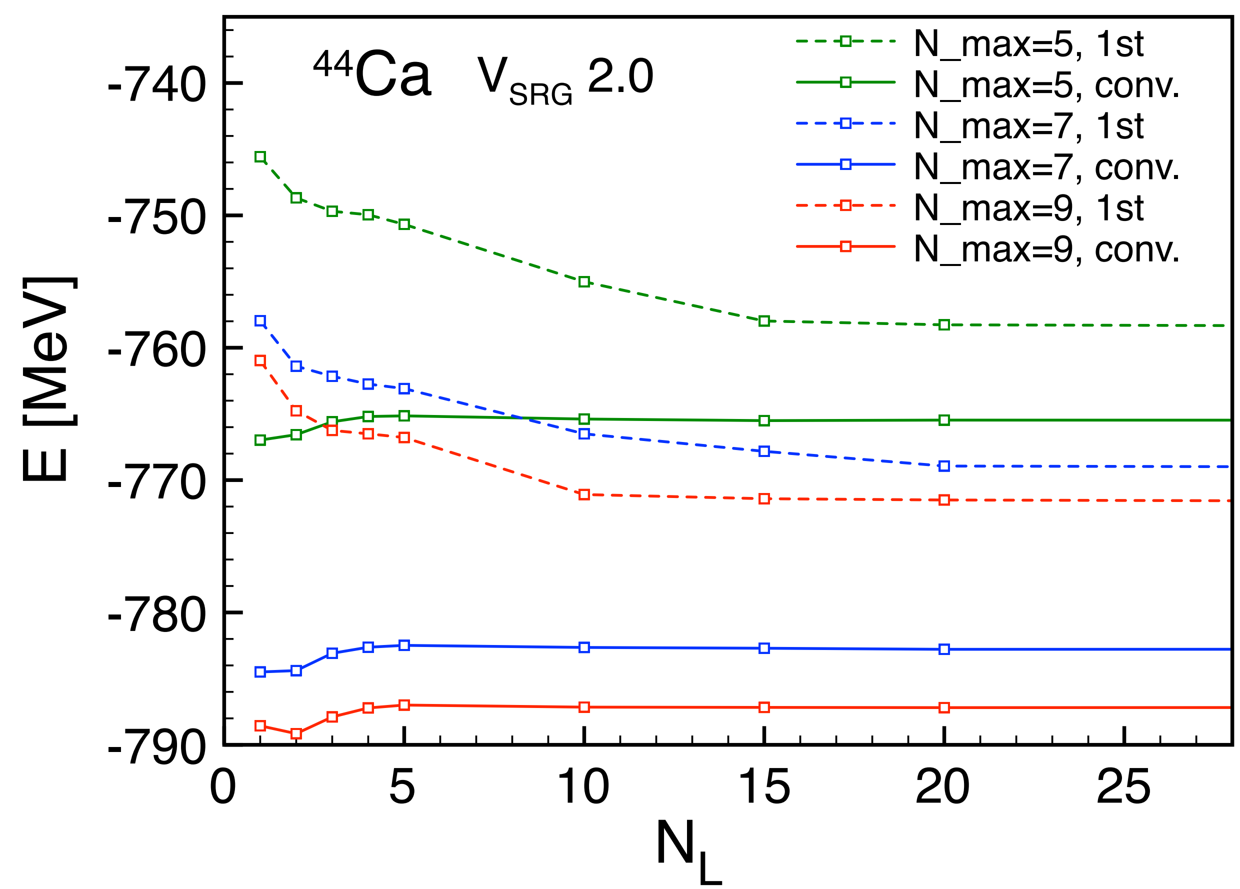
➟ Conserves moments of spectral functions

➟ Equivalent to exact diagonalization for $N_L \to \dim(E)$

Testing Lanczos projection

✺ Good convergence towards exact diagonalization

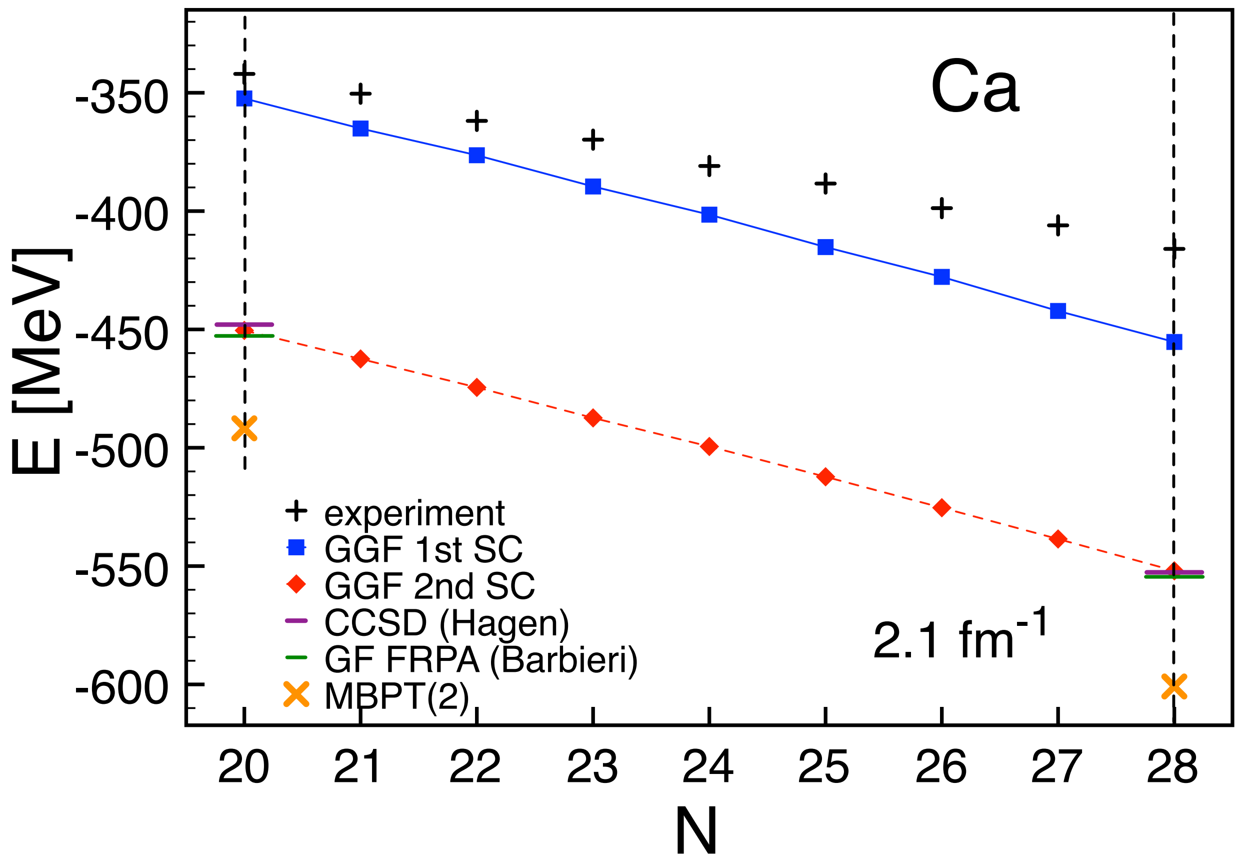


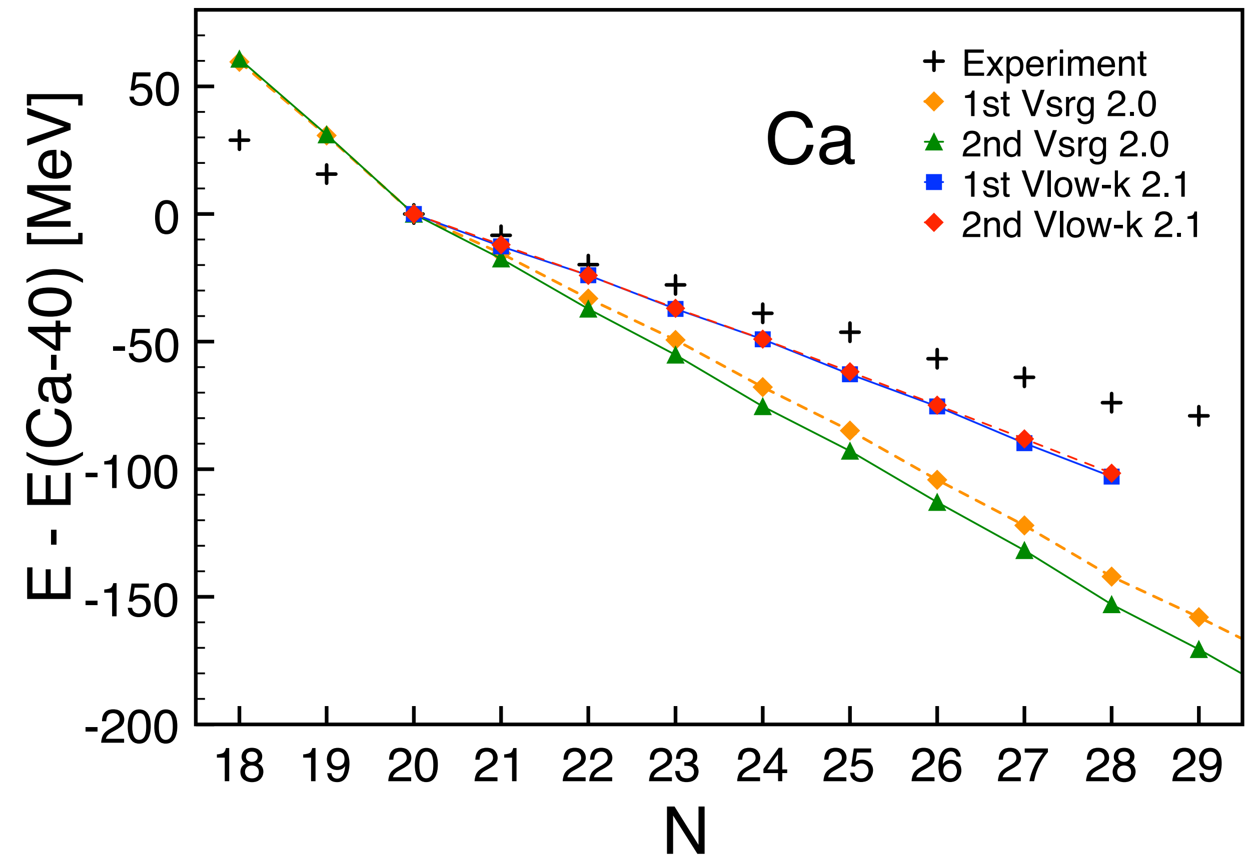


➟ Self-consistency cures results for low N_L

Binding energies

✺ Systematic along isotopic/isotonic chains become available





➟ Overbinding with A: traces need for (at least) NNN forces

Spectrum and spectroscopic factors

✳ Separation energy spectrum

$$G^{11}_{ab}(\omega) = \sum_k \left\{ \frac{\mathcal{U}^k_a \, \mathcal{U}^{k*}_b}{\omega - \omega_k + i\eta} + \frac{\bar{\mathcal{V}}^{k*}_a \, \bar{\mathcal{V}}^k_b}{\omega + \omega_k - i\eta} \right\}$$

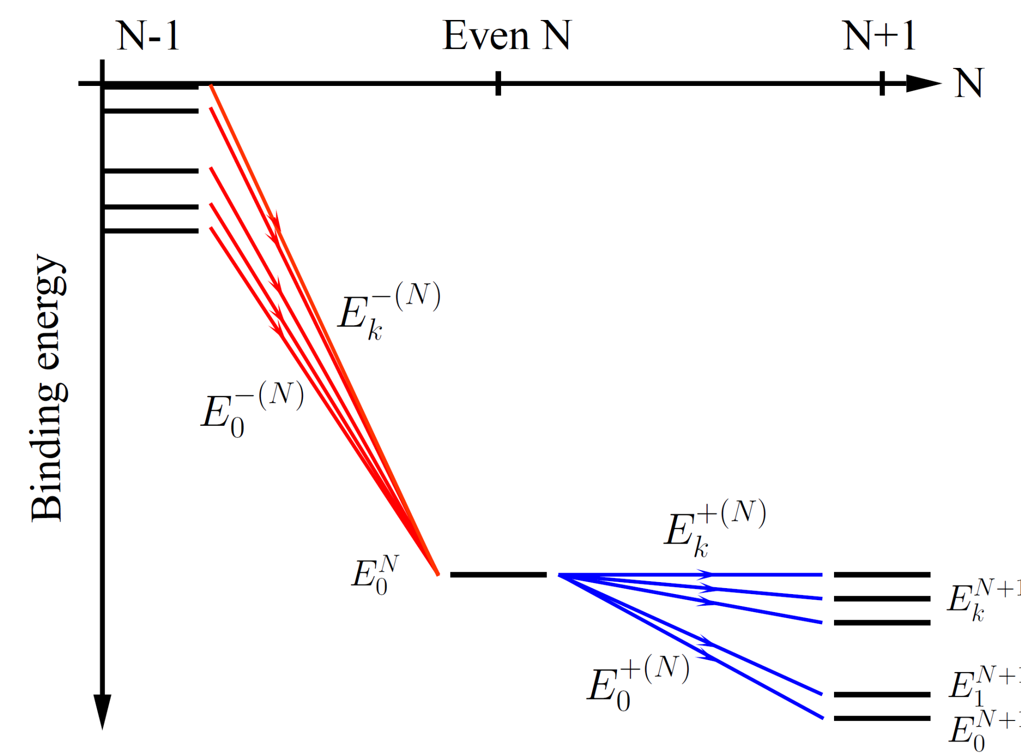
Lehmann representation

where
$$\begin{cases} \mathcal{U}^{k*}_a \equiv \langle \Psi_k | a^\dagger_a | \Psi_0 \rangle \\ \mathcal{V}^{k*}_a \equiv \langle \Psi_k | \bar{a}_a | \Psi_0 \rangle \end{cases}$$

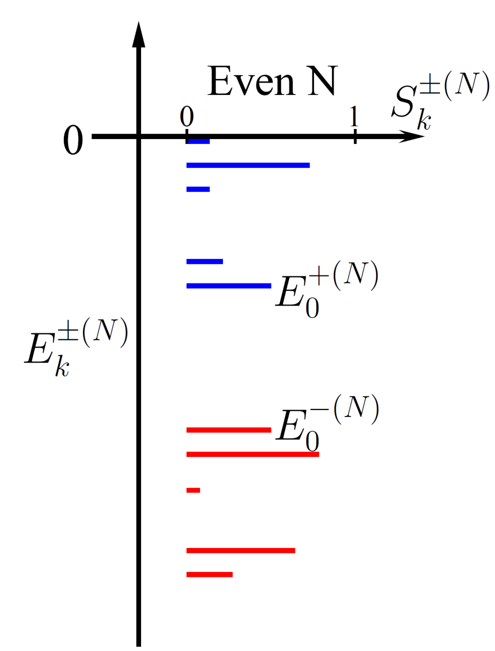
and
$$\begin{cases} E^{+\,(N)}_k \equiv E^{N+1}_k - E^N_0 \\ E^{-\,(N)}_k \equiv E^N_0 - E^{N-1}_k \end{cases}$$

✳ Spectroscopic factors

$$\mathcal{S}^+_k \equiv \sum_a \left| \langle \psi_k | a^\dagger_a | \psi_0 \rangle \right|^2 = \sum_a \left| \mathcal{U}^k_a \right|^2$$
$$\mathcal{S}^-_k \equiv \sum_a \left| \langle \psi_k | a_a | \psi_0 \rangle \right|^2 = \sum_a \left| \mathcal{V}^k_a \right|^2$$

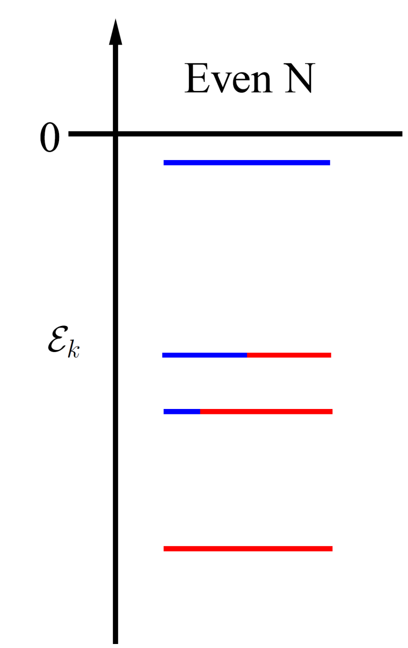


Separation energies + transfer strengths



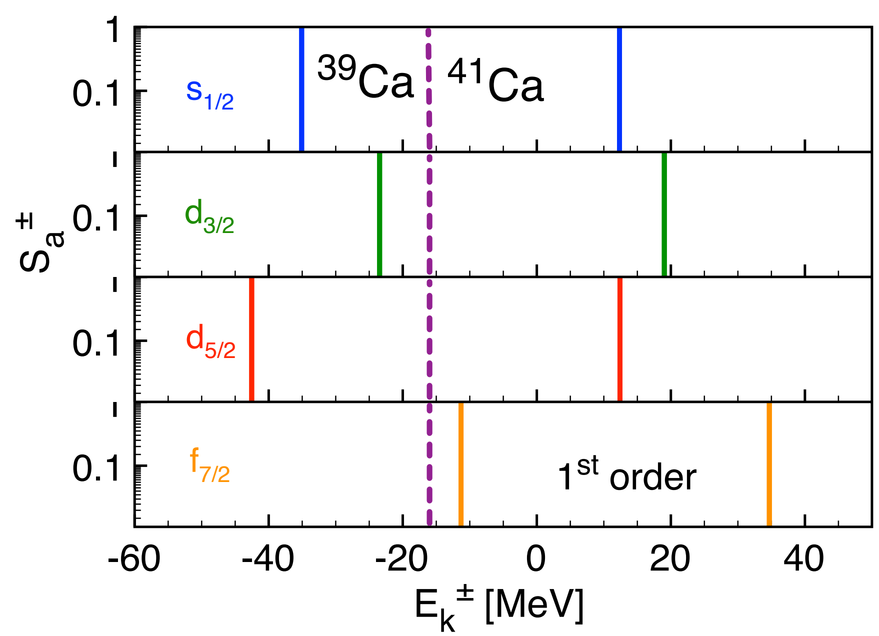
Centroids

ESPE



Spectral function

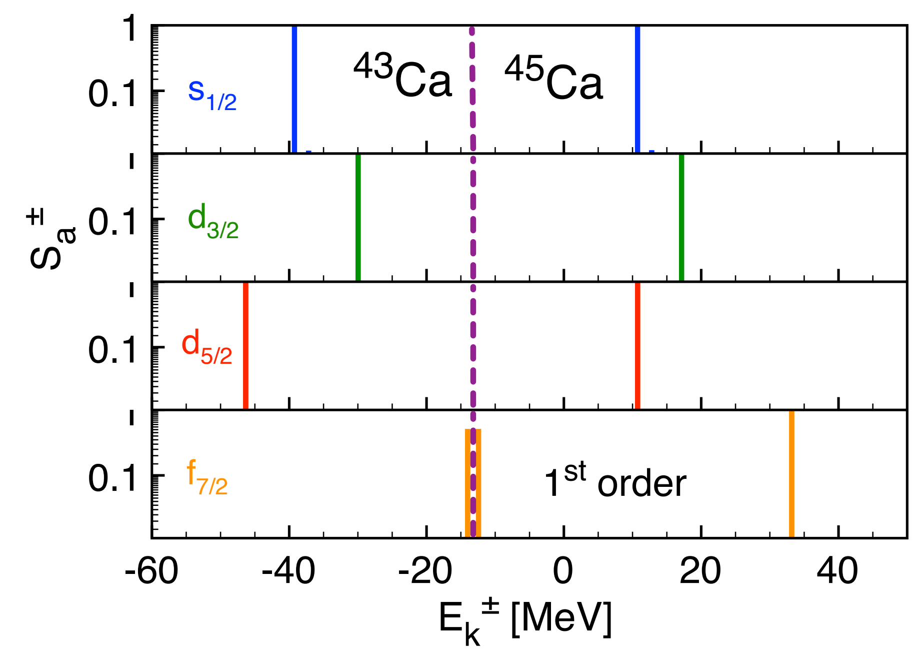
Dyson 1st order (HF)



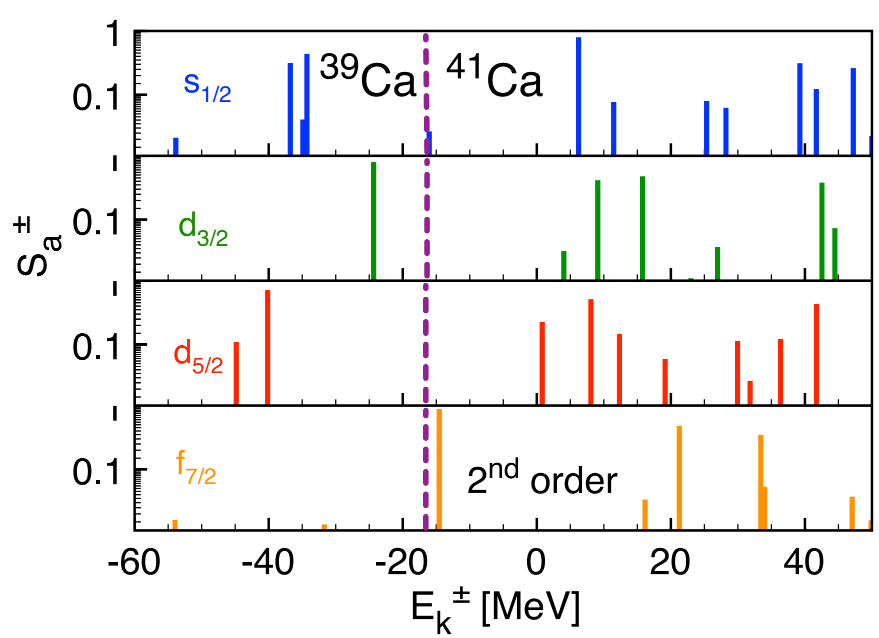
Fragmentation

Static pairing

Gorkov 1st order (HFB)

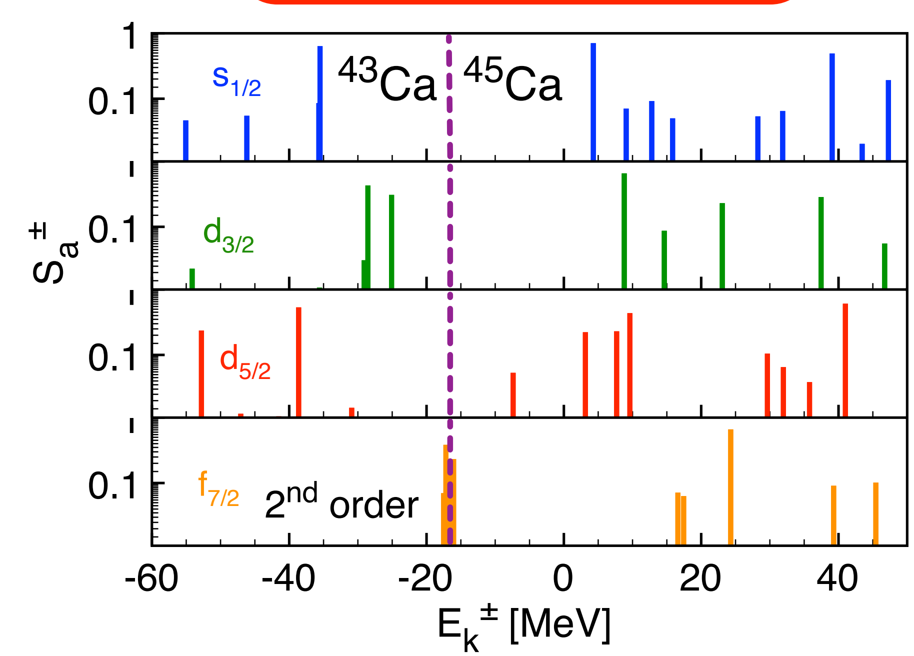


Dyson 2nd order



Dynamical fluctuations

Gorkov 2nd order



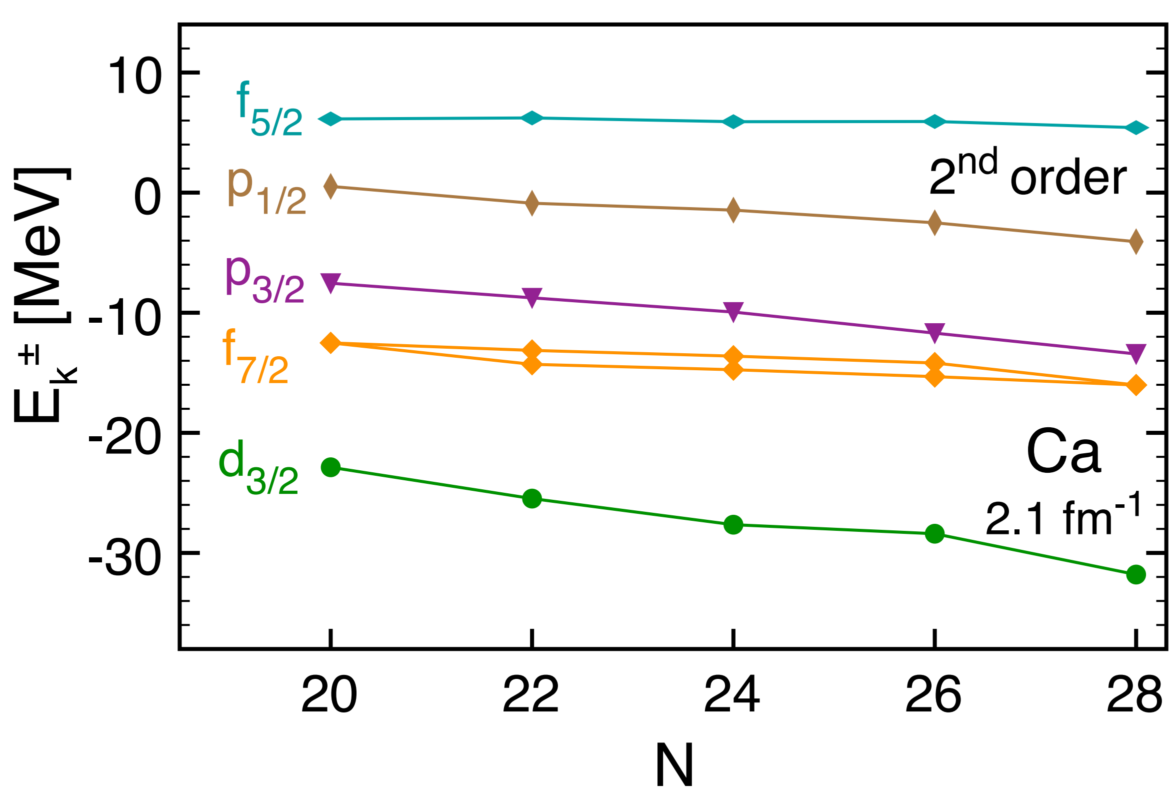
Shell structure evolution

✺ ESPE collect fragmentation of “single-particle” strengths from both N±1

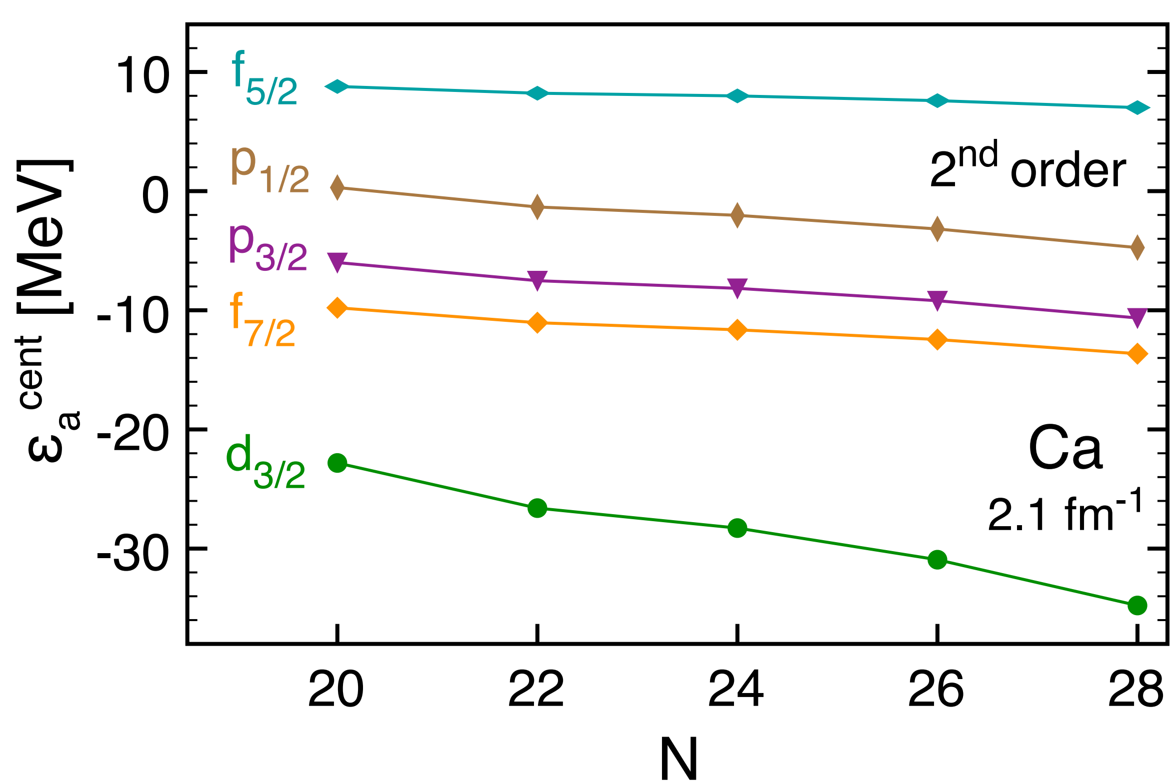
$$\epsilon_a^{cent} \equiv h_{ab}^{cent}\,\delta_{ab} = t_{aa} + \sum_{cd} \bar{V}^{NN}_{acad}\,\rho^{[1]}_{dc} + \sum_{cdef} \bar{V}^{NNN}_{acdaef}\,\rho^{[2]}_{efcd} \equiv \sum_k \mathcal{S}_k^{+a} E_k^+ + \sum_k \mathcal{S}_k^{-a} E_k^-$$

[Baranger 1970, Duguet *et al*. 2011]

Quasiparticle peaks

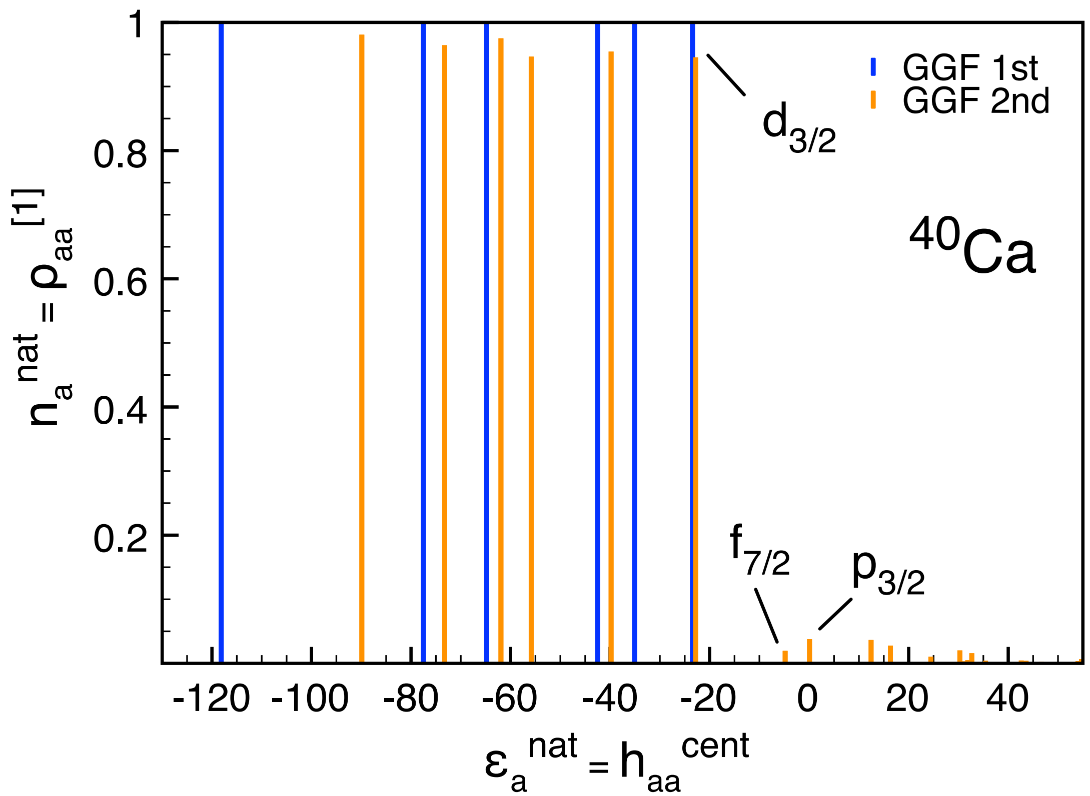


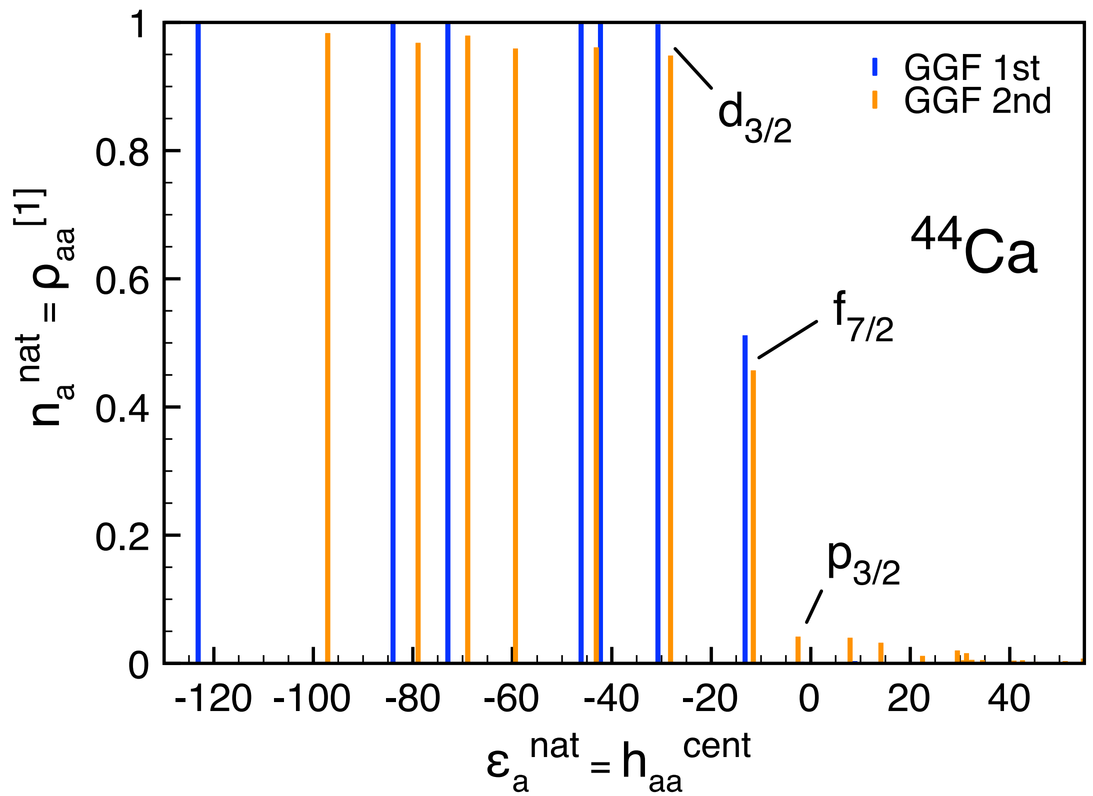
Centroids



Natural single-particle occupation

- Natural orbit *a*: $\rho_{ab}^{[1]} = n_a^{nat}\, \delta_{ab}$
- Associated energy: $\varepsilon_a^{nat} = h_{aa}^{cent}$





- Dynamical correlations similar for doubly-magic and semi-magic
- Static pairing essential to open-shells

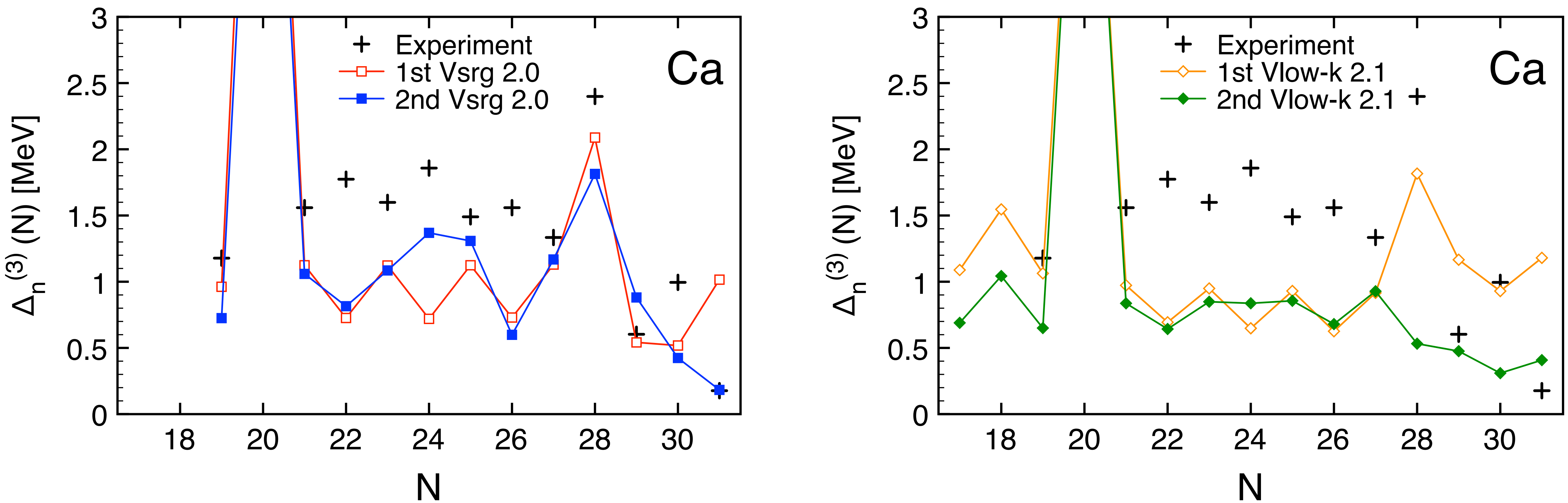
Pairing gap

✳ Three-point mass differences

$$\Delta_n^{(3)}(N) = \boxed{\frac{(-1)^N}{2}\frac{\partial\,\mu_n}{\partial\,N}} + \boxed{\Delta_n}$$

Generates O-E oscillations

Actual pairing gaps



☝ Proof-of-principle only (larger model space needed!)

➠ Systematic underestimation of experimental gaps

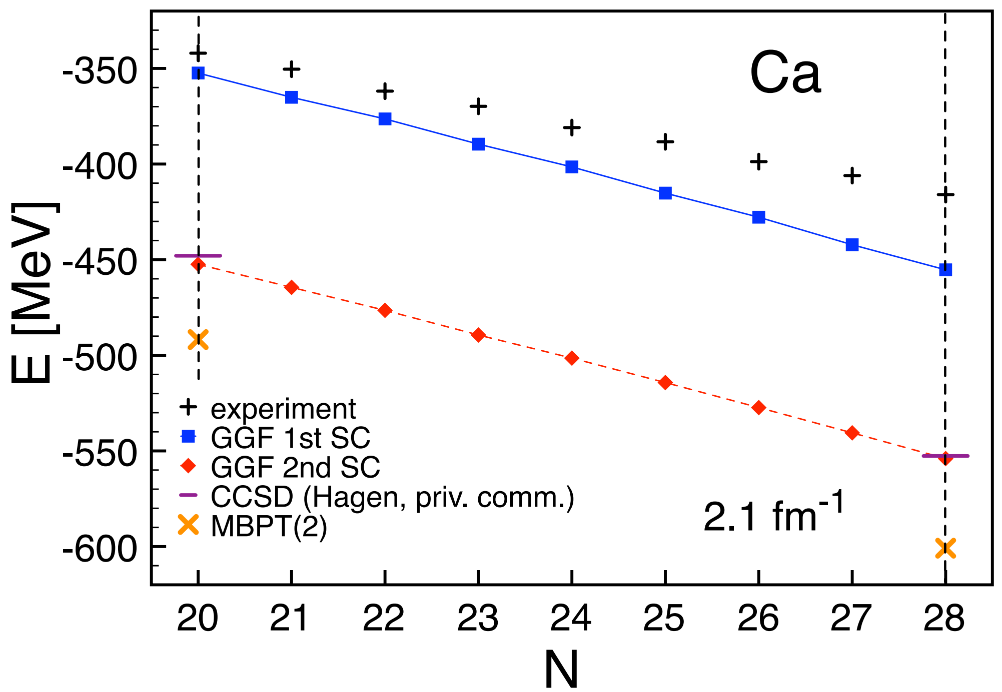
➠ Missing 3rd order and NNN should change picture qualitatively

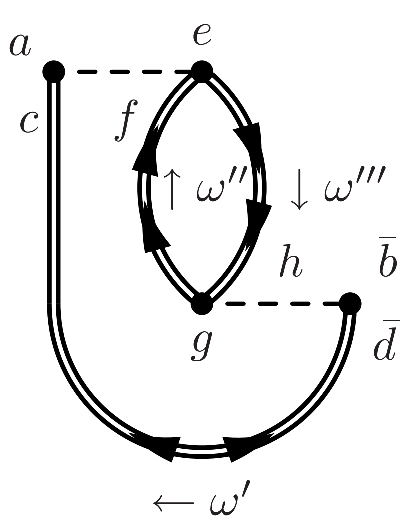
Conclusions & Outlook

✷ Gorkov-Green's functions:
first ab-initio open-shell calculations

✷ Provide optical potentials
for reaction models

✷ Provide constraints for next-generation
Energy Density Functionals





✷ Implementation of three-body forces

✷ Formulation of particle-number restored Gorkov theory

✷ Improvement of the self-energy expansion