Ab-initio Green's function calculations of open-shell medium-mass nuclei

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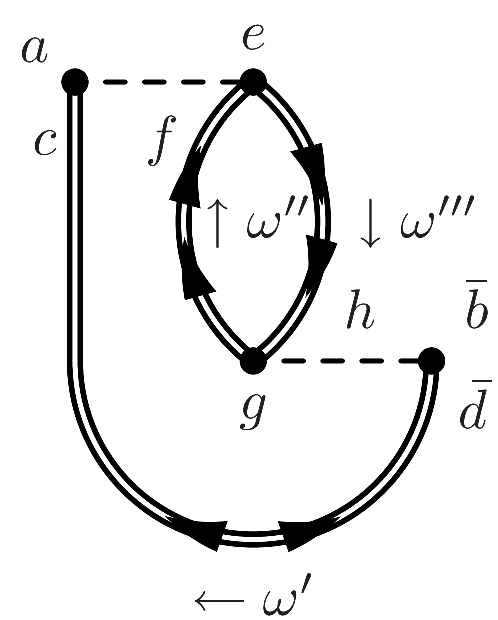


Based on:

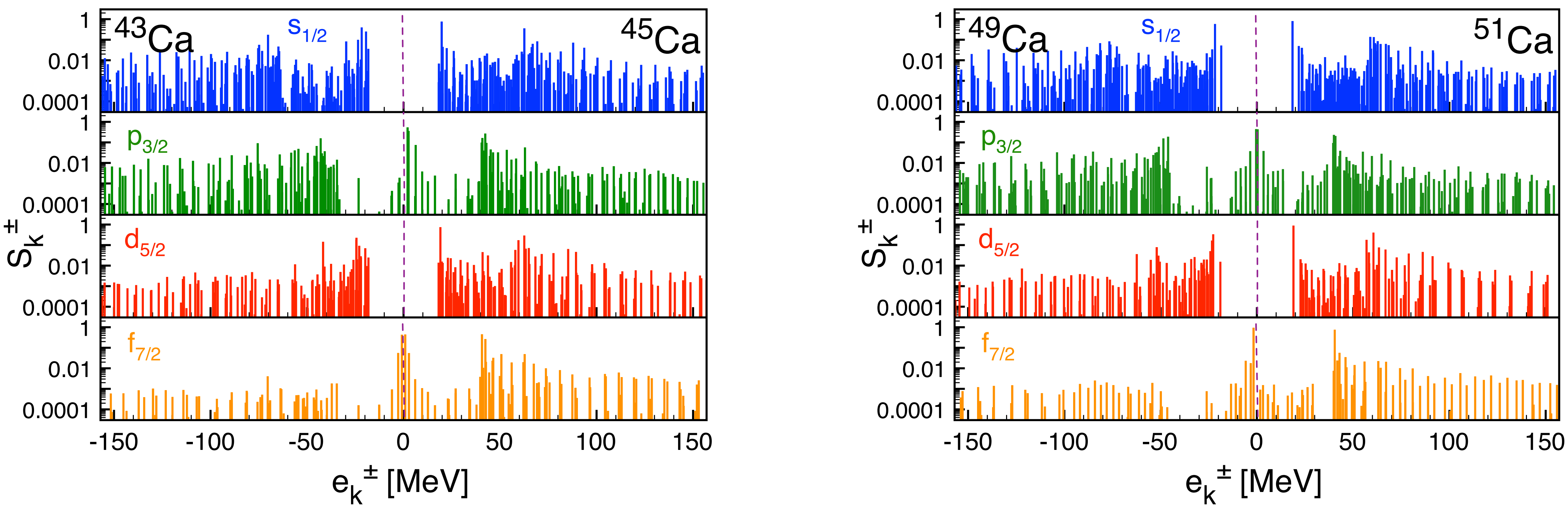
VS, Duguet, Barbieri, PRC 84 064317 (2011)

EURORIB 12

Abano Terme, 22 May 2012

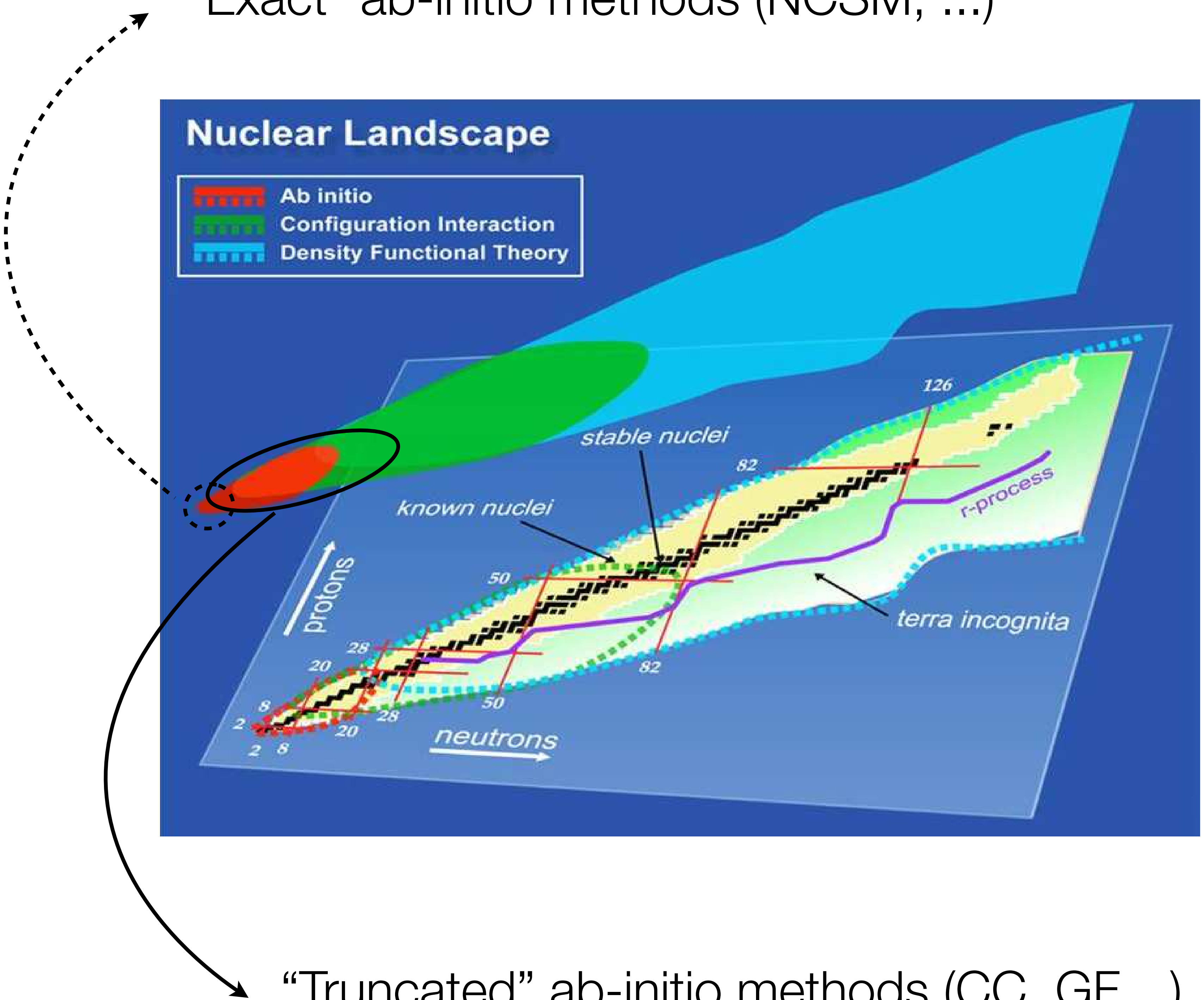
Punch line

✺ First ab-initio calculations of open-shell, medium-mass nuclei



Theoretical approaches to the nuclear chart

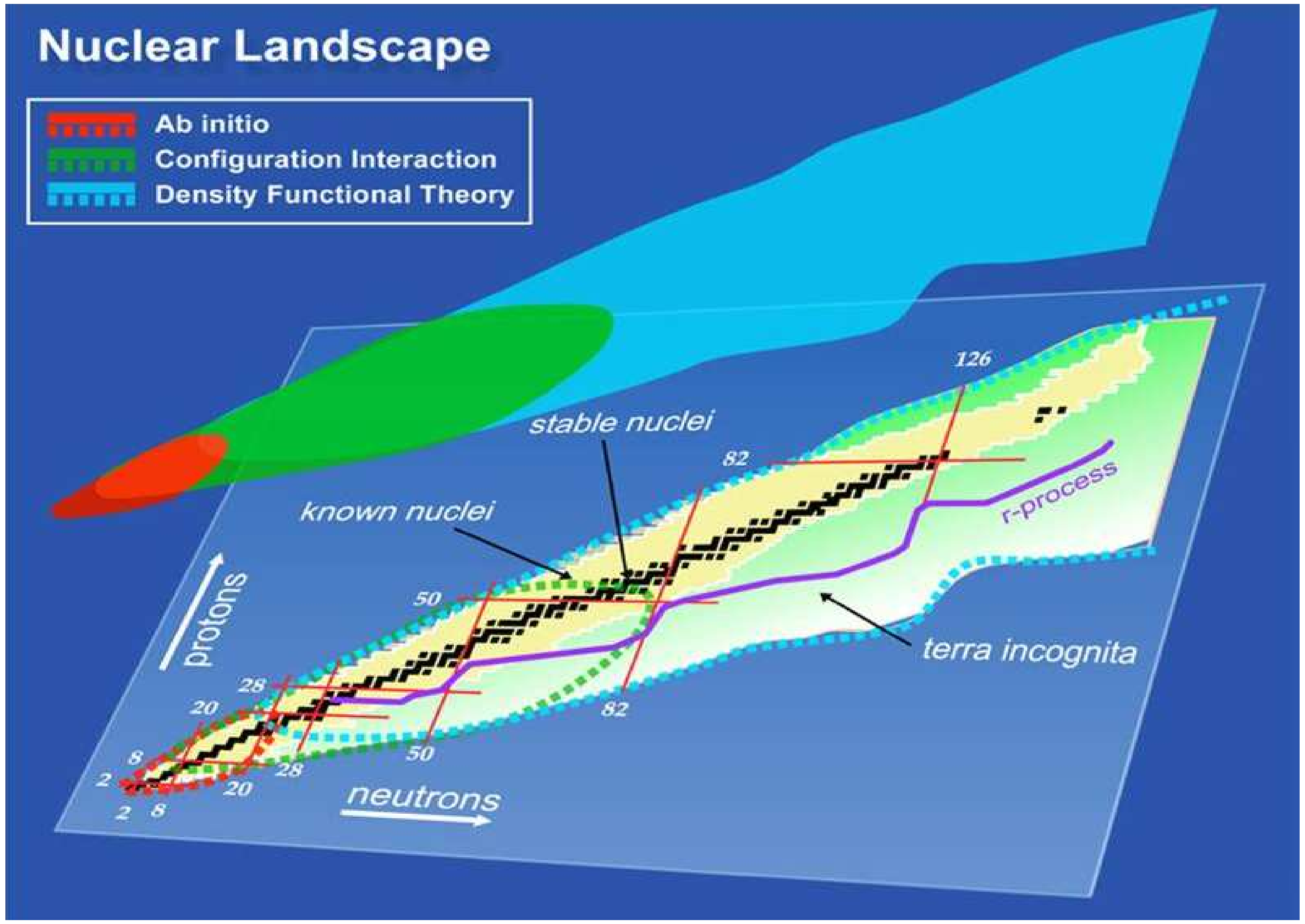
“Exact” ab-initio methods (NCSM, ...)



“Truncated” ab-initio methods (CC, GF, ..)

Towards a unified description of nuclei

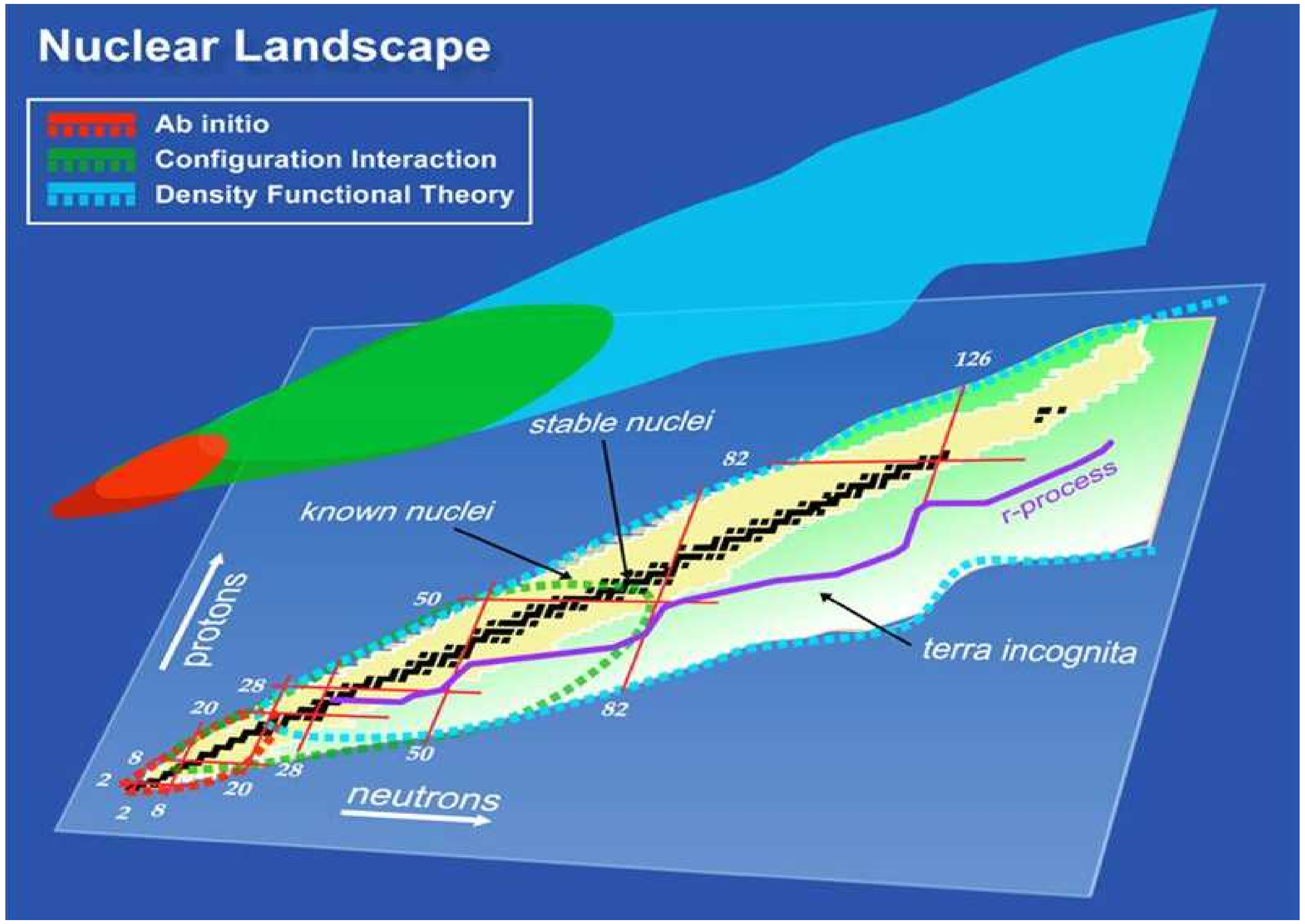
- ✤ How to extend to open-shell?
- ✤ How to link with EDF?
- ✤ How to calculate reactions?

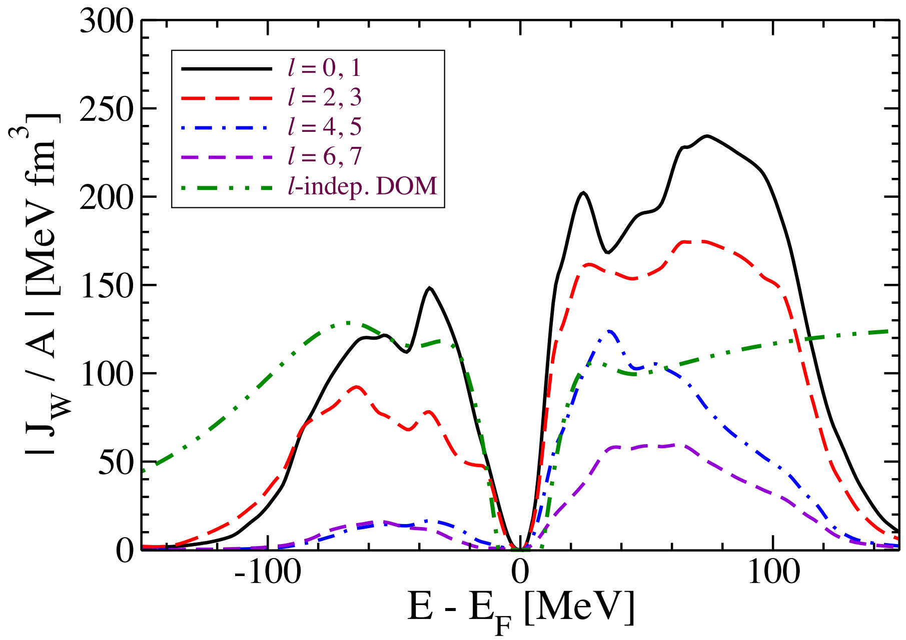


Towards a unified description of nuclei

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





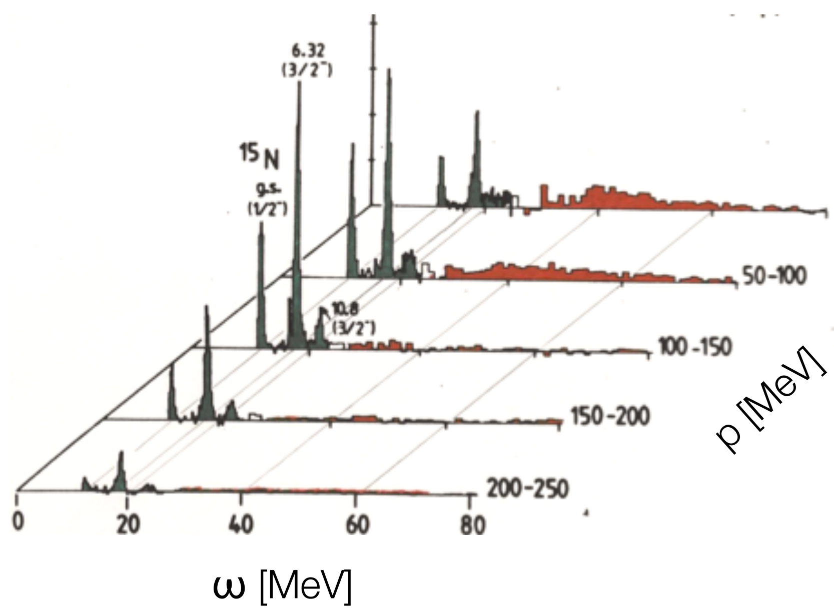
[Waldecker, Barbieri, Dickhoff 2011]

Green's functions

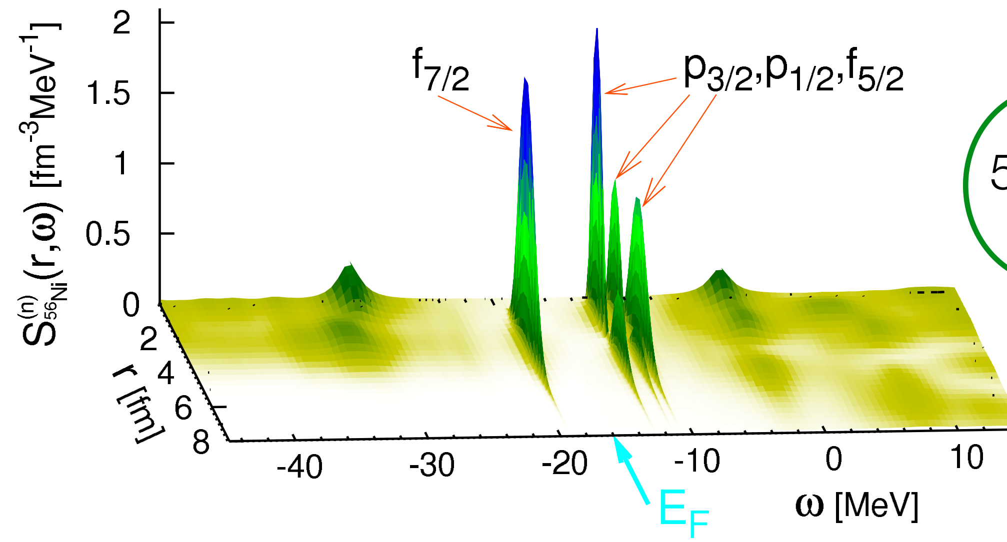
- Spectral function

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

^{16}O



[Mougey *et al.* 1980]



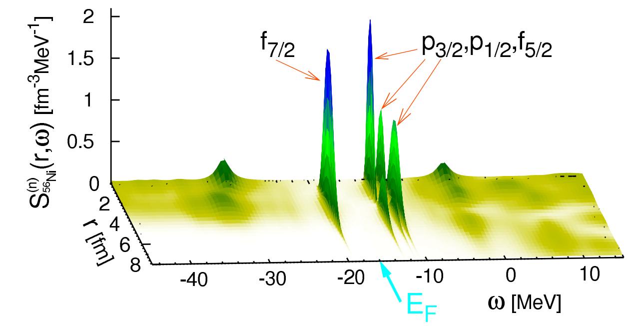
^{56}Ni

[Barbieri 2009]

Green’s functions

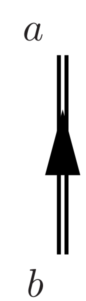
- Spectral function

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



- Green’s function

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



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

- Contains all structure information probed by nucleon transfer

$$G_{ab}(\omega) \equiv \sum_k \frac{\langle \psi_0^N | a_a | \psi_k^{N+1} \rangle \langle \psi_k^{N+1} | a_b^\dagger | \psi_0^N \rangle}{\omega - (E_k^{N+1} - E_0^N) + i\eta} + \sum_k \frac{\langle \psi_0^N | a_b^\dagger | \psi_k^{N-1} \rangle \langle \psi_k^{N-1} | a_a | \psi_0^N \rangle}{\omega - (E_0^N - E_k^{N-1}) - i\eta}$$

Gorkov Green's functions

✺ Formulate the expansion scheme around a Bogoliubov vacuum

→ Zeroth order already incorporates pairing

→ Breaking (and restoration) of particle number

✺ Gorkov equations

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

✺ Calculation scheme

✔ Start from NN (+NNN) realistic interaction

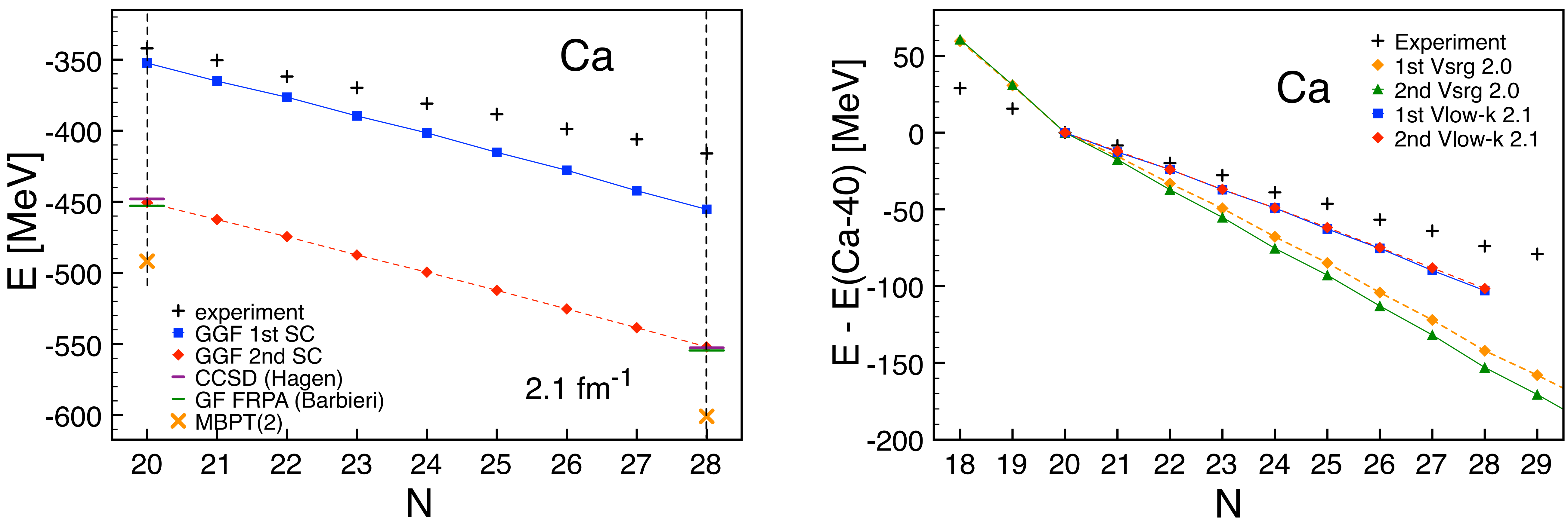
✔ No core, no adjustable parameters

✔ Choose self-energy truncation (2nd order)

Method able to tackle any semi-magic nucleus with A < 100

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

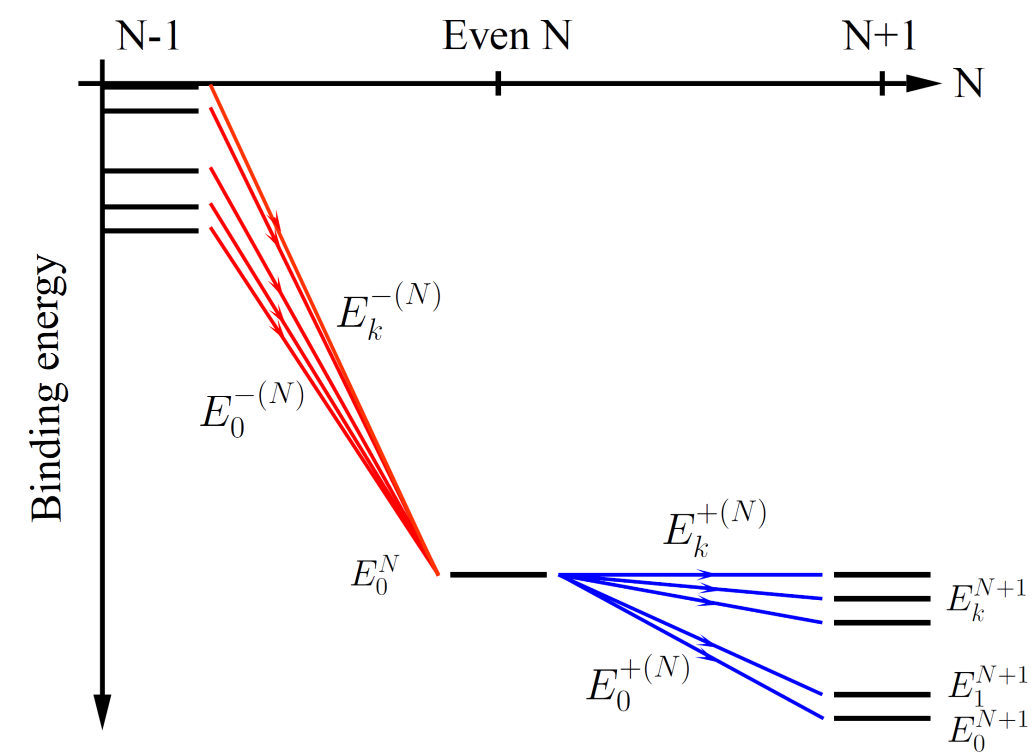
where
$$\begin{cases} \mathcal{U}^{k*}_a \equiv \langle \Psi_k | a^\dagger_a | \Psi_0 \rangle \\ \mathcal{V}^{k*}_a \equiv \langle \Psi_k | \bar{a}_a | \Psi_0 \rangle \end{cases}$$

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

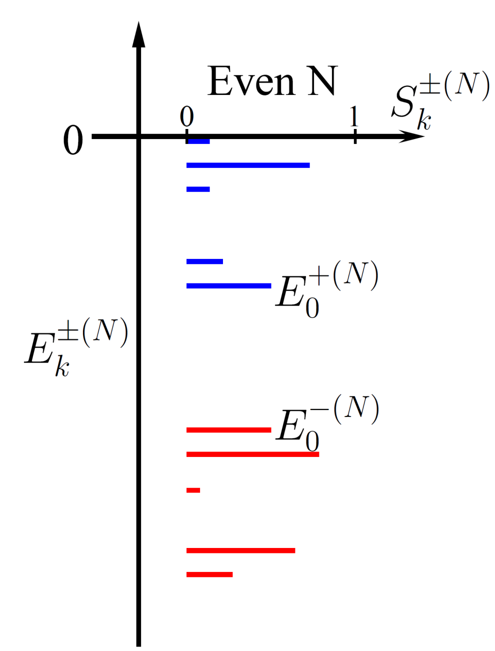
✺ Spectroscopic factors

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

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

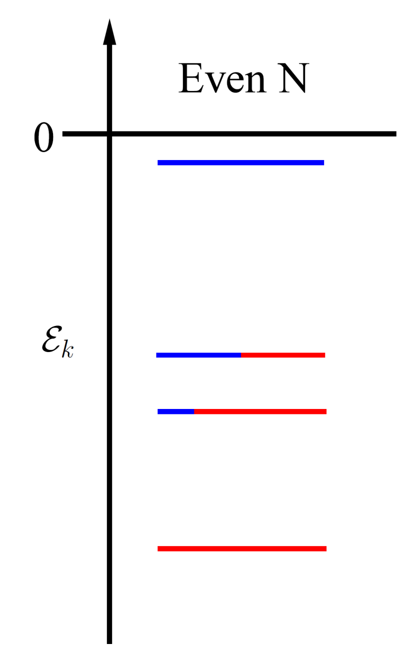


Separation energies + transfer strengths



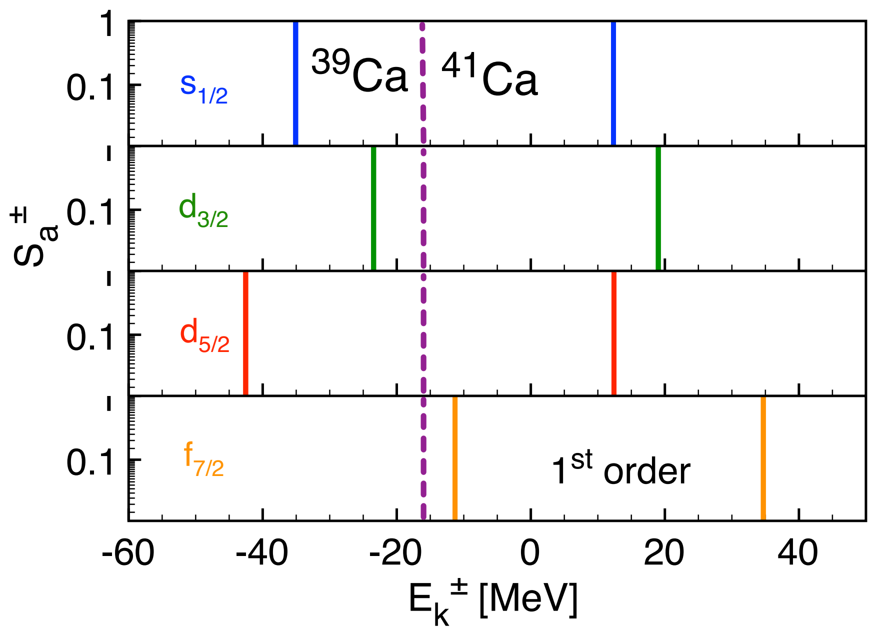
Centroids

ESPE



Spectral function

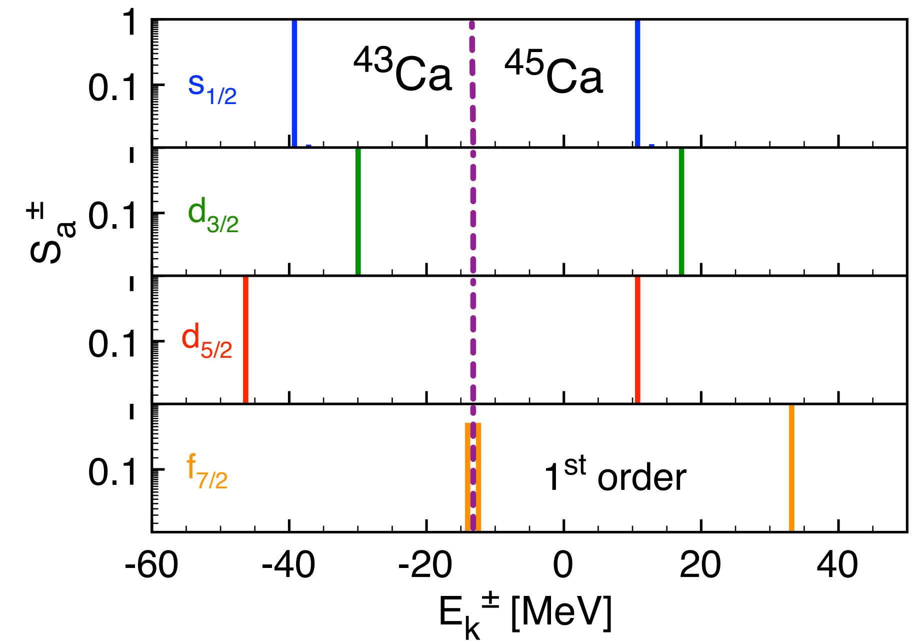
Dyson 1st order (HF)



Fragmentation

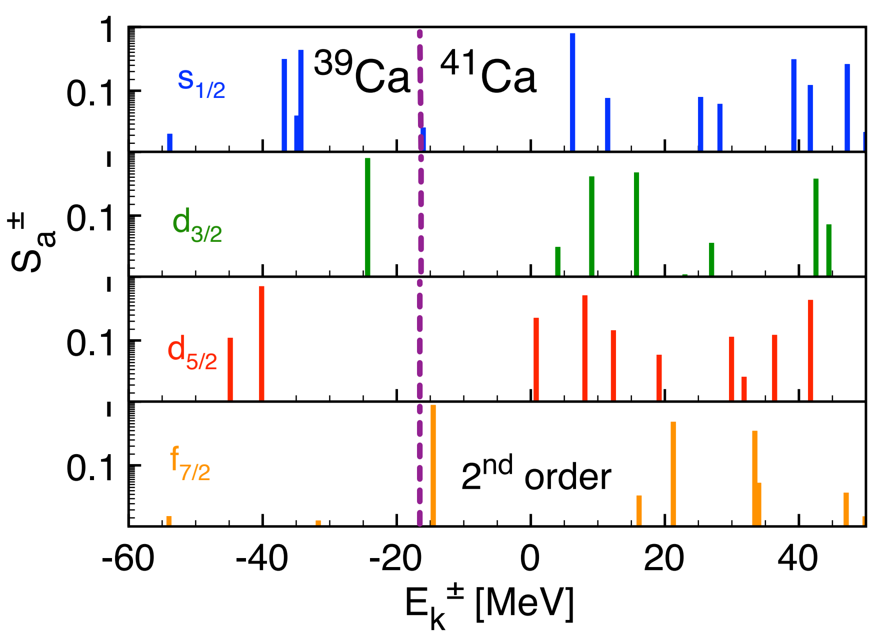
Static pairing

Gorkov 1st order (HFB)

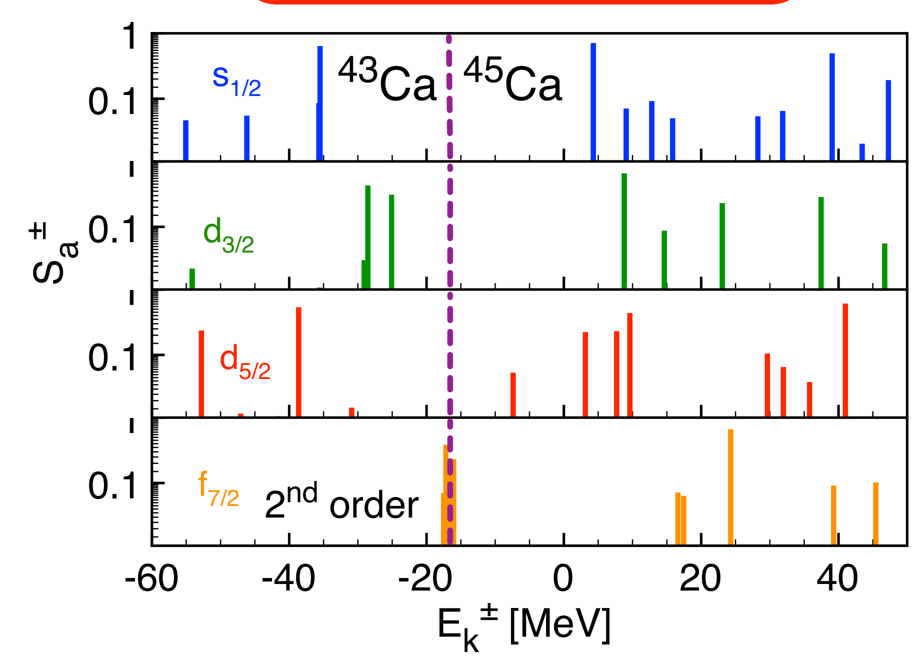


Dynamical fluctuations

Dyson 2nd order



Gorkov 2nd order



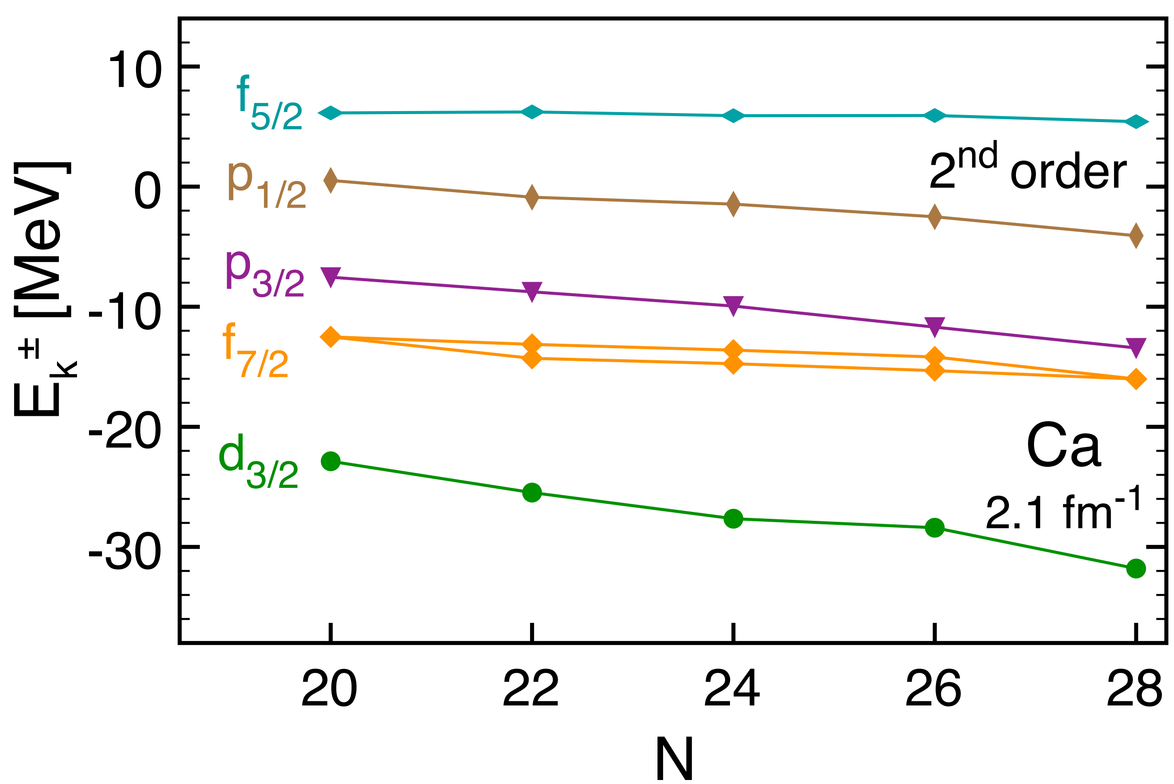
Shell structure evolution

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

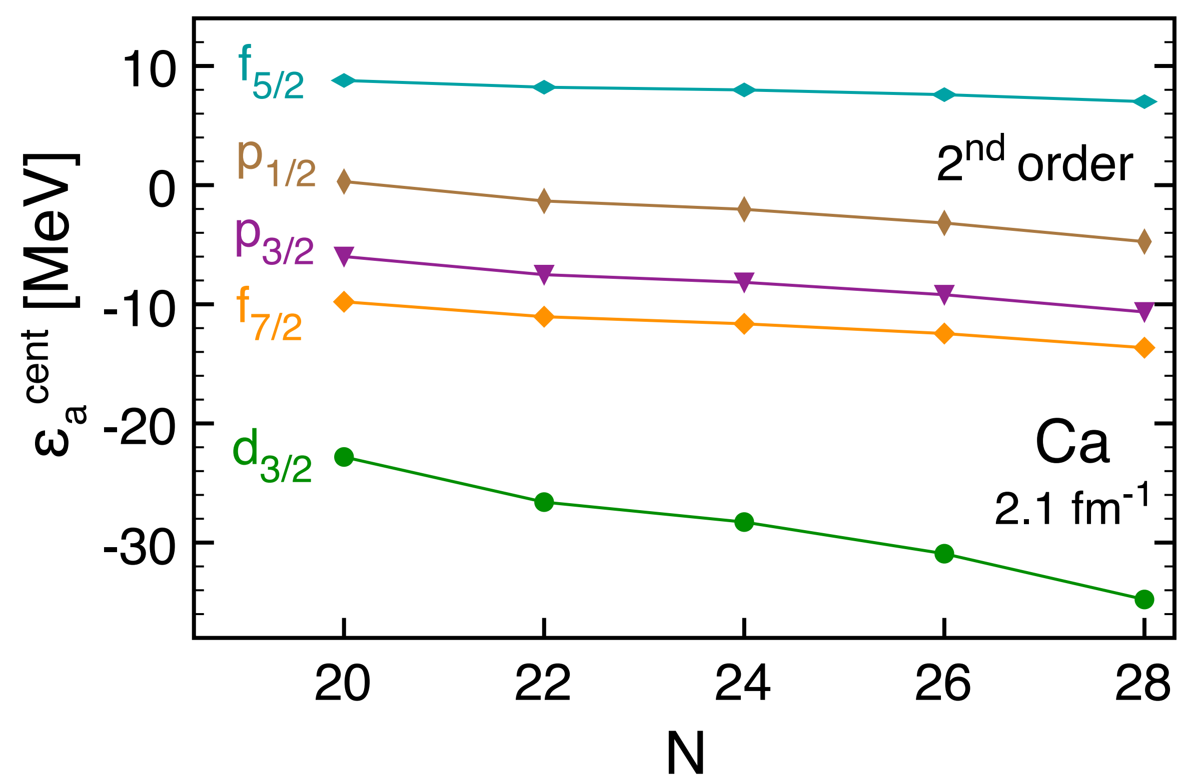
$$\epsilon_a^{cent} \equiv h_{ab}^{cent}\,\delta_{ab} = t_{aa} + \sum_{cd} \bar{V}^{NN}_{acad}\,\rho^{[1]}_{dc} + \sum_{cdef} \bar{V}^{NNN}_{acdaef}\,\rho^{[2]}_{efcd} \equiv \sum_k \mathcal{S}_k^{+a} E_k^{+} + \sum_k \mathcal{S}_k^{-a} E_k^{-}$$

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

Quasiparticle peaks

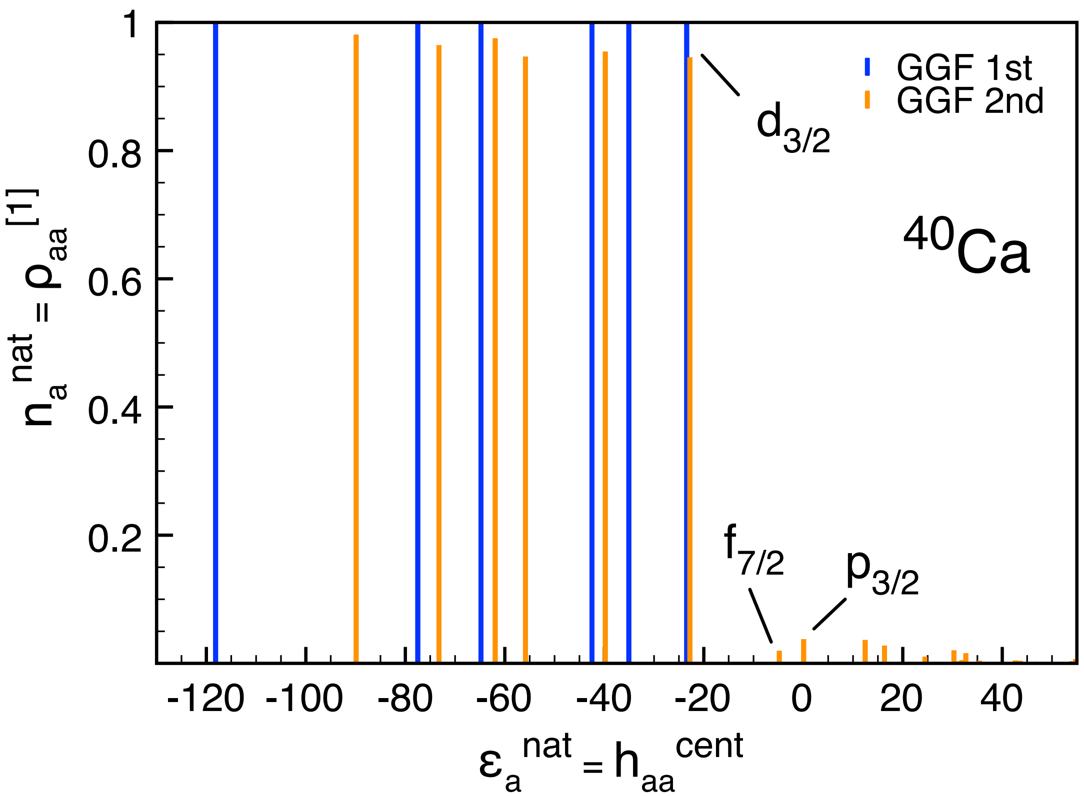


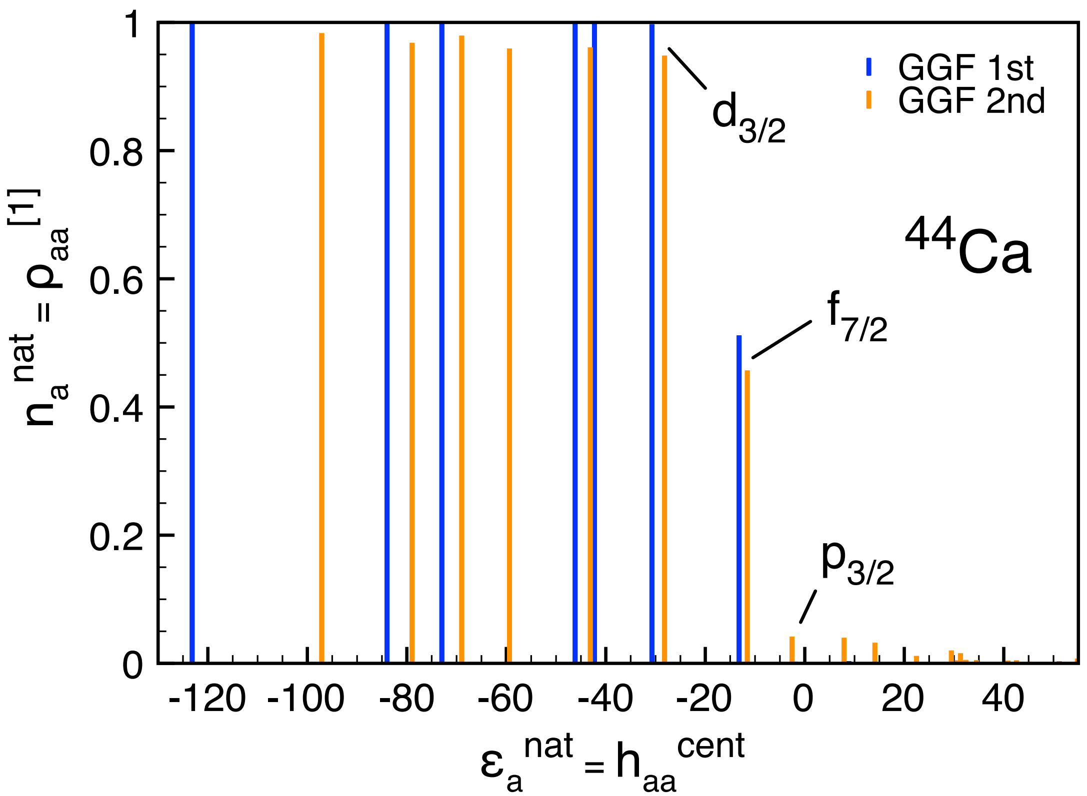
Centroids



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

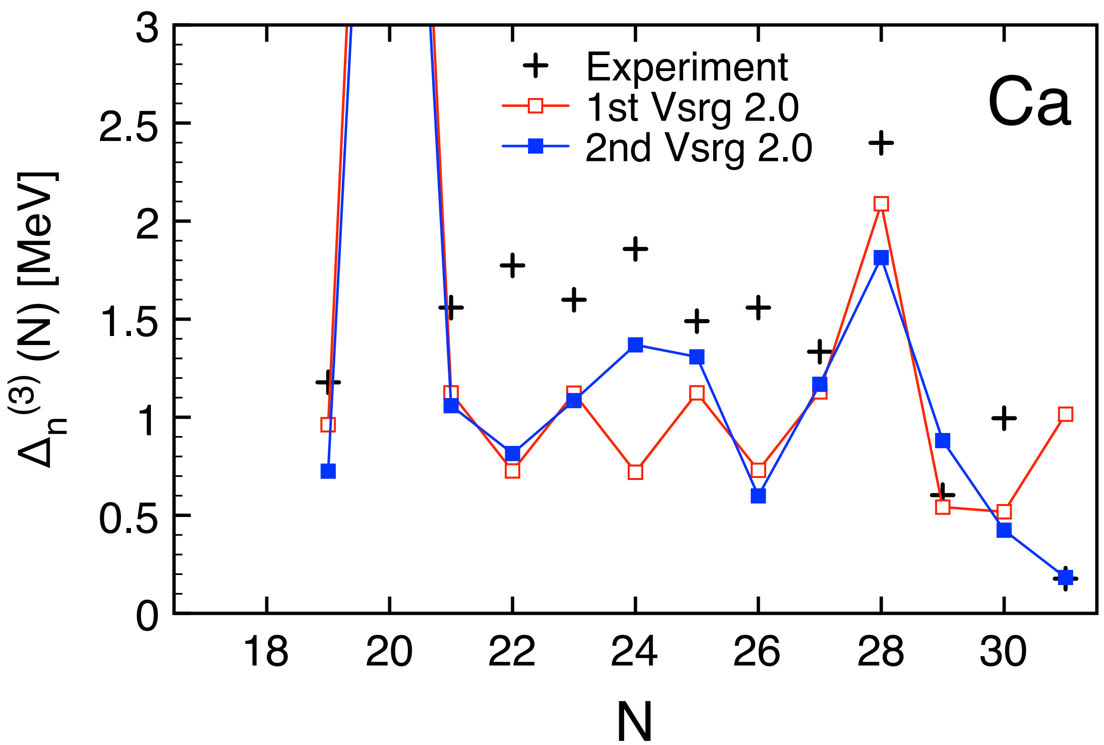
Pairing gap

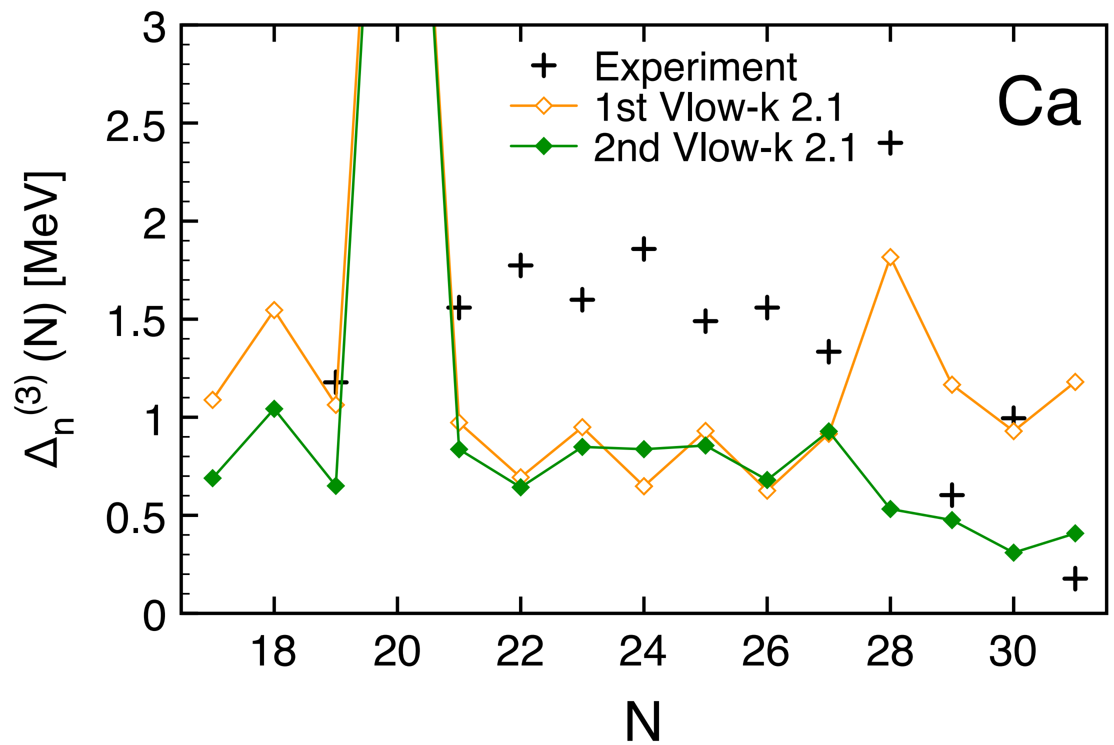
✳ Three-point mass differences

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

Generates O-E oscillations

Actual pairing gaps





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

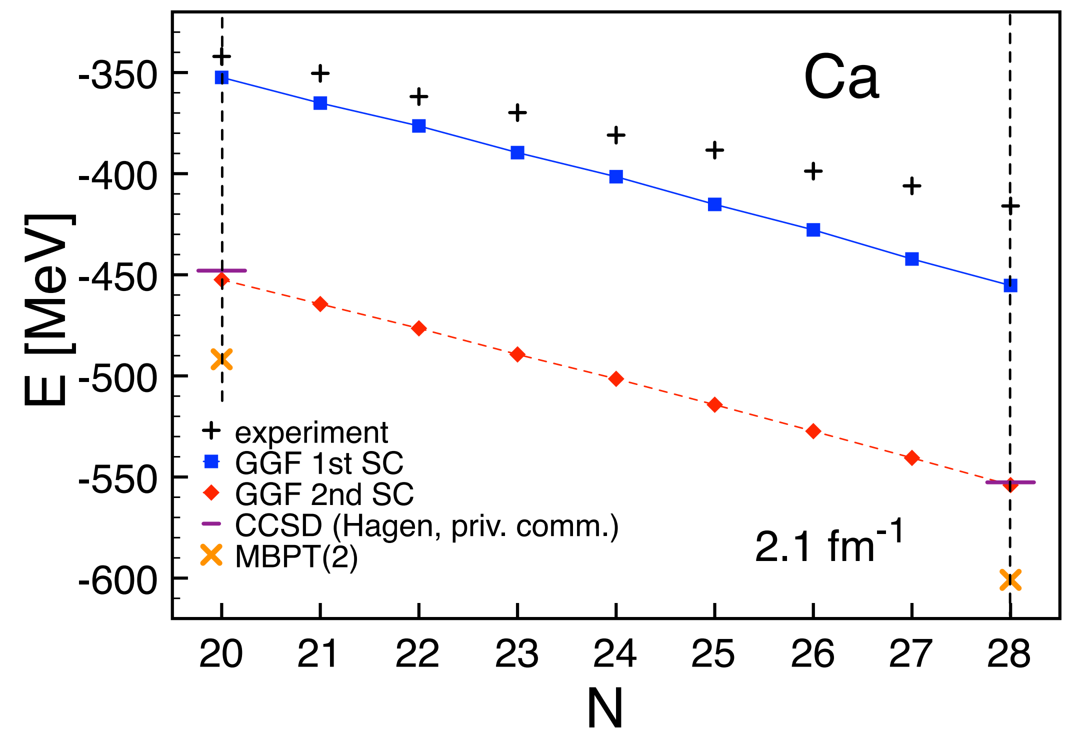
➟ Systematic underestimation of experimental gaps

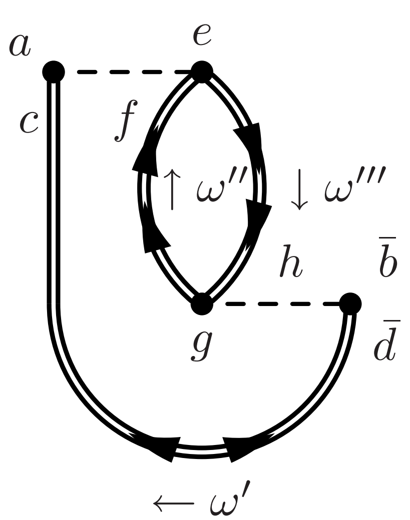
➟ Missing 3rd order and NNN should change picture qualitatively

Conclusions & Outlook

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

- Long term project:
  proof of principle available





Next steps:

- Implementation of three-body forces
- Formulation of particle-number restored Gorkov theory
- Improvement of the self-energy expansion

Appendix

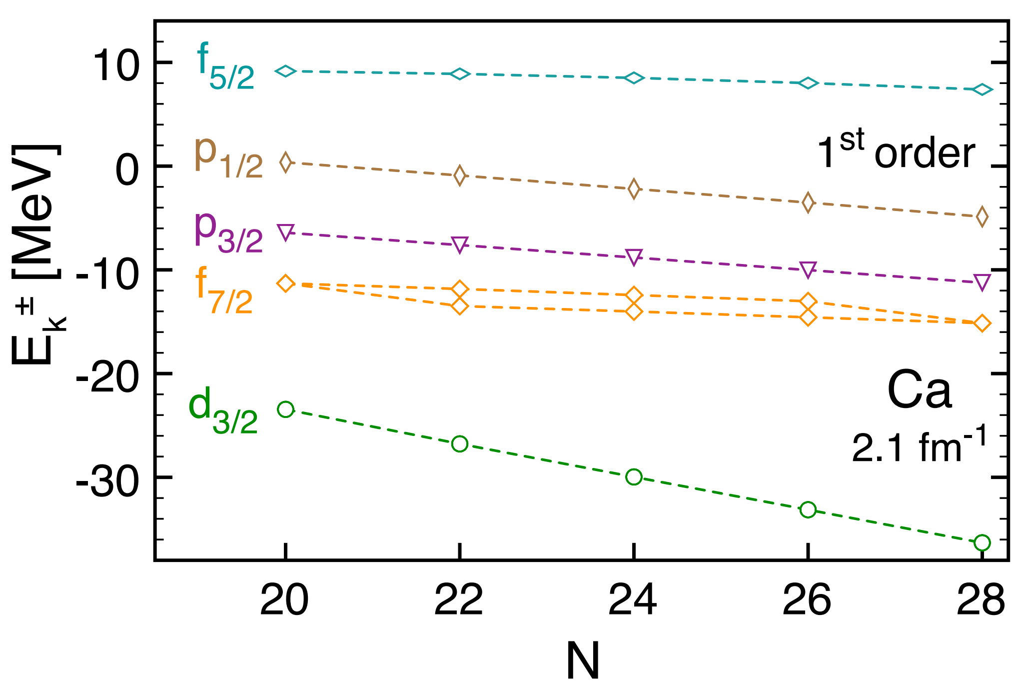
Shell structure evolution

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

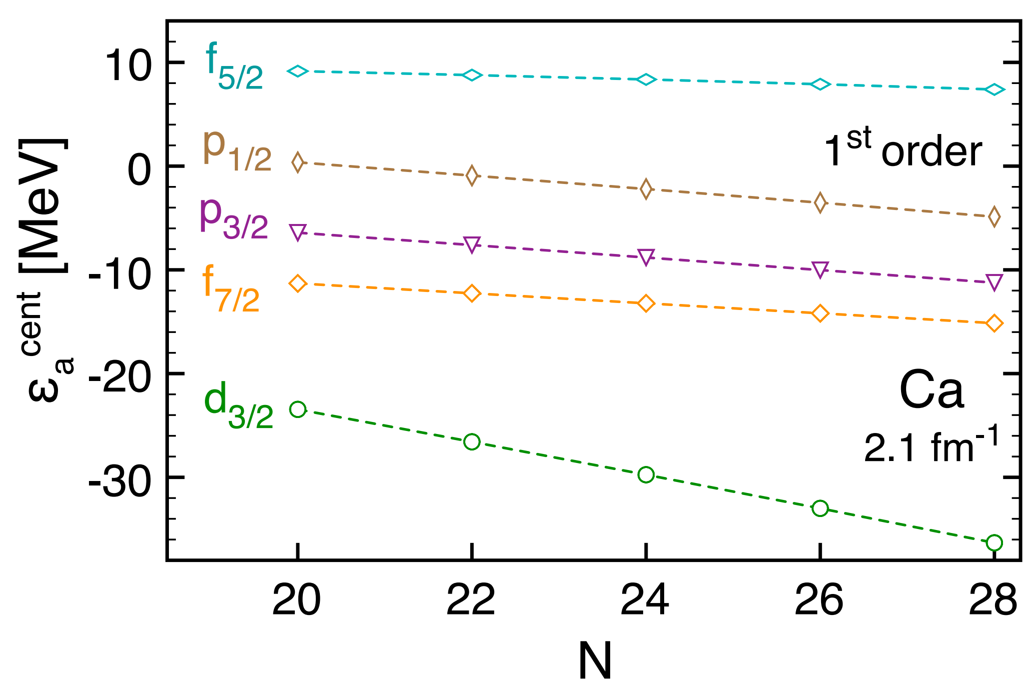
$$\epsilon_a^{cent} \equiv h_{ab}^{cent}\,\delta_{ab} = t_{aa} + \sum_{cd} \bar{V}_{acad}^{NN}\,\rho_{dc}^{[1]} + \sum_{cdef} \bar{V}_{acdaef}^{NNN}\,\rho_{efcd}^{[2]} \equiv \sum_k \mathcal{S}_k^{+a} E_k^{+} + \sum_k \mathcal{S}_k^{-a} E_k^{-}$$

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

Quasiparticle peaks



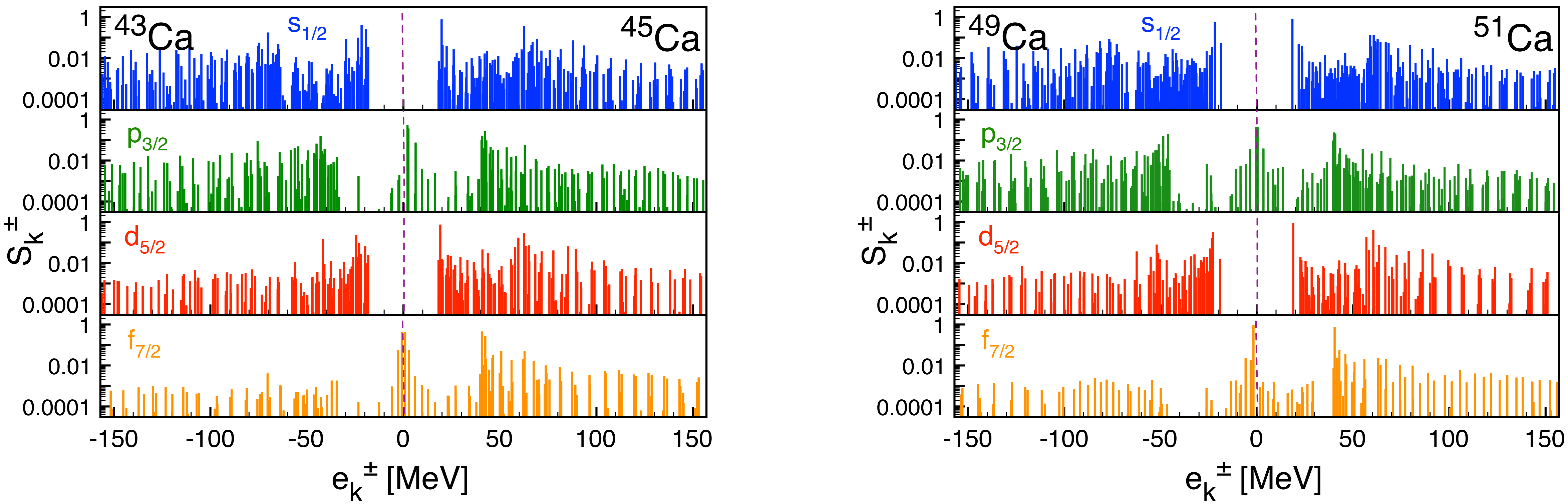
Centroids



➟ ESPE not to be confused with quasiparticle peak

➟ Particularly true for low-lying state in open-shell due to pairing

Spectral function



Observables

- One-body observables with $\hat{O} = \sum_{ab} O_{ab}\, a_a^\dagger\, a_b$

$$\langle \hat{O} \rangle = \sum_{ab} \int \frac{d\omega}{2\pi}\, O_{ab}\, G_{ab}(\omega)$$

➟ e.g. kinetic energy $\langle \hat{T} \rangle = \sum_{ab} \int \frac{d\omega}{2\pi}\, t_{ab}\, G_{ab}(\omega)$

- Koltun sum rule

$$\langle \hat{H} \rangle = E_0 = \sum_{ab} \int \frac{d\omega}{2\pi}\, \left[t_{ab} + \omega\, \delta_{ab} \right]\, G_{ab}(\omega)$$

➟ Two-body observable computed from the one-body propagator

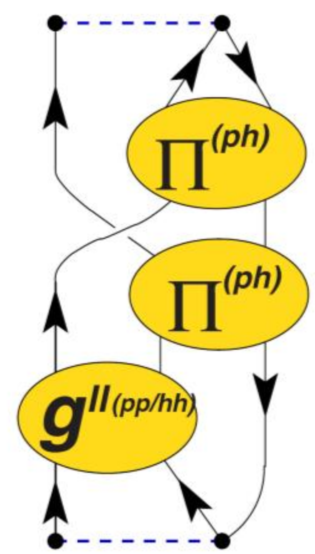
Applications to doubly-magic nuclei

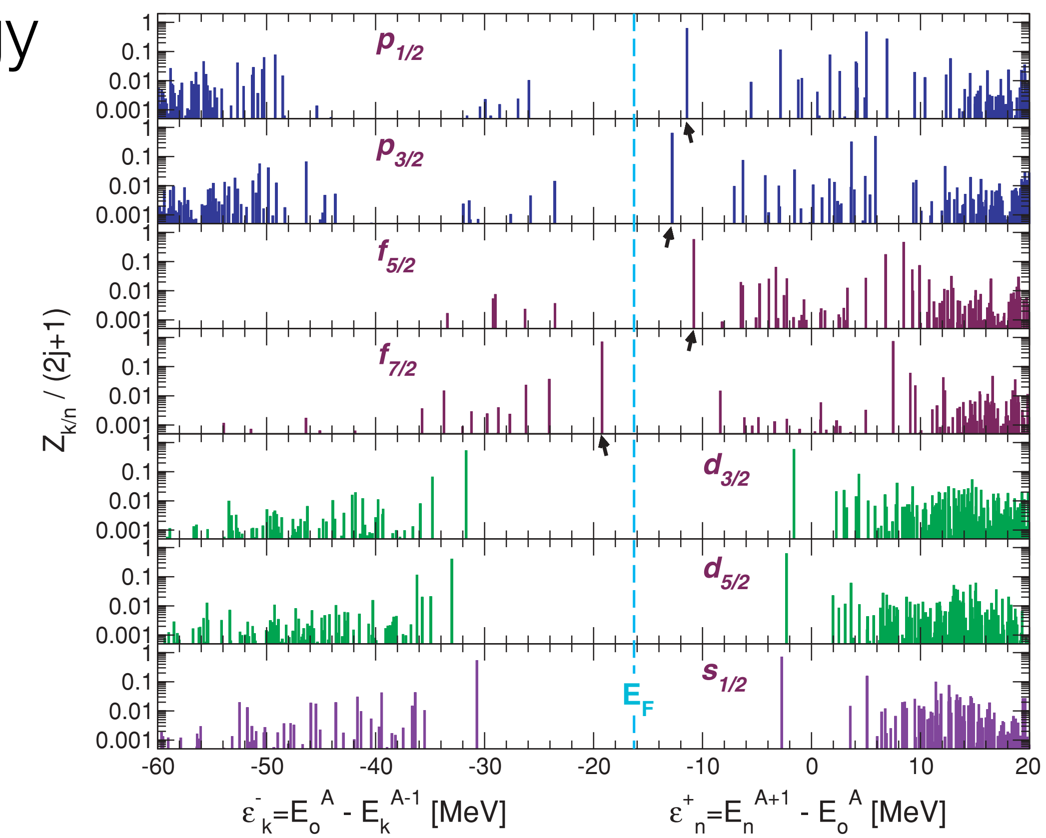
✺ Faddeev-RPA approximation for the self-energy

collective vibrations

particle-vibration coupling

[Barbieri *et al*. 2004-2009]





✺ Successful in medium-mass doubly-magic systems

Expansion breaks down when pairing instabilities appear

Explicit configuration mixing

Single-reference: Bogoliubov (Gorkov)

Lehmann representation

✵ Set eigenstates of Ω $\quad \Omega|\Psi_k\rangle = \Omega_k|\Psi_k\rangle$

define

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

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

✵ Lehmann representation

$$G_{ab}^{11}(\omega) = \sum_k \left\{ \frac{\bar{\mathcal{U}}_a^k \bar{\mathcal{U}}_b^{k*}}{\omega - \omega_k + i\eta} + \frac{\mathcal{V}_a^{k*} \mathcal{V}_b^k}{\omega + \omega_k - i\eta} \right\} \qquad G_{ab}^{21}(\omega) = \sum_k \left\{ \frac{\bar{\mathcal{V}}_a^k \bar{\mathcal{U}}_b^{k*}}{\omega - \omega_k + i\eta} + \frac{\mathcal{U}_a^{k*} \mathcal{V}_b^k}{\omega + \omega_k - i\eta} \right\}$$

$$G_{ab}^{12}(\omega) = \sum_k \left\{ \frac{\bar{\mathcal{U}}_a^k \bar{\mathcal{V}}_b^{k*}}{\omega - \omega_k + i\eta} + \frac{\mathcal{V}_a^{k*} \mathcal{U}_b^k}{\omega + \omega_k - i\eta} \right\} \qquad G_{ab}^{22}(\omega) = \sum_k \left\{ \frac{\bar{\mathcal{V}}_a^k \bar{\mathcal{V}}_b^{k*}}{\omega - \omega_k + i\eta} + \frac{\mathcal{U}_a^{k*} \mathcal{U}_b^k}{\omega + \omega_k - i\eta} \right\}$$

where $\omega_k \equiv \Omega_k - \Omega_0$ and

$$E_k^+ \equiv +\omega_k + \mu$$
$$E_k^- \equiv -\omega_k + \mu$$

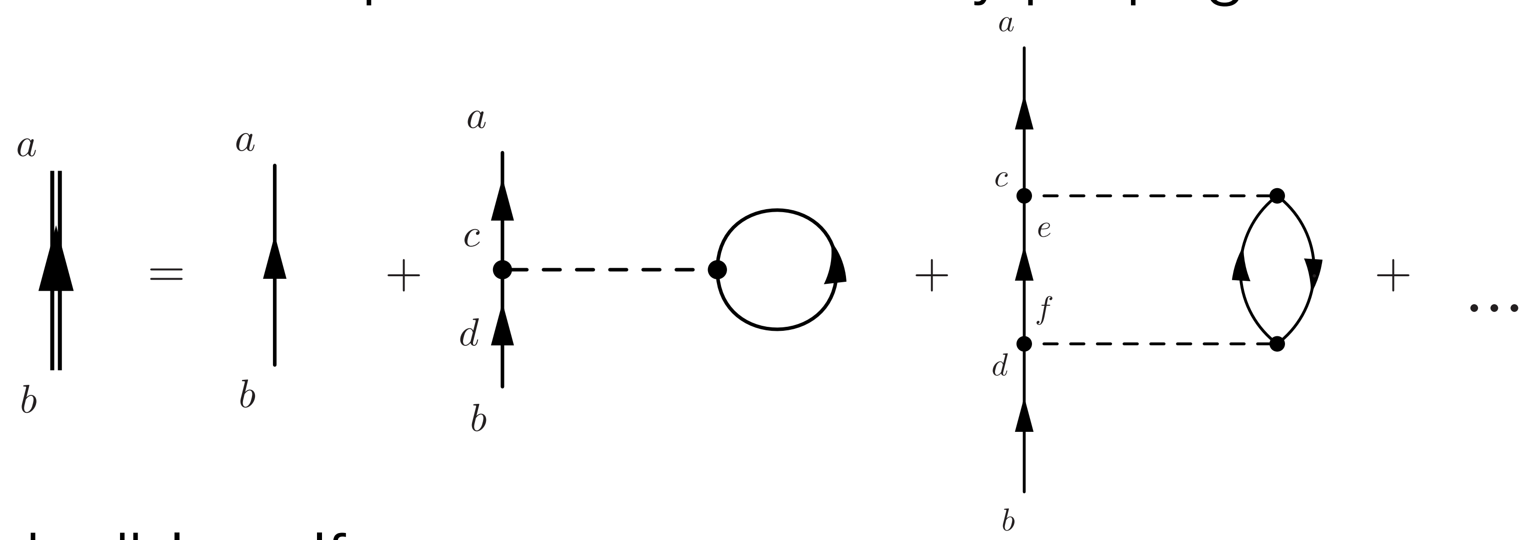
✵ Generalized spectroscopic factors

$$\mathcal{S}_k^+ \equiv \sum_a \left|\langle\psi_k|a_a^\dagger|\psi_0\rangle\right|^2 = \sum_a \left|\mathcal{U}_a^k\right|^2$$

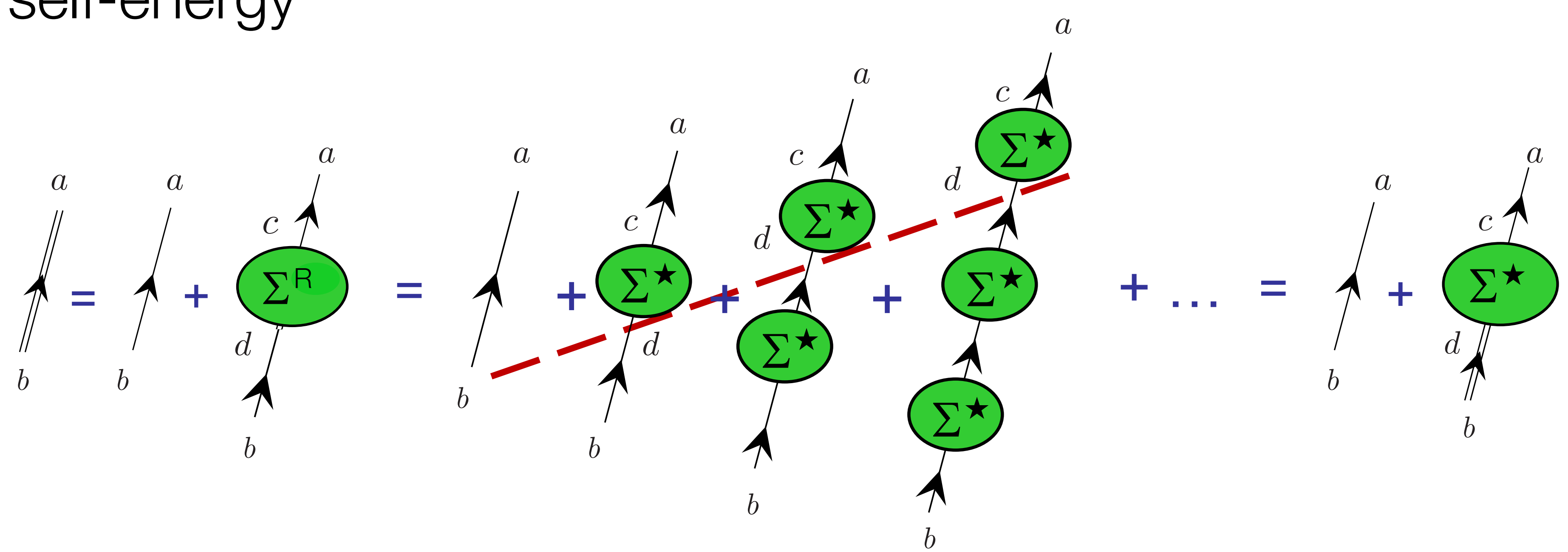
$$\mathcal{S}_k^- \equiv \sum_a \left|\langle\psi_k|a_a|\psi_0\rangle\right|^2 = \sum_a \left|\mathcal{V}_a^k\right|^2$$

Dyson equation & self-energy

- Perturbative expansion of one-body propagator



- Irreducible self-energy



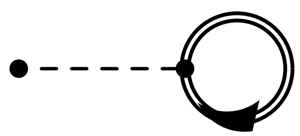
- Dyson equation

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

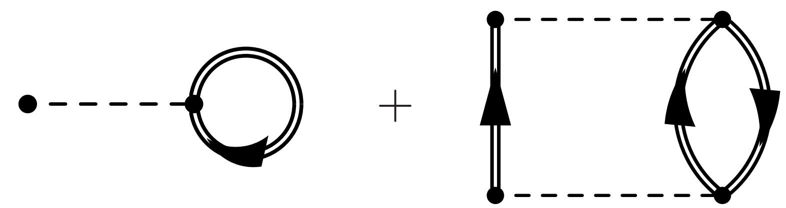
Solving Dyson equation

- Different approximations to the self-energy (**self-consistent** approaches)

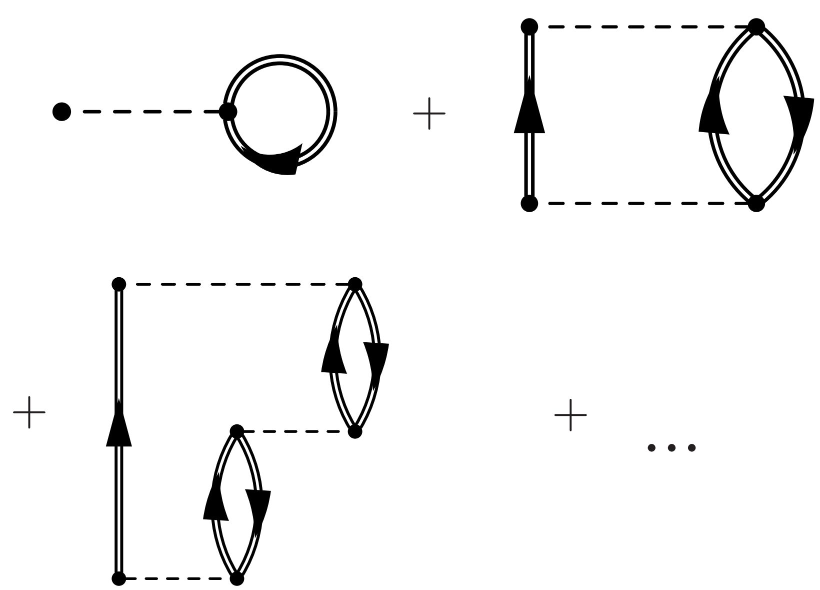
➟ Hartree-Fock



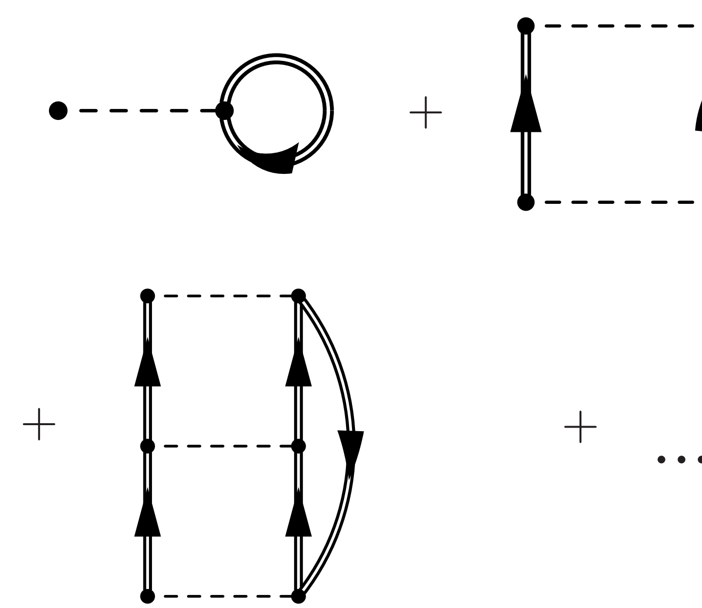
➟ Second order



➟ RPA



➟ Ladder (or T-matrix)



Gorkov equations (2)

✺ Gorkov equations $\xrightarrow{\text{Lehmann}}$ energy-dependent eigenvalue problem

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

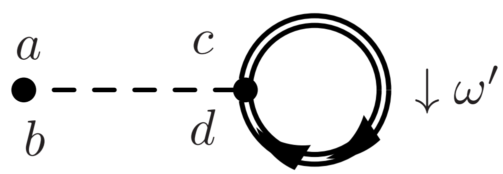
- $\Sigma^{g_1 g_2}(\omega)$ play the role of energy-dependent potentials
- Iterative problem: the number of poles ω_k grows with iterations
- Constraint: correct number of particles in average $N = \sum_{a,k} \left|\mathcal{V}^k_a\right|^2$
- Normalization condition $\sum_a \left(\mathcal{V}^k_a \; \mathcal{U}^k_a \right) \begin{pmatrix} \mathcal{V}^{k*}_a \\ \mathcal{U}^{k*}_a \end{pmatrix} = 1 + \sum_{ab} \left(\mathcal{V}^k_a \; \mathcal{U}^k_a \right) \frac{\partial \Sigma_{ab}(\omega)}{\partial \omega}\Big|_{-\omega_k} \begin{pmatrix} \mathcal{V}^{k*}_a \\ \mathcal{U}^{k*}_a \end{pmatrix}$

Objective
- Short term ➟ **Self-consistent** second order
- Longer term ➟ **Self-consistent** Faddeev-QRPA

1st order diagrams and HFB limit

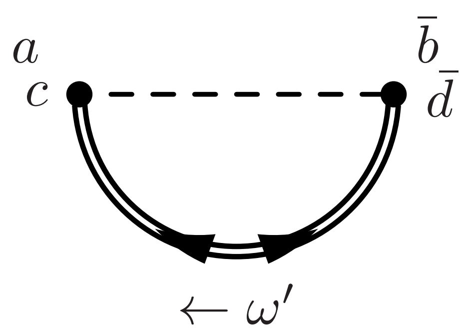
✹ Energy-independent self-energy

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



$$\Sigma_{ab}^{11\,(1)} = \sum_{cd,k} \bar{V}_{acbd}\, \mathcal{V}_d^{k*}\, \mathcal{V}_c^{k} \equiv \Lambda_{ab} = -\Sigma_{ab}^{22\,(1)}$$

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



$$\Sigma_{ab}^{12\,(1)} = \frac{1}{2} \sum_{cd,k} \bar{V}_{a\bar{b}c\bar{d}}\, \mathcal{V}_c^{k*}\, \mathcal{U}_d^{k} \equiv \tilde{h}_{ab} = \left[\Sigma_{ba}^{21\,(1)}\right]^*$$

✹ HFB problem is recovered ⟶ energy-independent eigenvalue problem

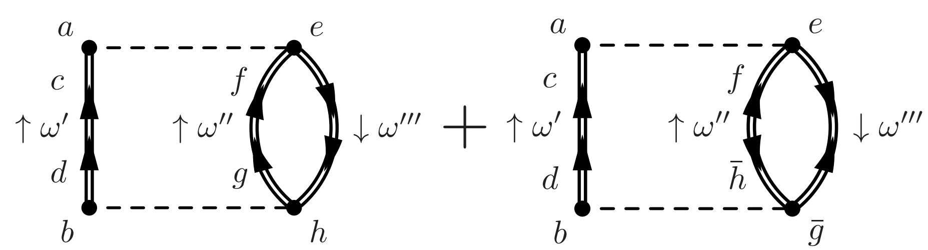
$$\sum_b \begin{pmatrix} t_{ab} + \Lambda_{ab} - \mu\,\delta_{ab} & \tilde{h}_{ab} \\ \tilde{h}^{\dagger}_{ab} & -t_{ab} - \Lambda_{ab} + \mu\,\delta_{ab} \end{pmatrix} \begin{pmatrix} U_b^k \\ V_b^k \end{pmatrix} = \omega_k \begin{pmatrix} U_a^k \\ V_a^k \end{pmatrix}$$

with the normalization condition $$\sum_a \left|U_a^k\right|^2 + \sum_a \left|V_a^k\right|^2 = 1$$

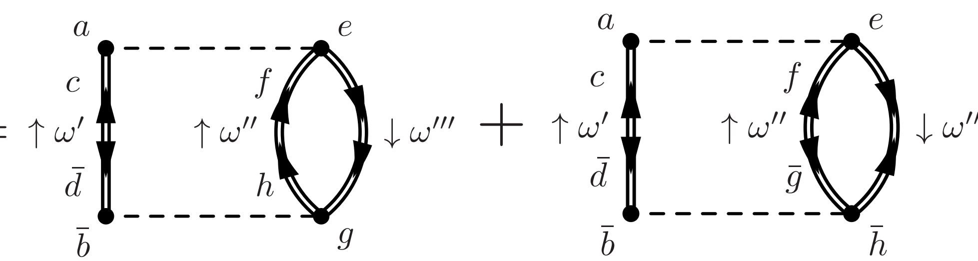
2nd order diagrams

✷ Energy-dependent self-energy

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



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



$$\Sigma_{ab}^{11\,(2)}(\omega) = \sum_{k_1 k_2 k_3} \left\{ \frac{\mathcal{C}_a^{k_1 k_2 k_3}\, \mathcal{C}_b^{k_1 k_2 k_3\,\dagger}}{\omega - E_{k_1 k_2 k_3} + i\eta} + \frac{\mathcal{D}_a^{k_1 k_2 k_3\,\dagger}\, \mathcal{D}_b^{k_1 k_2 k_3}}{\omega + E_{k_1 k_2 k_3} + i\eta} \right\}$$

$$\Sigma_{ab}^{12\,(2)}(\omega) = -\sum_{k_1 k_2 k_3} \left\{ \frac{\mathcal{C}_a^{k_1 k_2 k_3}\, \mathcal{D}_b^{k_1 k_2 k_3}}{\omega - E_{k_1 k_2 k_3} + i\eta} + \frac{\mathcal{D}_a^{k_1 k_2 k_3\,\dagger}\, \mathcal{C}_b^{k_1 k_2 k_3\,\dagger}}{\omega + E_{k_1 k_2 k_3} + i\eta} \right\}$$

$$\mathcal{C}_a^{k_1 k_2 k_3} \equiv \frac{1}{\sqrt{6}} \sum_{\{1,2,3\}} \sum_{ijk} \bar{V}_{akij}\, \bar{\mathcal{U}}_i^{k_1} \bar{\mathcal{U}}_j^{k_2} \mathcal{V}_k^{k_3}$$

$$\mathcal{D}_a^{k_1 k_2 k_3} \equiv \frac{1}{\sqrt{6}} \sum_{\{1,2,3\}} \sum_{ijk} \bar{V}_{akij}\, \mathcal{V}_i^{k_1} \mathcal{V}_j^{k_2} \bar{\mathcal{U}}_k^{k_3}$$

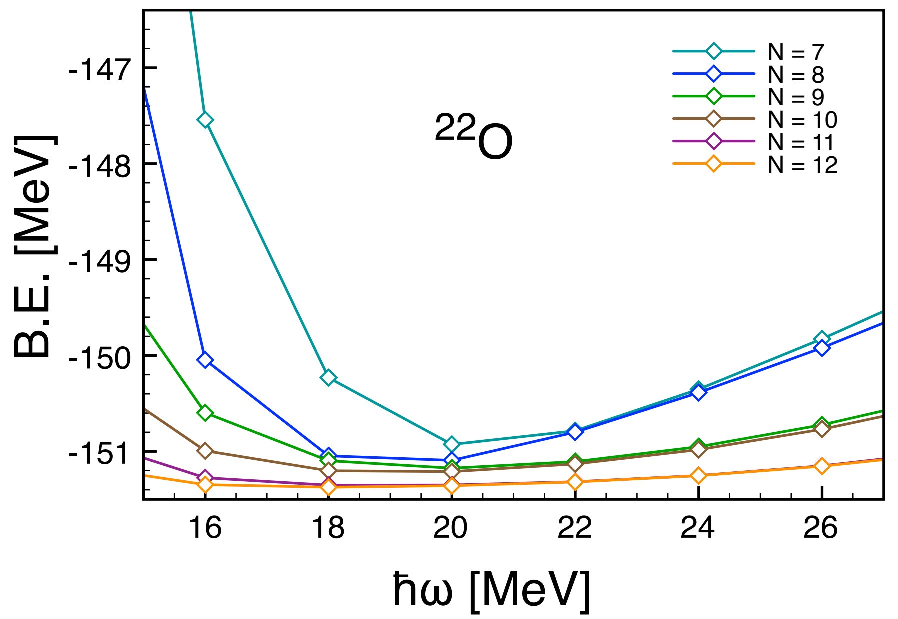
✷ Recast known energy dependence into new quantities

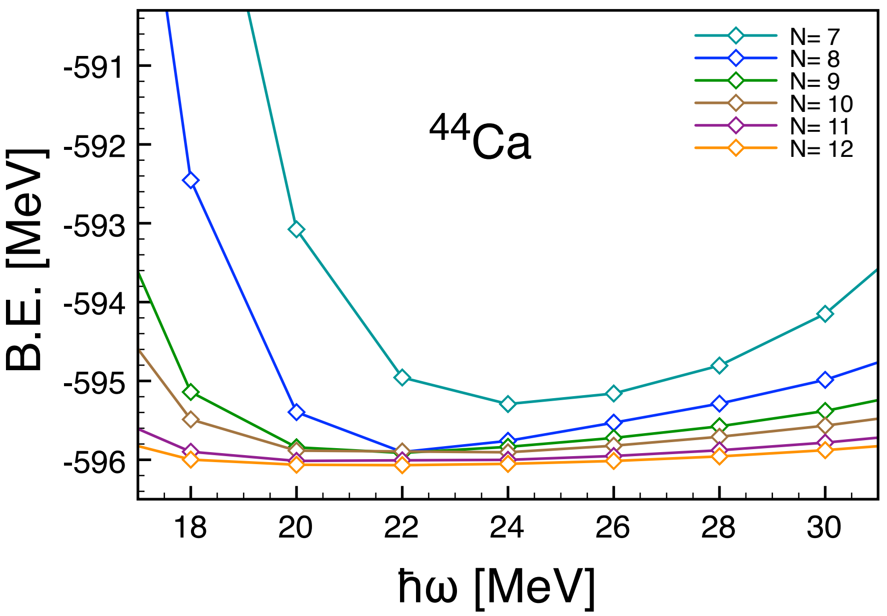
$$(\omega_k - E_{k_1 k_2 k_3})\, \mathcal{W}_k^{k_1 k_2 k_3} \equiv \sum_a \left[\mathcal{C}_a^{k_1 k_2 k_3\,\dagger}\, \mathcal{U}_a^k - \mathcal{D}_a^{k_1 k_2 k_3}\, \mathcal{V}_a^k \right]$$

$$(\omega_k + E_{k_1 k_2 k_3})\, \mathcal{Z}_k^{k_1 k_2 k_3} \equiv \sum_a \left[-\mathcal{D}_a^{k_1 k_2 k_3}\, \mathcal{U}_a^k + \mathcal{C}_a^{k_1 k_2 k_3\,\dagger}\, \mathcal{V}_a^k \right]$$

Convergence

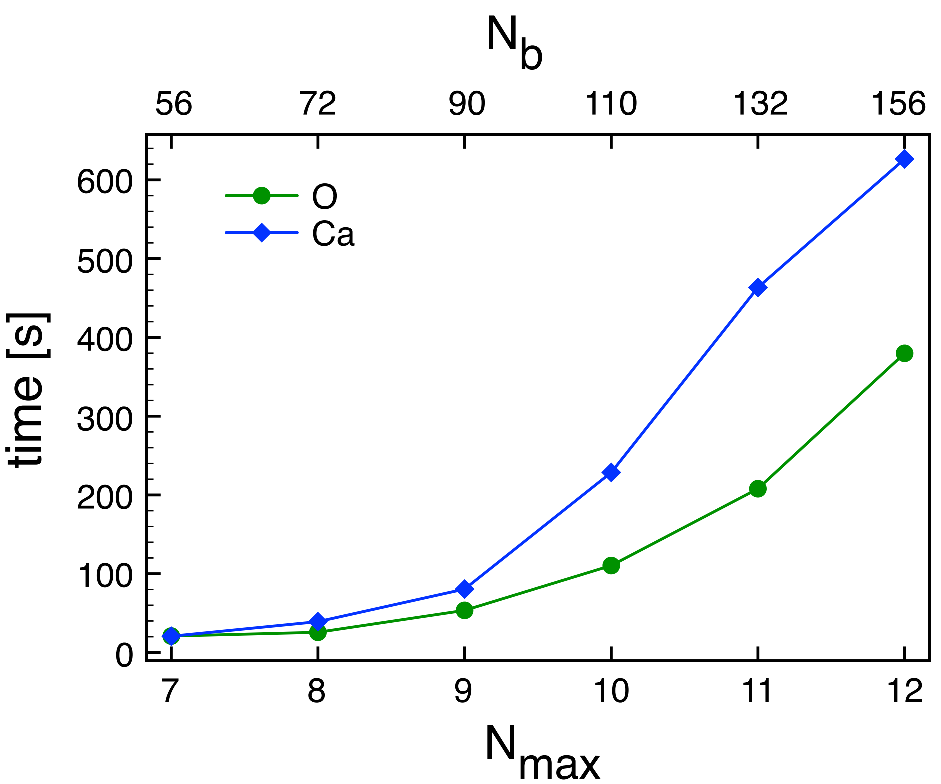
- Convergence tests in medium-mass systems





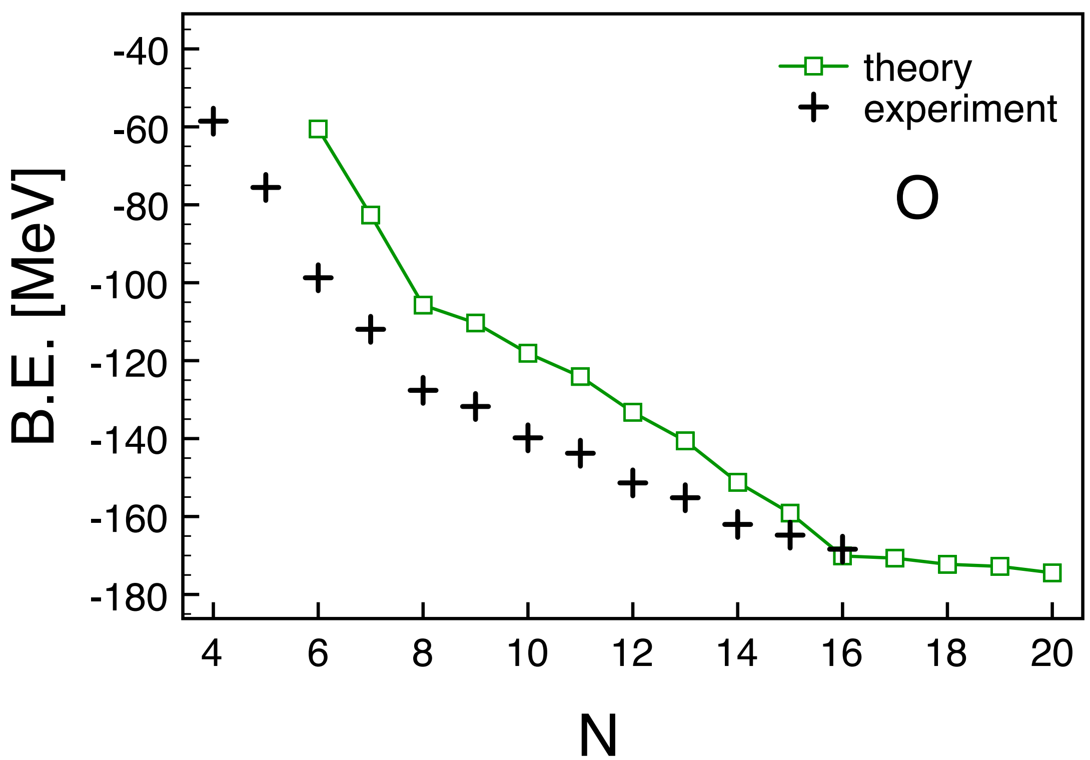
➟ 11 to 12 major shells sufficient

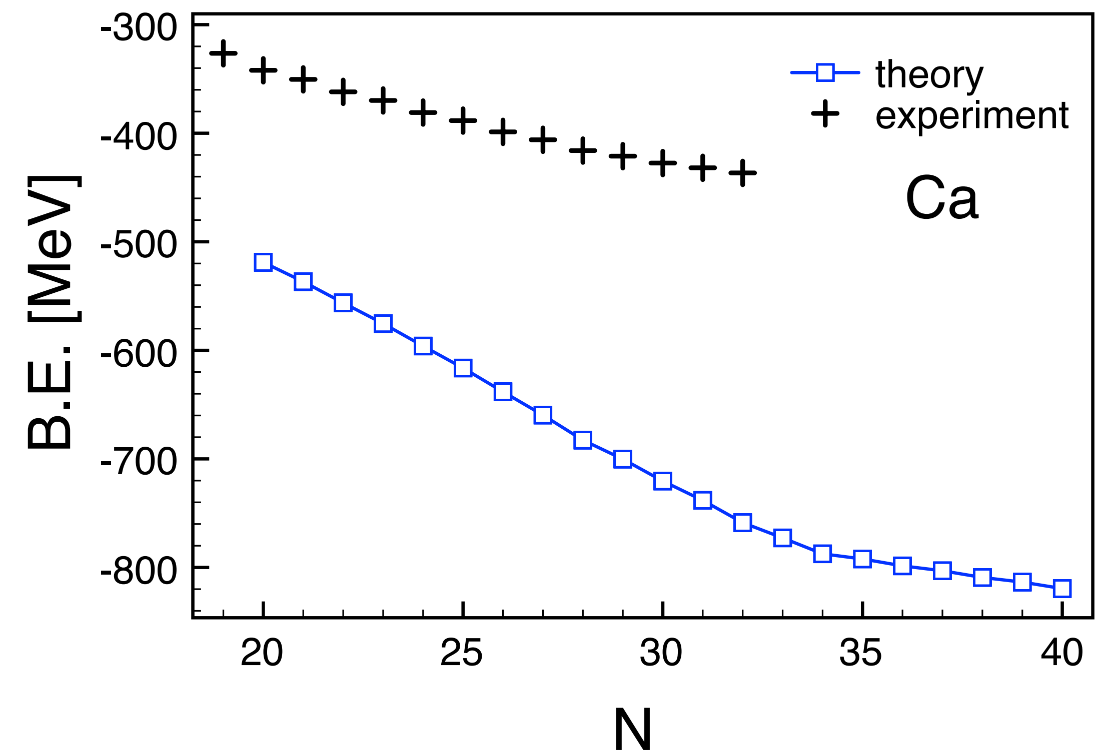
- CPU time to convergence (on a single processor)



Binding energy

- Total binding energies





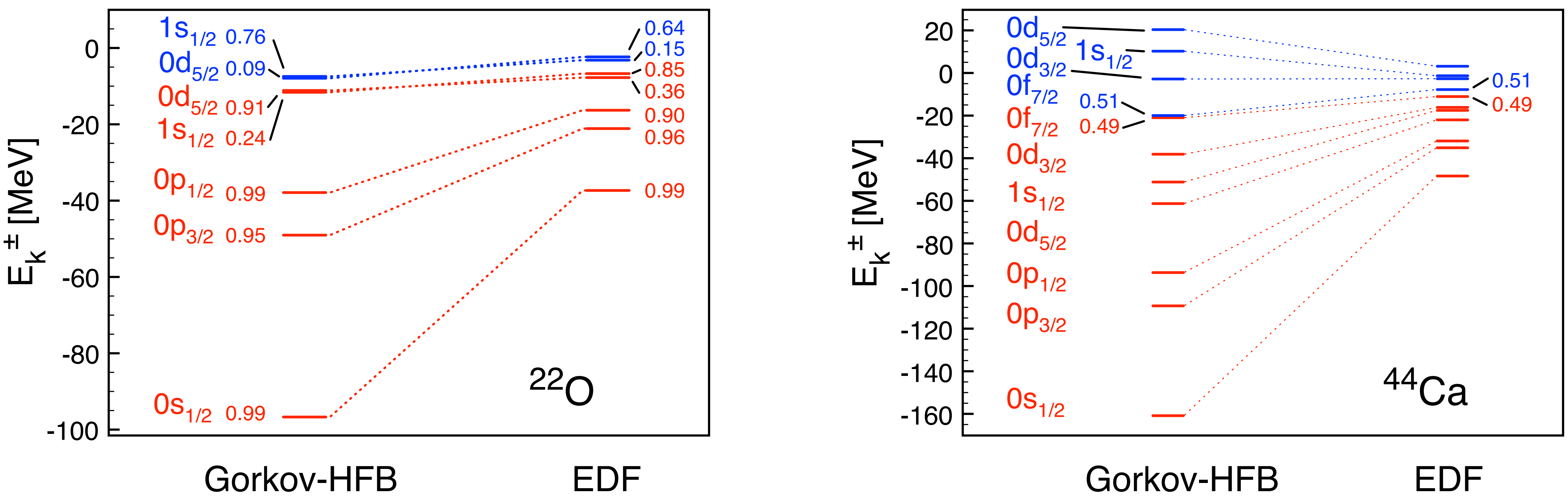
➡ Nucleus is bound at HFB level

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

➡ Isospin trend: trace of NNN/higher-order physics?

Single-particle-like spectrum

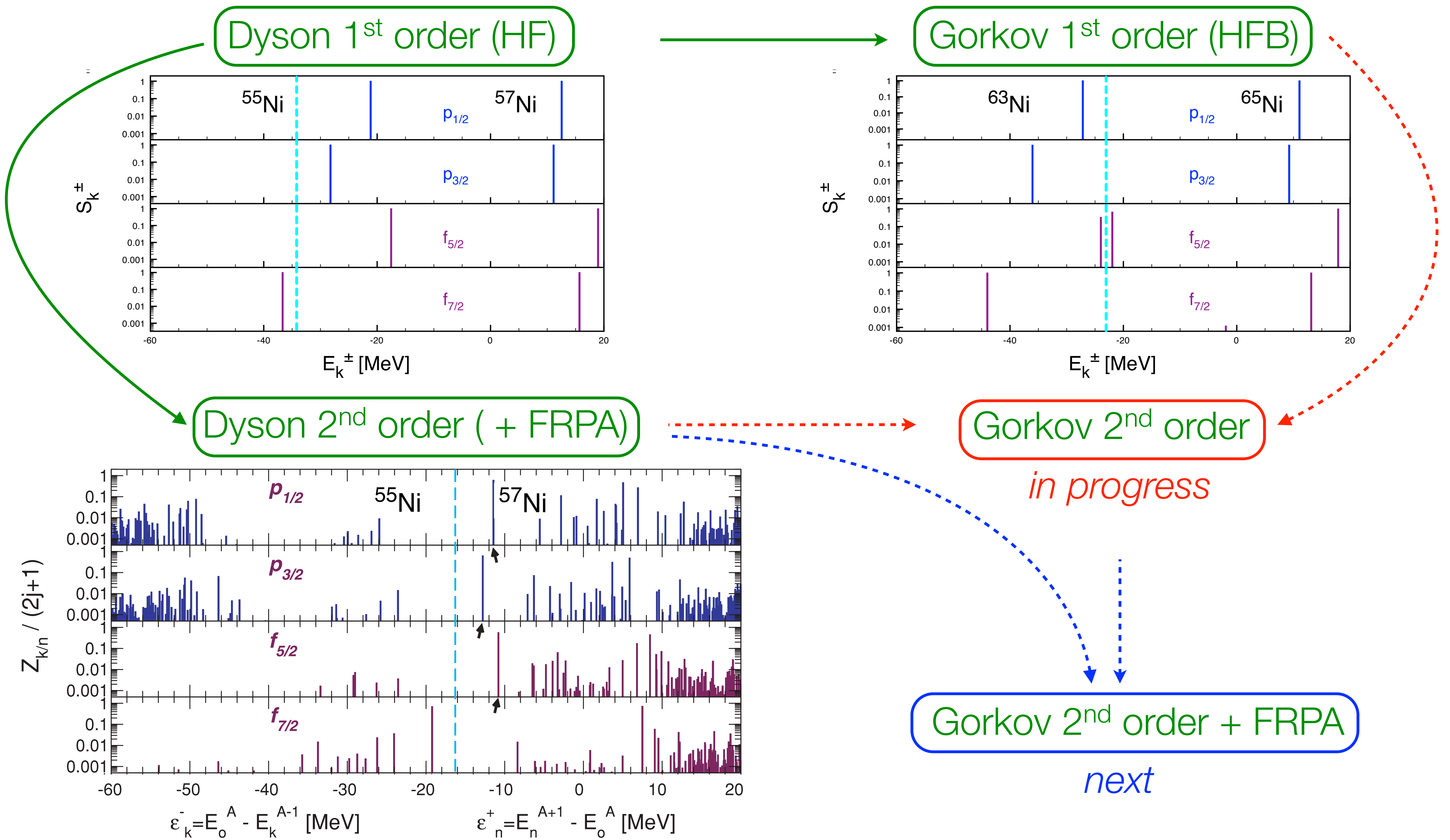
- Gorkov-HFB spectrum vs Skyrme-EDF quasi-particle spectrum ($S^{\pm}_{k} > 0.01$)



➟ Ordering of levels & spectroscopic factors consistent with Skyrme-EDF

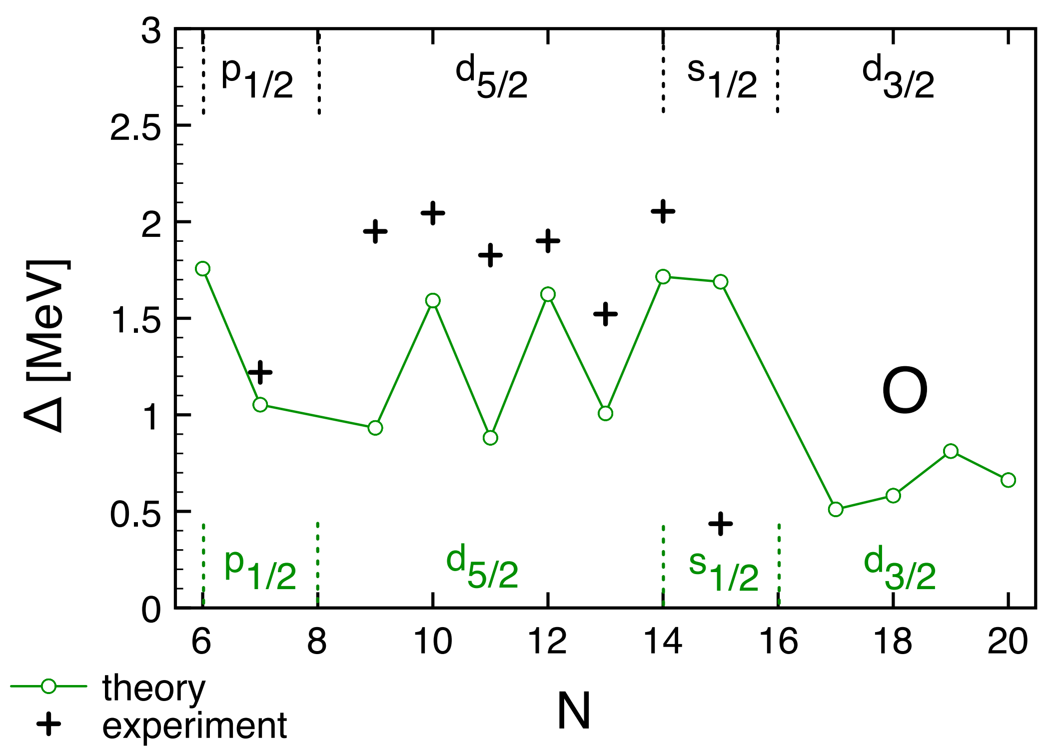
➟ Levels much more spread: trace of missing NNN physics in $\Sigma^{11(1)}$ mocked up in EDF

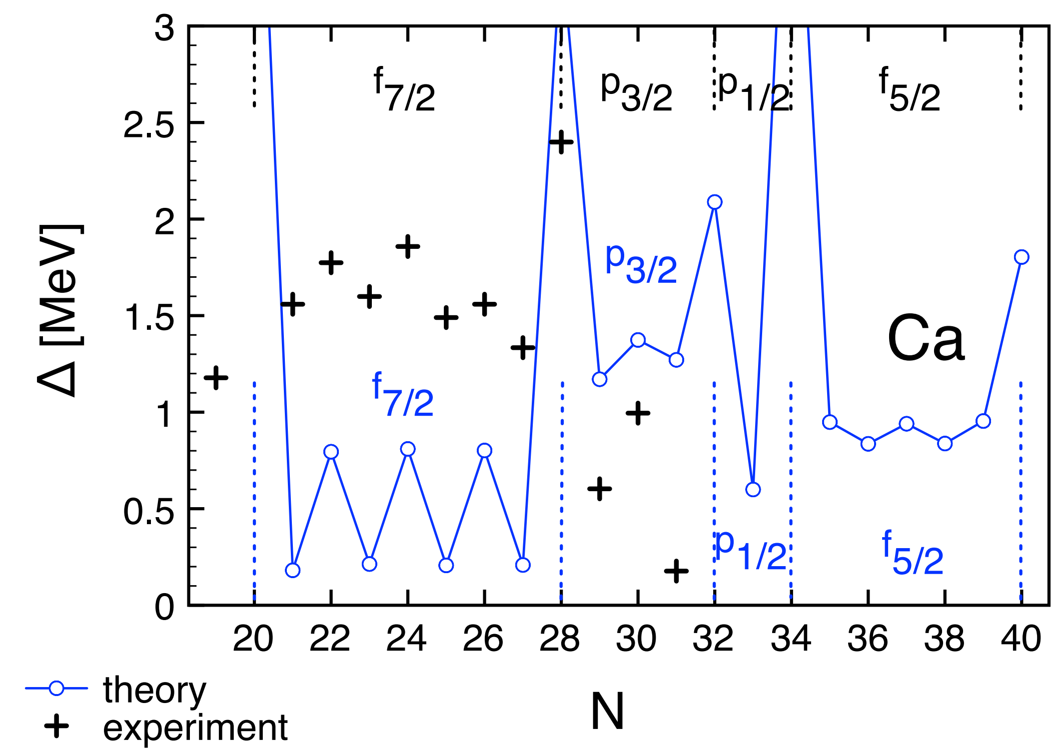
Spectral function



Gaps

- Gaps as three-point mass differences



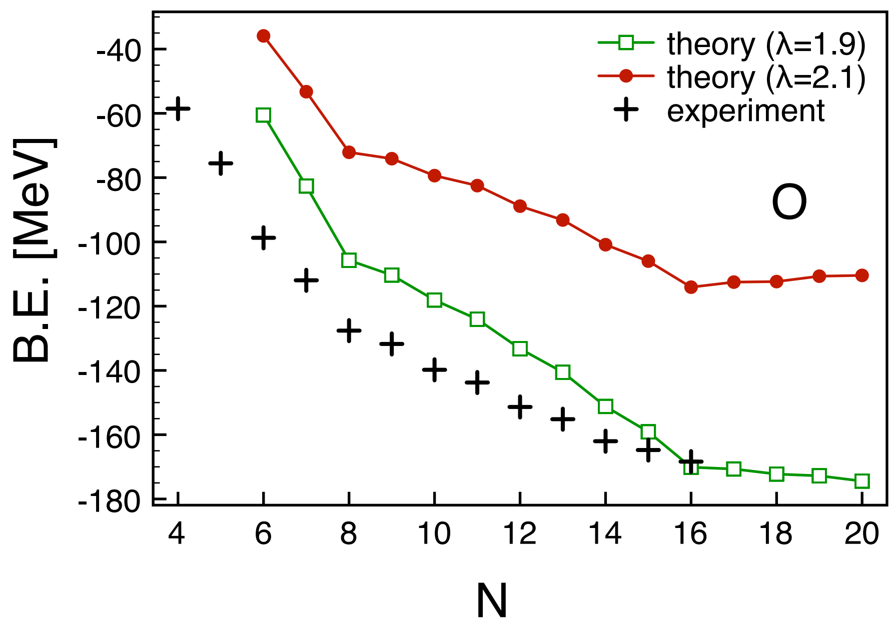


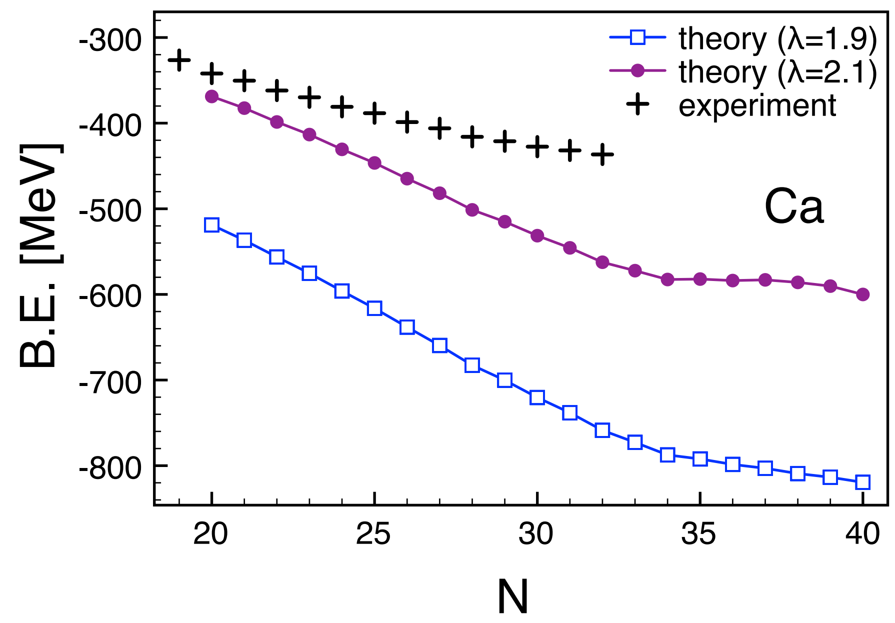
➟ Correct odd-even trend but too large oscillations

➟ Systematic underestimation of experimental gaps

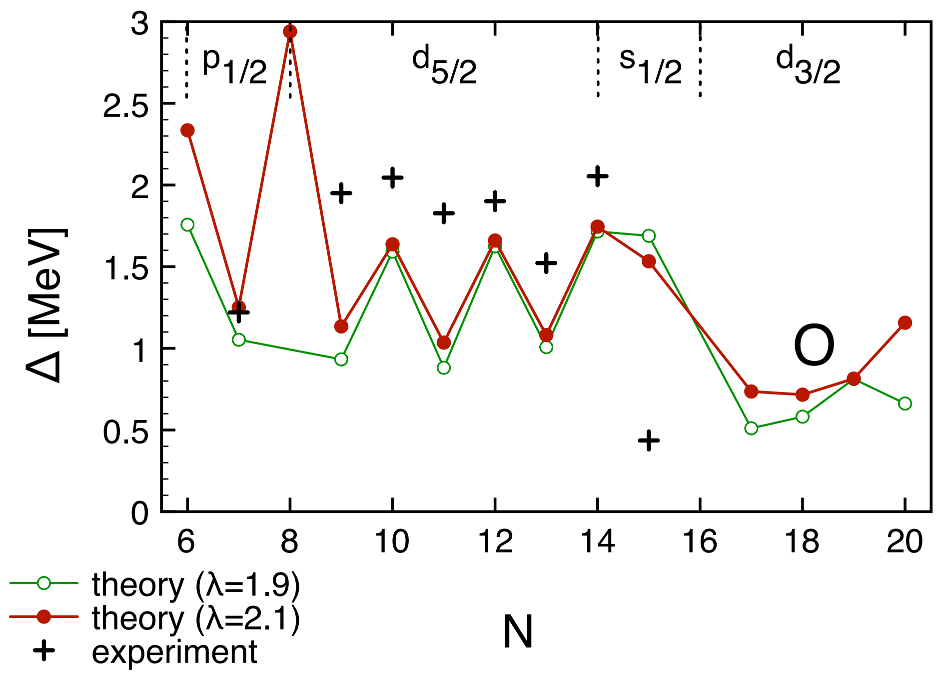
Cutoff dependence (1)

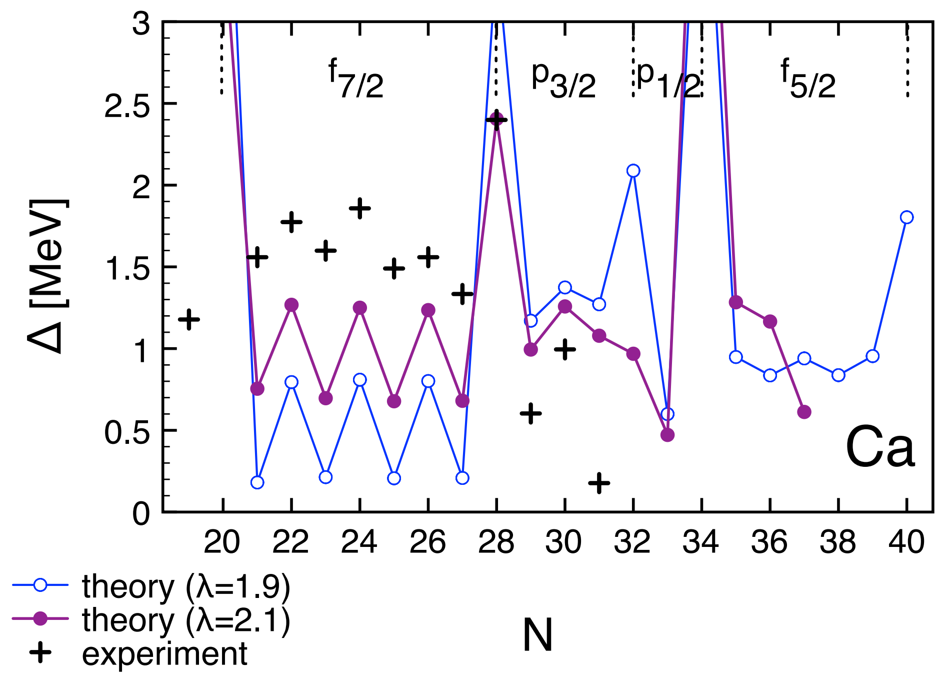
- Total binding energies





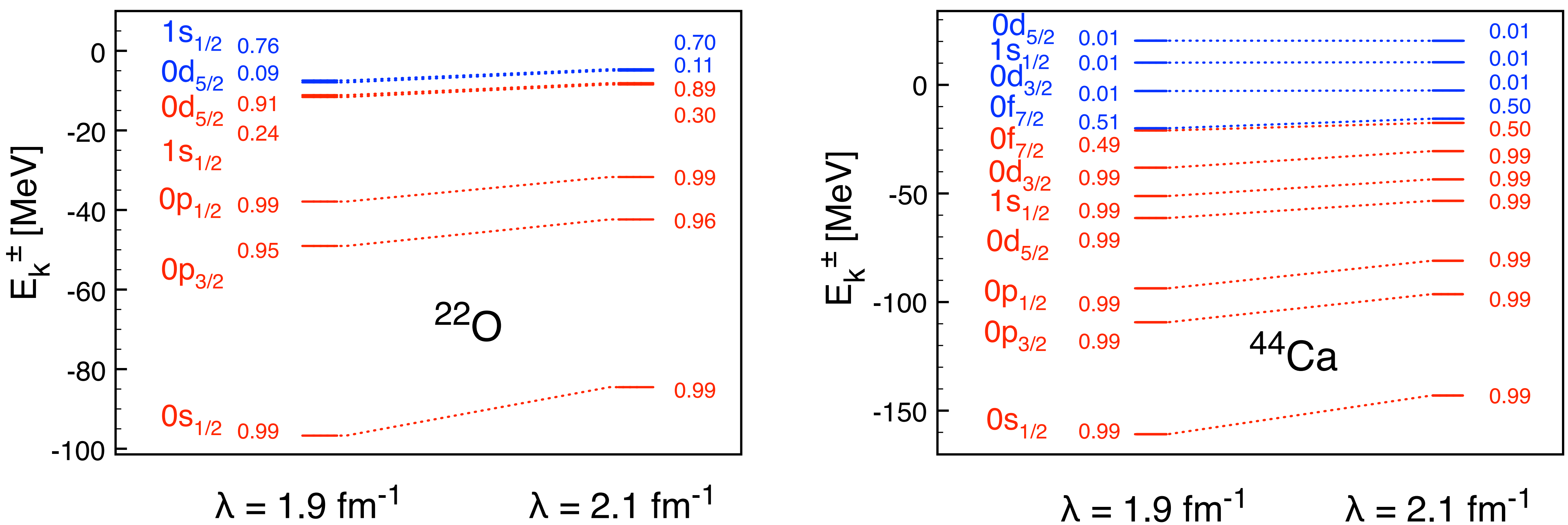
- Odd-even mass differences





Cutoff dependence (2)

✺ Single-particle-like spectrum ($S_k > 0.01$)



➟ Systematic shifts in both O and Ca

➟ Calculations in progress: complete study of cutoff dependence

➟ Inclusion of NNN mandatory at first order

Low-momentum nuclear interactions

RG

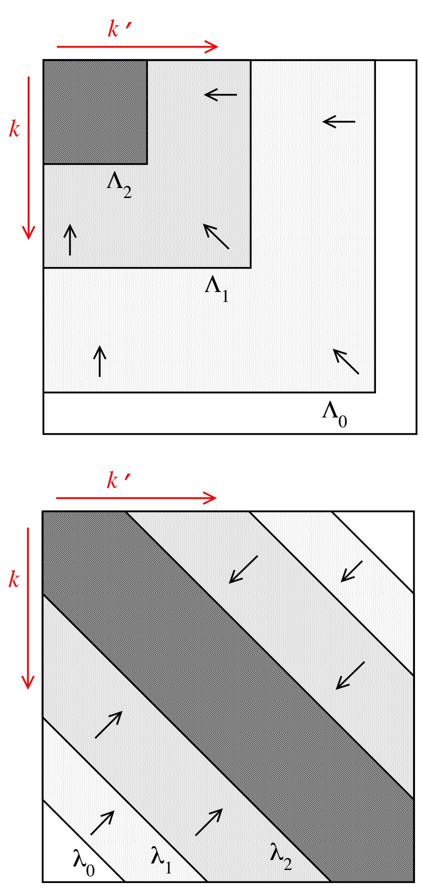
➟ Traditional “hard core” potentials → ➟ “Soft” NN and NNN interactions

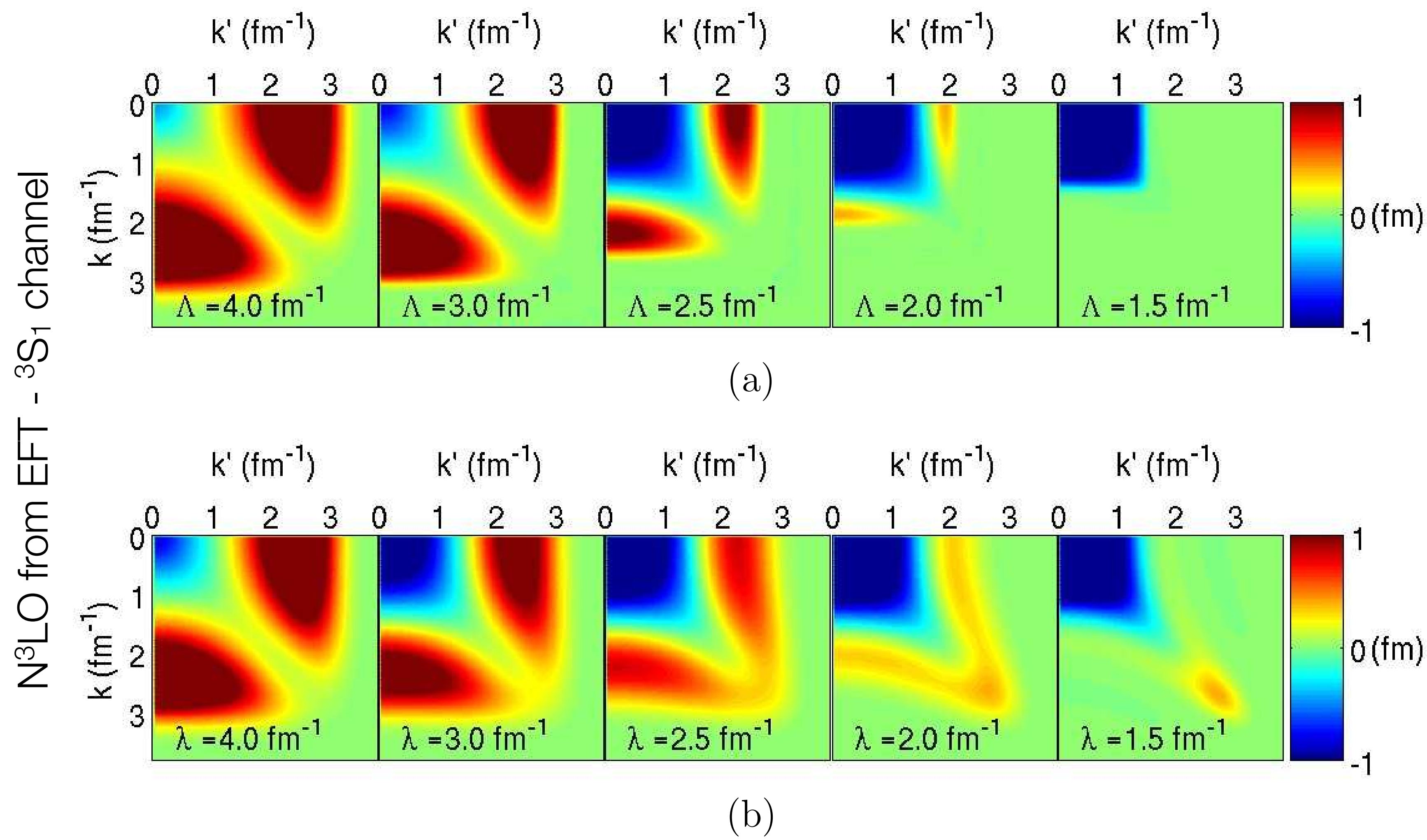
✺ Renormalization group transformations to decouple low and high momenta

(a) $V_{\text{low-k}}$

[Bogner, Furnstahl, Schwenk 2009]

(b) V_{SRG}

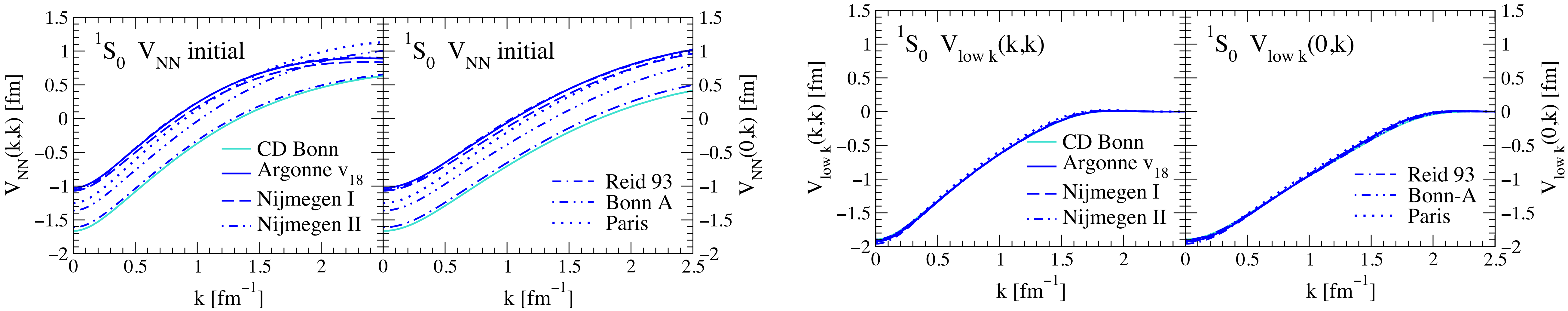




➟ NN scattering phase-shifts and deuteron binding energy conserved

Low-momentum nuclear interactions

- Universality



- RG transformations induce many-body forces

[Bogner, Furnstahl, Schwenk 2009]

- N-body observables are RG invariant if and only if

  1) Induced N-body (e.g. 3-body) forces are kept

  2) N-body calculation is exact

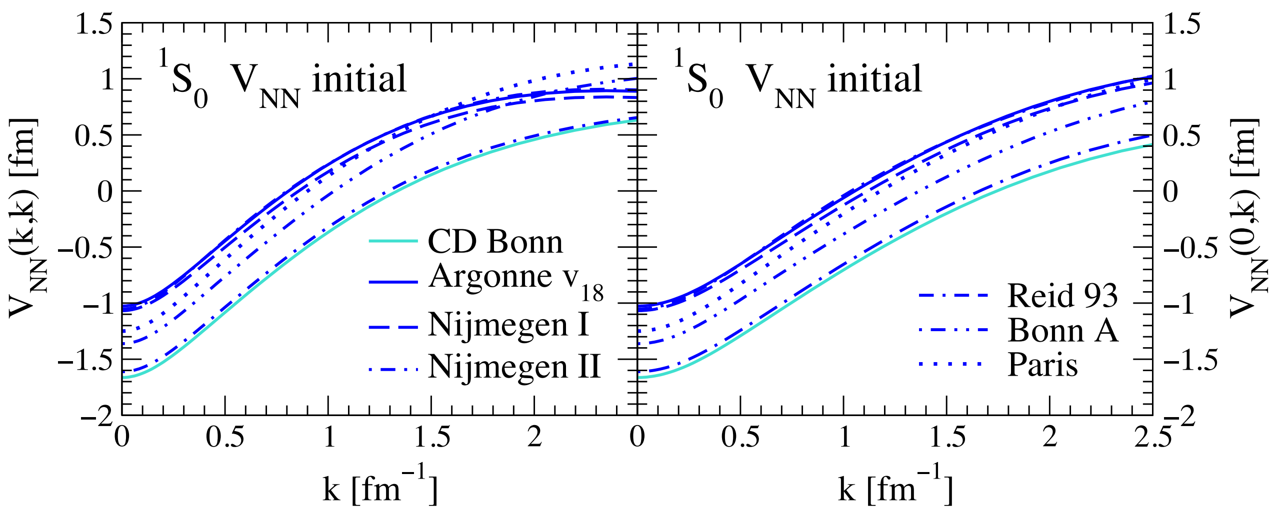
➡ RG cutoff dependence helps tracking

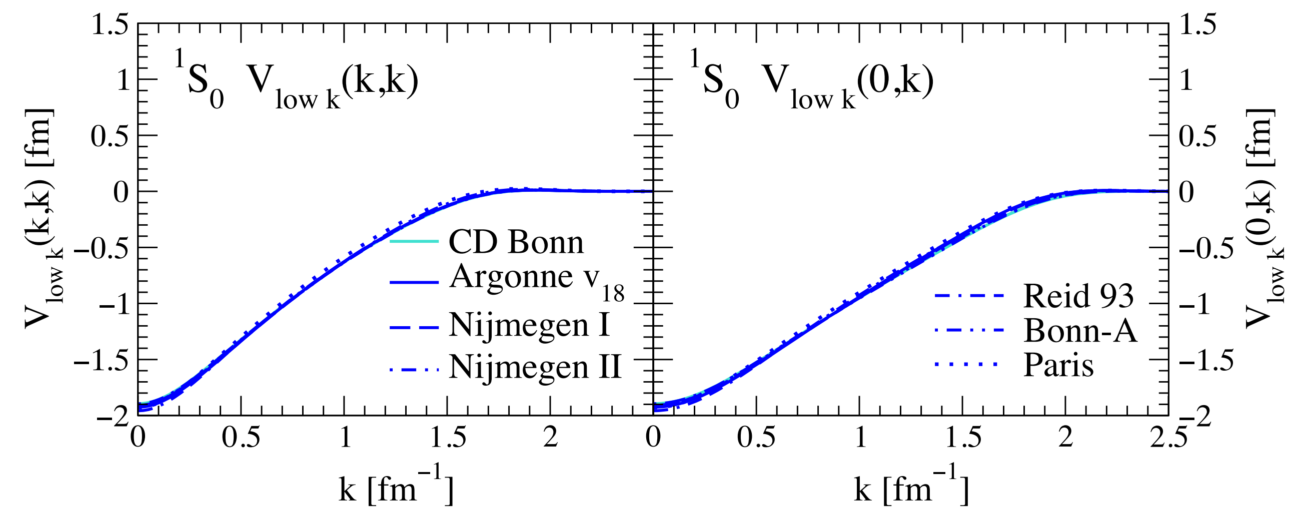
  1) Importance of omitted N-body forces

  2) Incomplete N-body calculation

Low-momentum nuclear interactions

- Universality

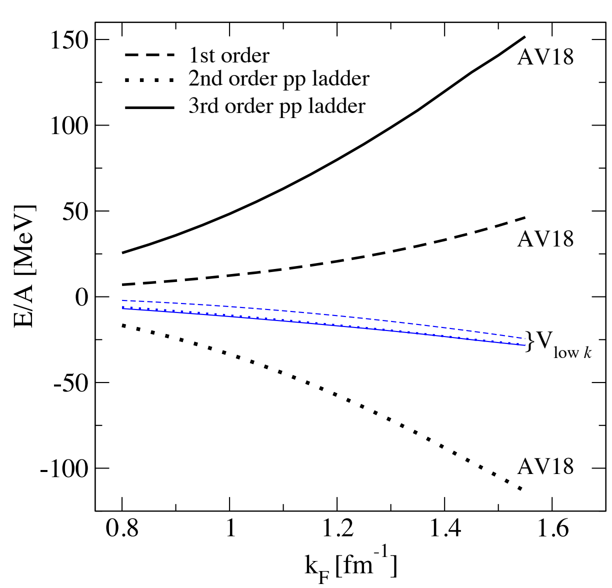


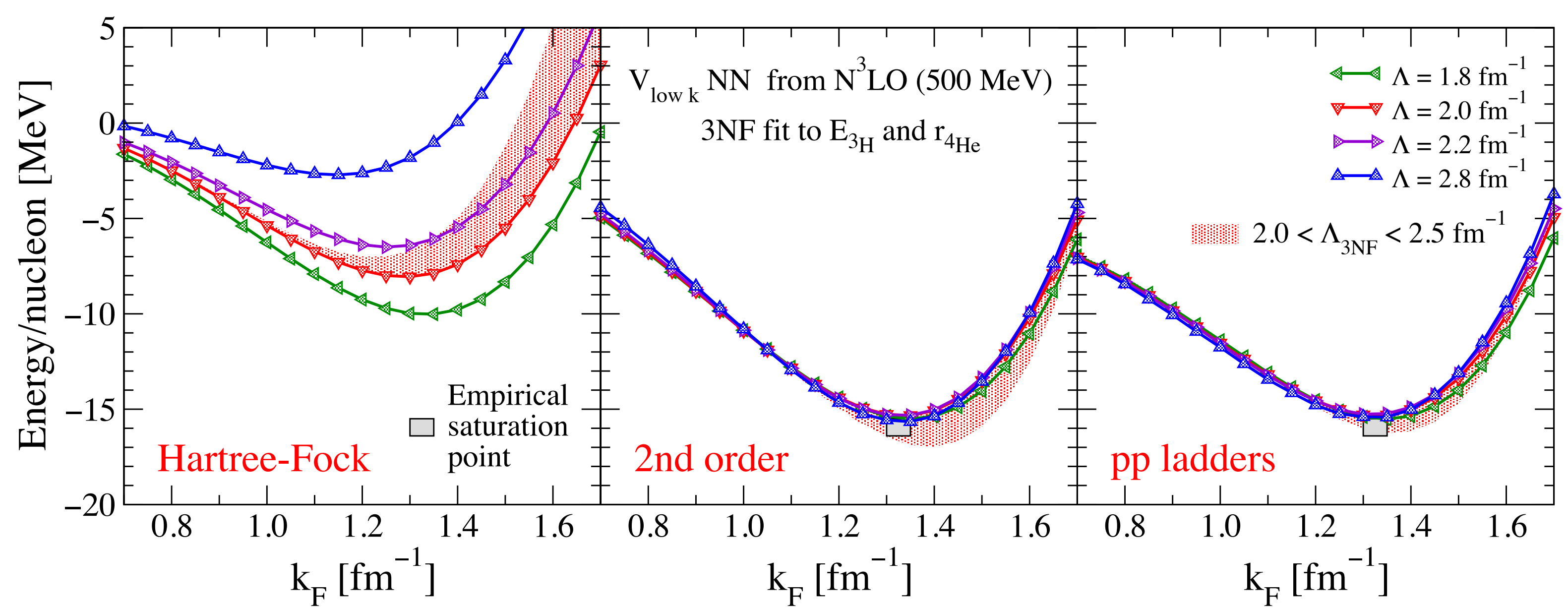


[Bogner, Furnstahl, Schwenk 2009]

- Perturbativeness?

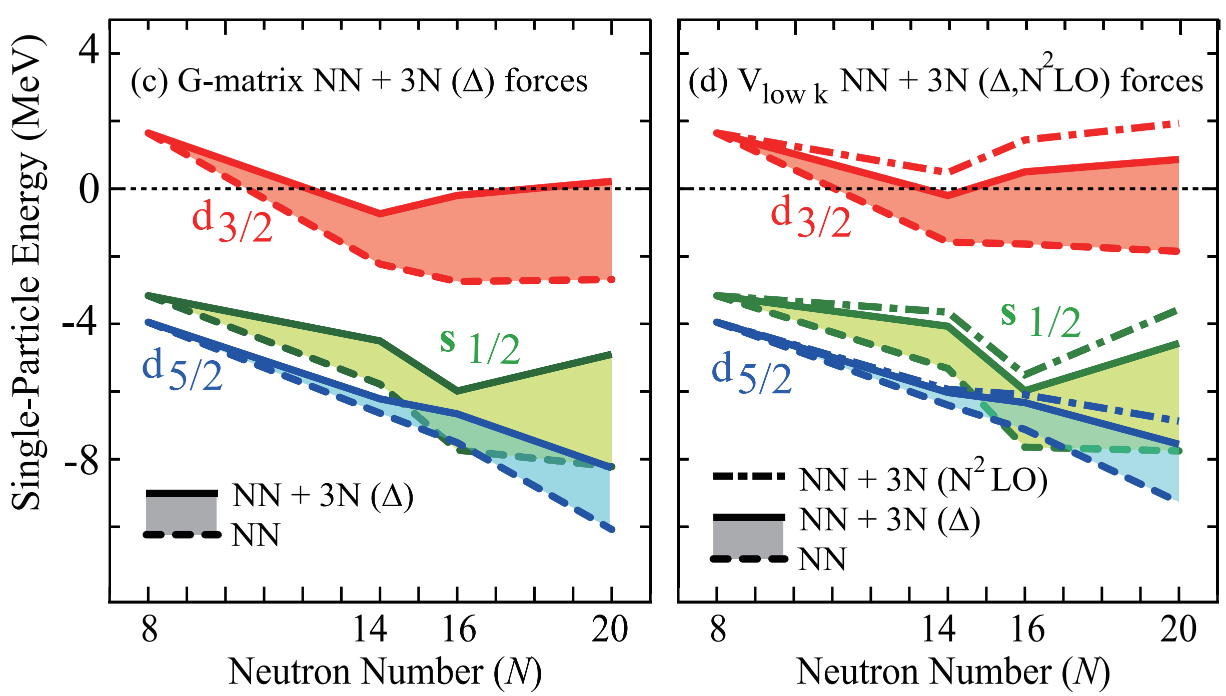
[Bogner, Furnstahl, Nogga, Schwenk 2009]





Three-body forces

- Realistic microscopic calculations cannot avoid the use of NNN forces
  - Binding energies, saturation properties and radii
  - Shell evolution
  - Spin-orbit splitting
  - Three-nucleon scattering



[Otsuka *et al.* 2010]

➟ Dripline location in O isotopes (^{24}O) possibly due to NNN physics

Three-body forces

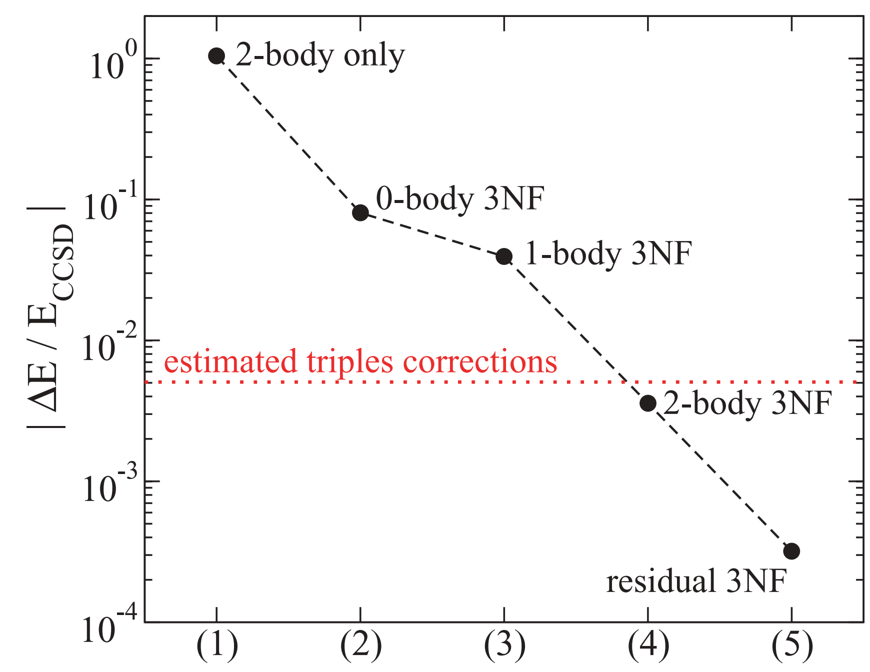
- Realistic microscopic calculations cannot avoid the use of NNN forces
  - Binding energies, saturation properties and radii
  - Shell evolution
  - Spin-orbit splitting
  - Three-nucleon scattering

- Currently: microscopic NNN interactions only in light systems and INM
  - Normal-ordered (average) part of NNN possibly sufficient

➠ Coupled-cluster in ^{4}He [Hagen *et al.* 2007]

➠ SCGF in INM [Somà, Bożek 2008]

➠ Perturbation theory in INM [Hebeler, Schwenk 2009]



Dyson equation & self-energy

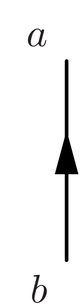
✳ Perturbative expansion of one-body propagator

- ➟ Introduce an auxiliary potential

$$U \equiv \sum_{ab} U_{ab}\, a_a^\dagger a_b$$

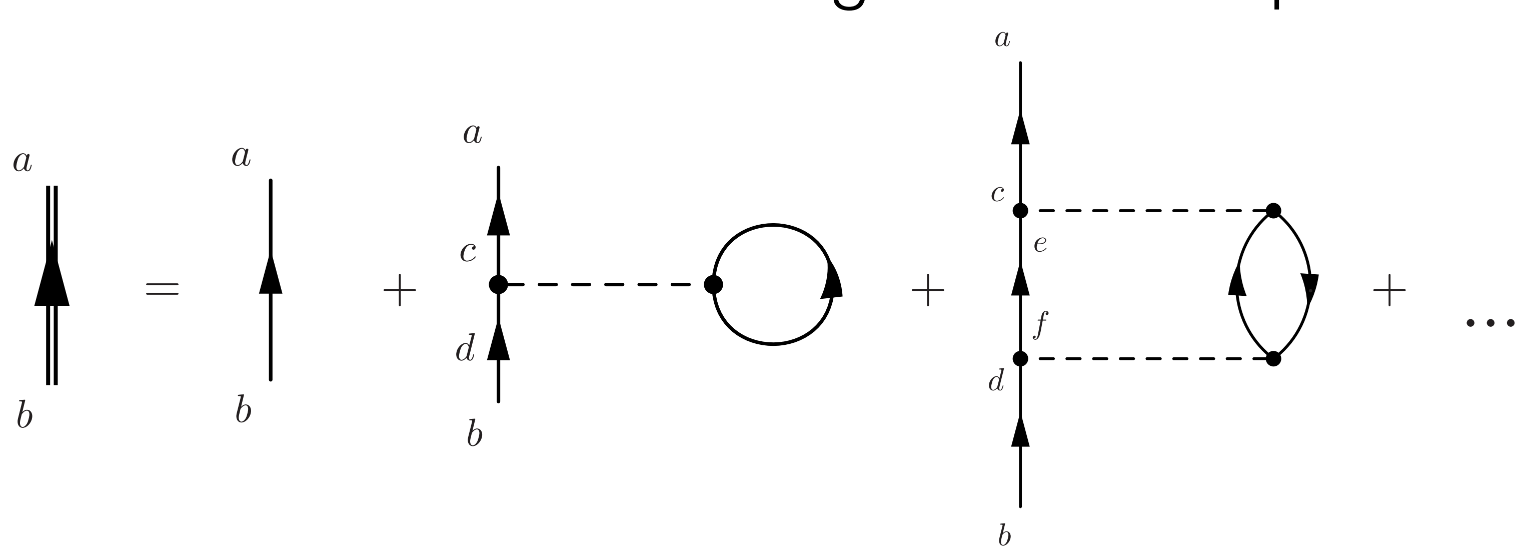
- ➟ Split the Hamiltonian

$$H = \underbrace{T + U}_{\equiv H_0} + \underbrace{V^{NN} + V^{NNN} - U}_{\equiv H_I}$$

- ➟ Define the unperturbed propagator $\equiv$ 

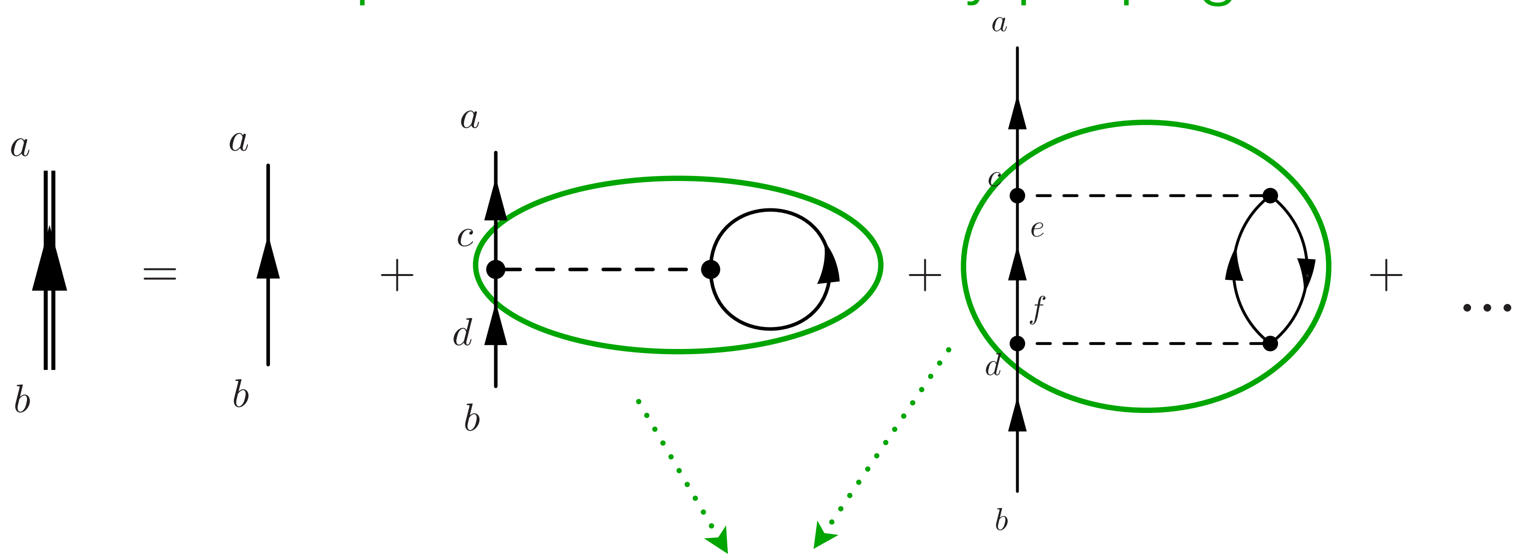
$$\left[G^{(0)}(\omega)\right]^{-1} \equiv \omega - H_0$$

- ➟ Expand G in terms of $G^{(0)}$ through interaction picture



Dyson equation & self-energy

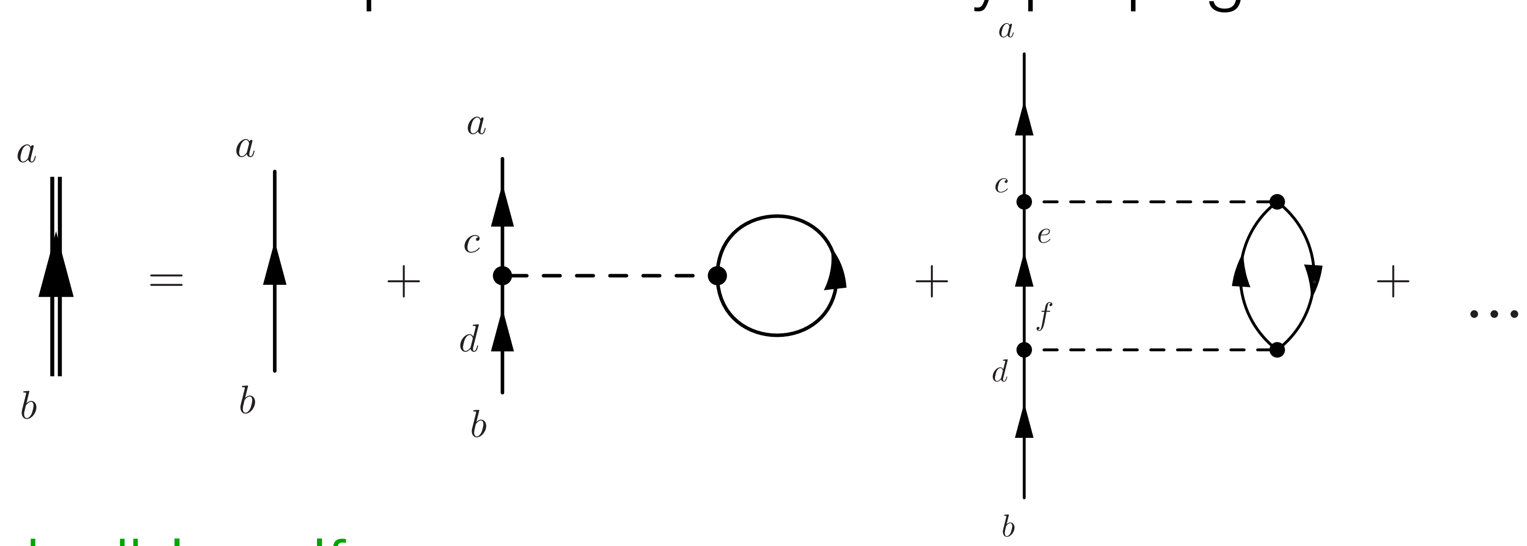
- Perturbative expansion of one-body propagator



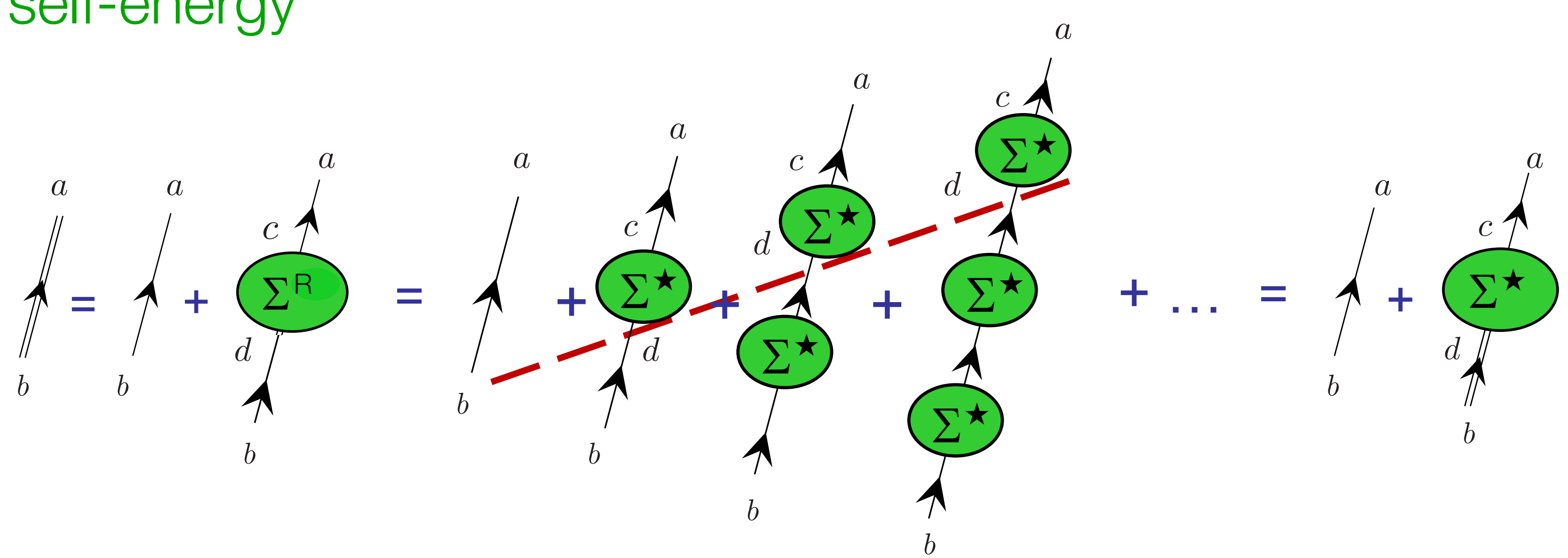
(reducible) self-energy $\Sigma^{R}_{cd}(\omega)$

Dyson equation & self-energy

- Perturbative expansion of one-body propagator

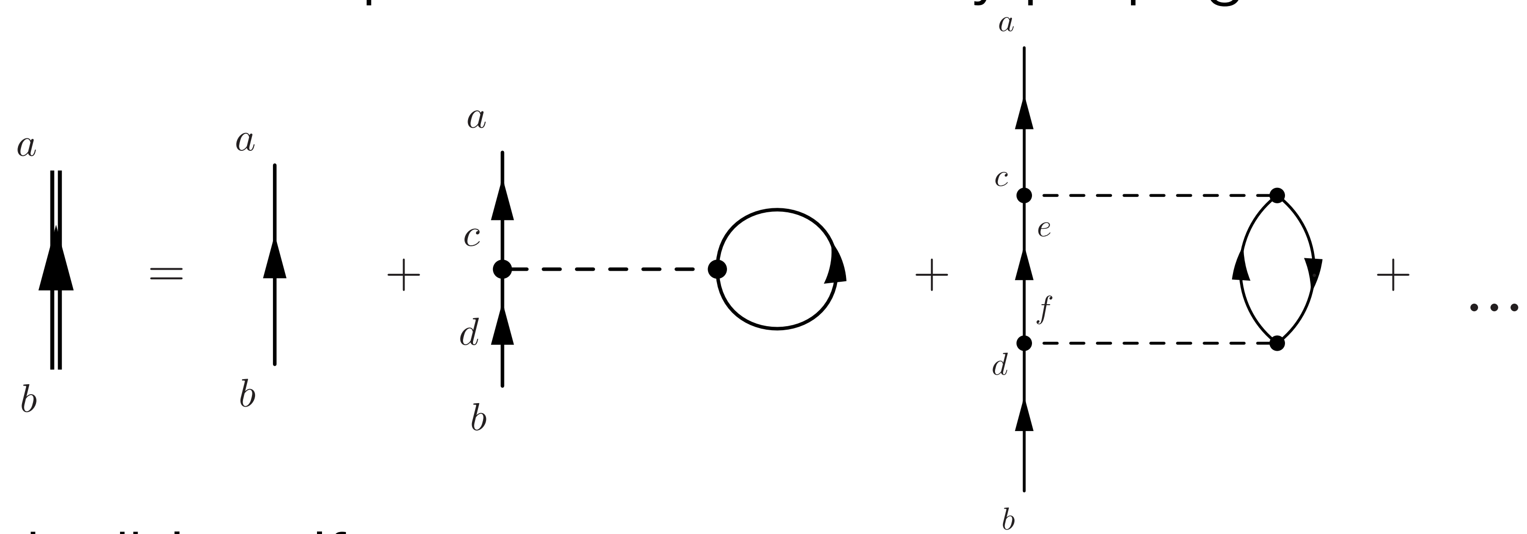


- Irreducible self-energy

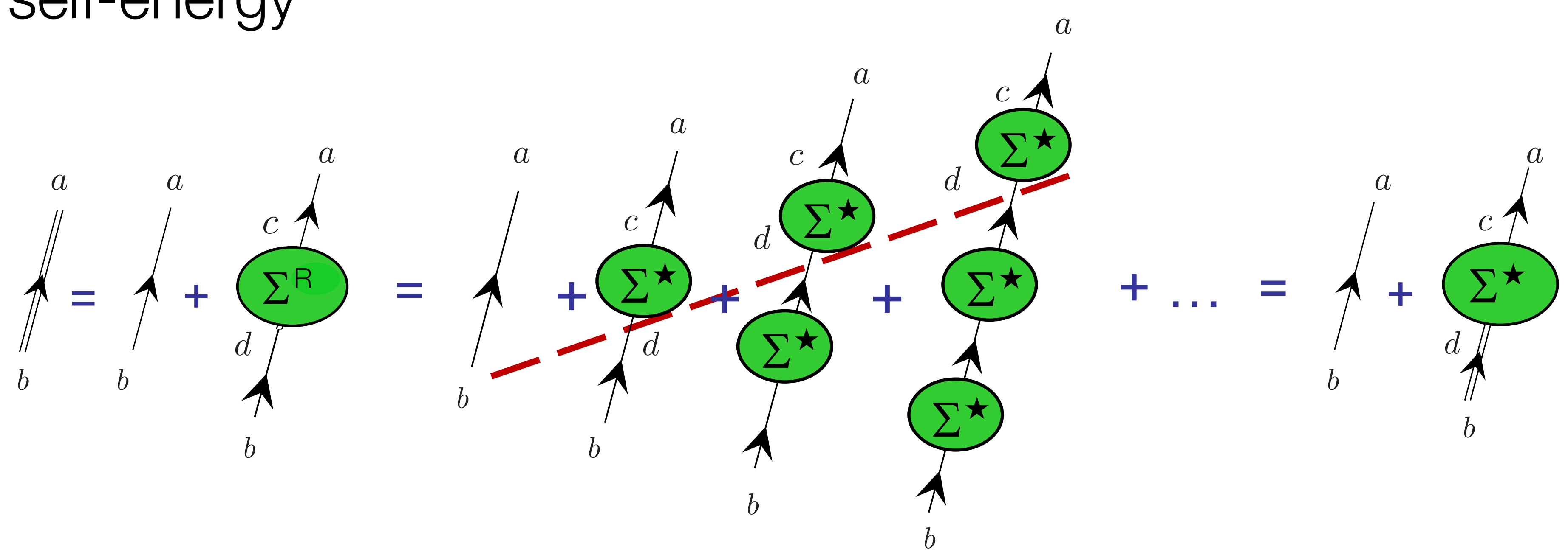


Dyson equation & self-energy

✴ Perturbative expansion of one-body propagator



✴ Irreducible self-energy



✴ Dyson equation

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

Single-particle (dual) basis

- Single-particle basis $\{a_b^\dagger\}$

  → separates in two blocks $\{b, \bar{b}\}$

  → anti-unitary transformation $b \underset{\eta_{\bar{b}}}{\overset{\eta_b}{\rightleftarrows}} \bar{b}$

Dual ⬇ basis

$$\bar{a}_b(t) \equiv \eta_b a_{\bar{b}}(t)$$

$$\bar{a}_b^\dagger(t) \equiv \eta_b a_{\bar{b}}^\dagger(t)$$

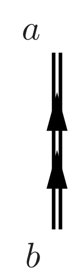
➠ Phase consistently included in all definitions

e.g. $\bar{V}^{NN}_{\bar{a}b\bar{c}d} \equiv \eta_a \, \eta_c \, \langle 1{:}\bar{a}; 2{:}b|V^{NN}|1{:}\bar{c}; 2{:}d\rangle - \eta_a \, \eta_c \, \langle 1{:}\bar{a}; 2{:}b|V^{NN}|1{:}d; 2{:}\bar{c}\rangle$

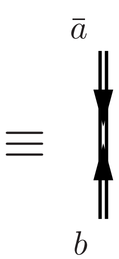
Gorkov-Green's functions

✺ Set of 4 Green's functions

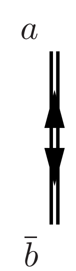
$$i\,G^{11}_{ab}(t,t') \equiv \langle\Psi_0|T\left\{a_a(t)a^\dagger_b(t')\right\}|\Psi_0\rangle \quad \equiv$$



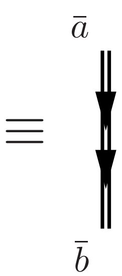
$$i\,G^{21}_{ab}(t,t') \equiv \langle\Psi_0|T\left\{\bar{a}^\dagger_a(t)a^\dagger_b(t')\right\}|\Psi_0\rangle \quad \equiv$$



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



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



[Gorkov 1958]

✺ Nambu matrix formalism

$$\mathbf{A}_a(t) \equiv \begin{pmatrix} a_a(t) \\ \bar{a}^\dagger_a(t) \end{pmatrix}$$

$$\mathbf{A}^\dagger_a(t) \equiv \begin{pmatrix} a^\dagger_a(t) & \bar{a}_a(t) \end{pmatrix}$$

$$i\,\mathbf{G}_{ab}(t,t') \equiv \langle\Psi_0|T\left\{\mathbf{A}_a(t)\mathbf{A}^\dagger_b(t')\right\}|\Psi_0\rangle = i\begin{pmatrix} G^{11}_{ab}(t,t') & G^{12}_{ab}(t,t') \\ G^{21}_{ab}(t,t') & G^{22}_{ab}(t,t') \end{pmatrix}$$

[Nambu 1960]

Derivation of Gorkov equations

✺ Separate **Ω** into an "unperturbed" one-body part and an interacting part

$$\Omega = \underbrace{T + U}_{\equiv \Omega_0} + \underbrace{V^{NN} + V^{NNN} - U}_{\equiv \Omega_I}$$

where $$U \equiv \sum_{ab} \left[U_{ab}\, a_a^\dagger a_b - U_{ab}\, \bar{a}_a \bar{a}_b^\dagger + \tilde{U}_{ab}\, a_a^\dagger \bar{a}_b^\dagger + \tilde{U}_{ab}^\dagger\, \bar{a}_a a_b \right]$$

⬇

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

Gorkov equations

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

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

Application to 0+ systems

✷ Use time-reversal transformation to define the dual basis

$$b \equiv (n, \pi, j, m, q)$$
$$\bar{b} \equiv (n, \pi, j, -m, q)$$

$$\bar{a}^{\dagger}_{n\pi jmq} \equiv \eta_{\pi jm}\, a^{\dagger}_{n\pi j-mq}$$
$$\bar{a}_{n\pi jmq} \equiv \eta_{\pi jm}\, a_{n\pi j-mq}$$

with $\eta_{\pi jm} \equiv \pi\,(-1)^{j+m}$

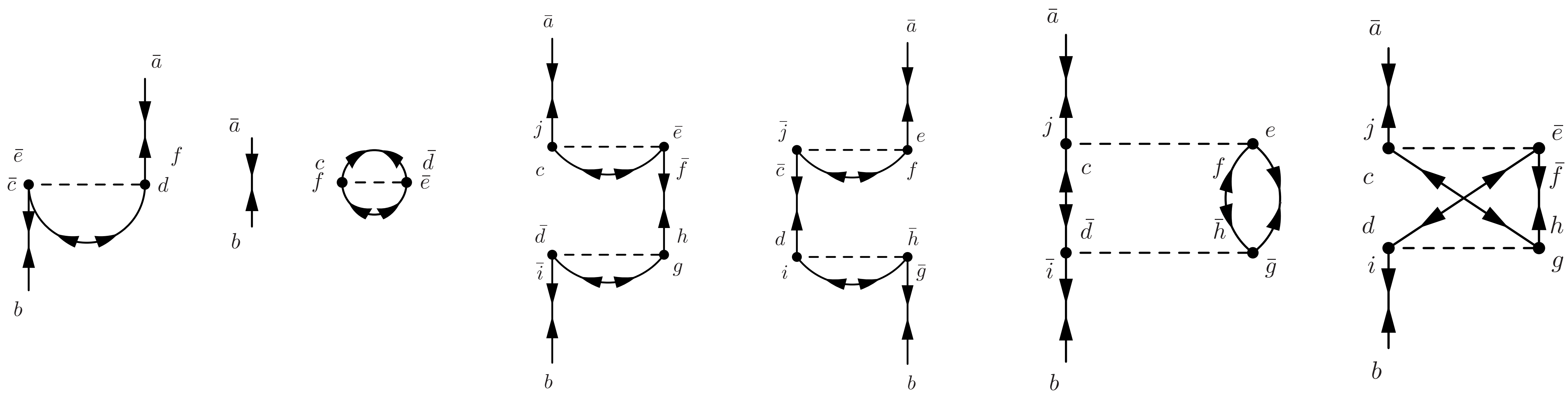
✷ Eigenvalue problem is block-diagonal in *j* and *l* as well as independent of *m*

$$\omega_k\, \mathcal{U}^{n_k}_{n_a\,[\alpha]} = \sum_{n_b} \Big[(t^{[\alpha]}_{n_a n_b} - \mu^{[q_a]}\,\delta_{n_a n_b} + \Lambda^{[\alpha]}_{n_a n_b})\, \mathcal{U}^{n_k}_{n_b\,[\alpha]} + \tilde{h}^{[\alpha]}_{n_a n_b}\, \mathcal{V}^{n_k}_{n_b\,[\alpha]} \Big]$$
$$+ \sum_{n_{k_1} n_{k_2} n_{k_3}} \sum_{\kappa_1 \kappa_2 \kappa_3} \sum_{J} \Big[\mathcal{C}^{n_{k_1} n_{k_2} n_{k_3}}_{n_a\,[\alpha\kappa_3\kappa_1\kappa_2]\,J}\, \mathcal{W}^{n_{k_1} n_{k_2} n_{k_3}}_{n_k\,[\kappa_3\kappa_1\kappa_2]\,J} - \mathcal{D}^{n_{k_1} n_{k_2} n_{k_3}\,\dagger}_{n_a\,[\alpha\kappa_3\kappa_1\kappa_2]\,J}\, \mathcal{Z}^{n_{k_1} n_{k_2} n_{k_3}}_{n_k\,[\kappa_3\kappa_1\kappa_2]\,J} \Big]$$

$$\omega_k\, \mathcal{V}^{n_k}_{n_a\,[\alpha]} = \sum_{n_b} \Big[-(t^{[\alpha]}_{n_a n_b} - \mu^{[q_a]}\,\delta_{n_a n_b} + \Lambda^{[\alpha]}_{n_a n_b})\, \mathcal{V}^{n_k}_{n_b\,[\alpha]} + \tilde{h}^{[\alpha]\,\dagger}_{n_a n_b}\, \mathcal{U}^{n_k}_{n_b\,[\alpha]} \Big]$$
$$+ \sum_{n_{k_1} n_{k_2} n_{k_3}} \sum_{\kappa_1 \kappa_2 \kappa_3} \sum_{J} \Big[-\mathcal{D}^{n_{k_1} n_{k_2} n_{k_3}\,\dagger}_{n_a\,[\alpha\kappa_3\kappa_1\kappa_2]\,J}\, \mathcal{W}^{n_{k_1} n_{k_2} n_{k_3}}_{n_k\,[\kappa_3\kappa_1\kappa_2]\,J} + \mathcal{C}^{n_{k_1} n_{k_2} n_{k_3}}_{n_a\,[\alpha\kappa_3\kappa_1\kappa_2]\,J}\, \mathcal{Z}^{n_{k_1} n_{k_2} n_{k_3}}_{n_k\,[\kappa_3\kappa_1\kappa_2]\,J} \Big]$$

Diagrammatic rules (1)

- To obtain all m-order terms in the expansion of G:
  1 ▪ Draw all
    i) topologically distinct connected direct diagrams
    ii) with m interaction lines
    iii) with $2m+1$ propagation lines (with two indices each)



(a) (b) (c) (d) (e) (f)

Diagrammatic rules (1)

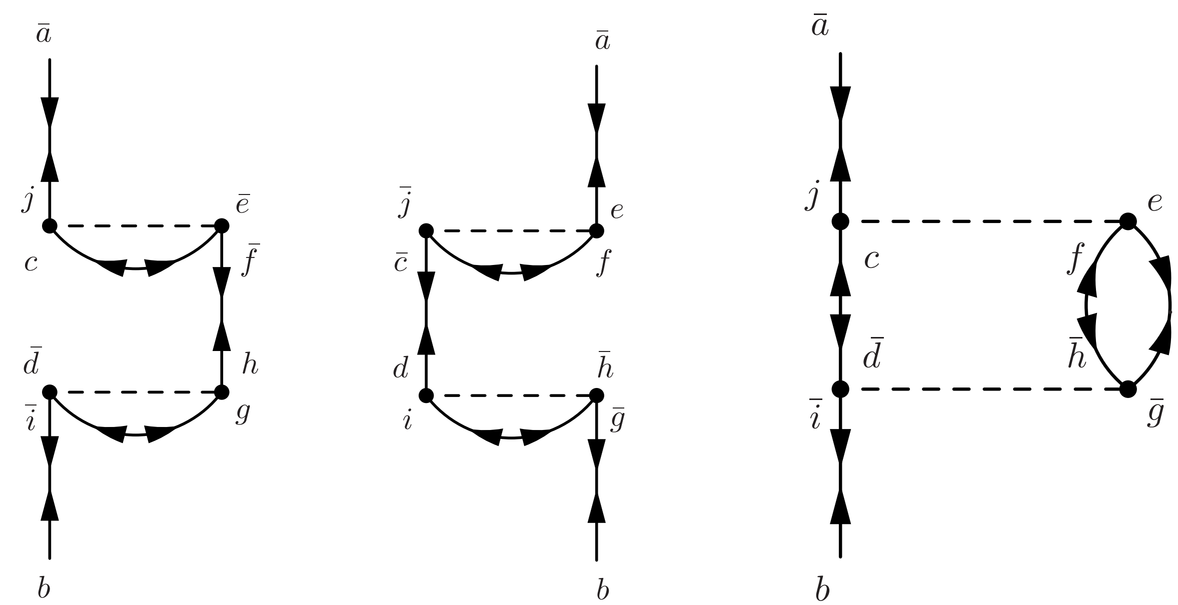
✺ To obtain all *m*-order terms in the expansion of G:

1 ▪ Draw all

i) topologically distinct connected direct diagrams

ii) with *m* interaction lines

iii) with 2*m*+1 propagation lines (with two indices each)



(c) (d) (e)

➠ Diagrams (c) and (d) are topologically equivalent

➠ Diagrams (c) and (e) are topologically distinct

Diagrammatic rules (1)

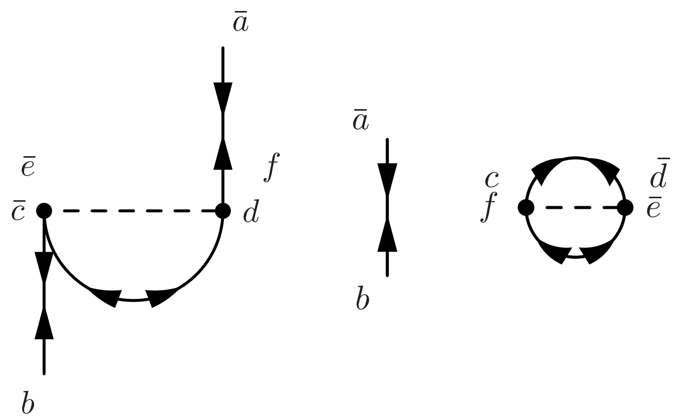
✺ To obtain all *m*-order terms in the expansion of G:

1 ▪ Draw all

i) topologically distinct connected direct diagrams

ii) with *m* interaction lines

iii) with 2*m*+1 propagation lines (with two indices each)



(a) (b)

➠ Diagram (a) is connected

➠ Diagram (b) is disconnected

Diagrammatic rules (1)

✺ To obtain all *m*-order terms in the expansion of G:

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i) topologically distinct connected direct diagrams

ii) with *m* interaction lines

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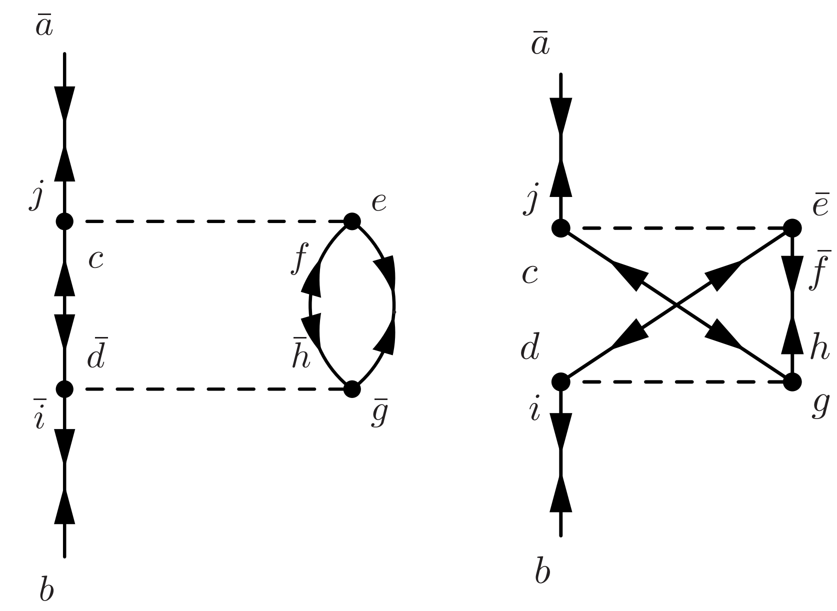
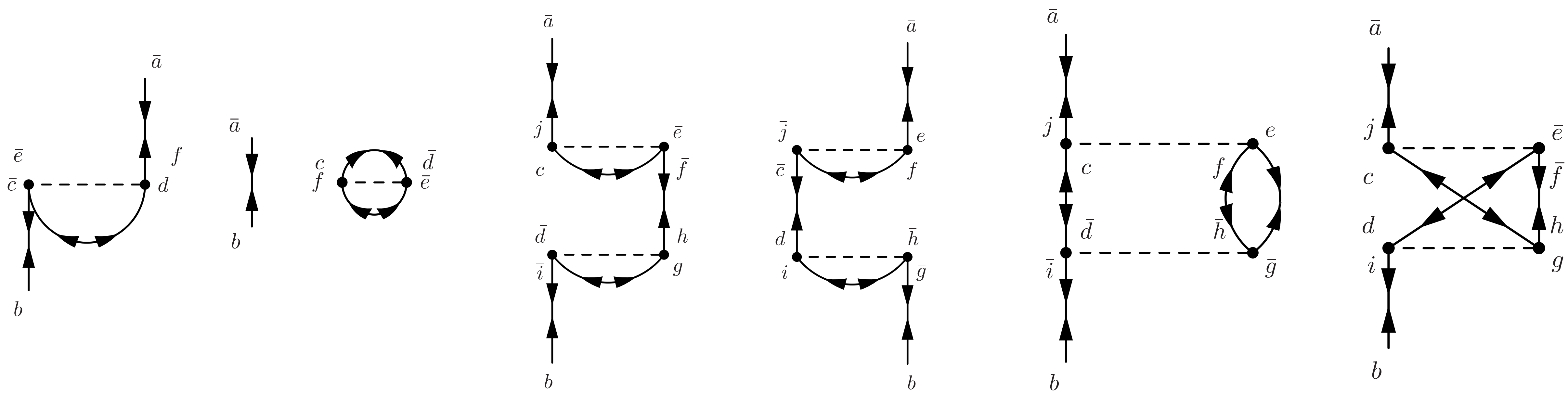


(e) (f)

➟ If one assumes diagram (e) to be direct, diagram (f) is its exchange

Diagrammatic rules (1)

- To obtain all m-order terms in the expansion of G:
  1 ▪ Draw all
    i) topologically distinct connected direct diagrams
    ii) with m interaction lines
    iii) with $2m+1$ propagation lines (with two indices each)



(a) (b) (c) (d) (e) (f)

2 ▪ Assign energy to each propagation line / energy is conserved at each vertex

Diagrammatic rules (2)

3 ■ Attribute $\bar{V}^{NN}_{abcd}$ to each interaction and $G_{ab}(\omega)$ to each propagator

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4 ▪ Write down factors

❶ i^m

❷ 1/2 for each pair of equivalent propagation lines (only antisymmetrized V)

❸ 1/2 for each anomalous propagator connecting the same interaction

❹ $(-1)^{N_C+N_A}$ where

a) N_C is the number of closed fermionic loops

b) N_A is the number of anomalous contractions

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5 ▪ Sum over all internal indices and integrate over all internal energies

Diagrammatic rules (3)

6 ▪ Derive the corresponding self-energy expansion by cutting external legs

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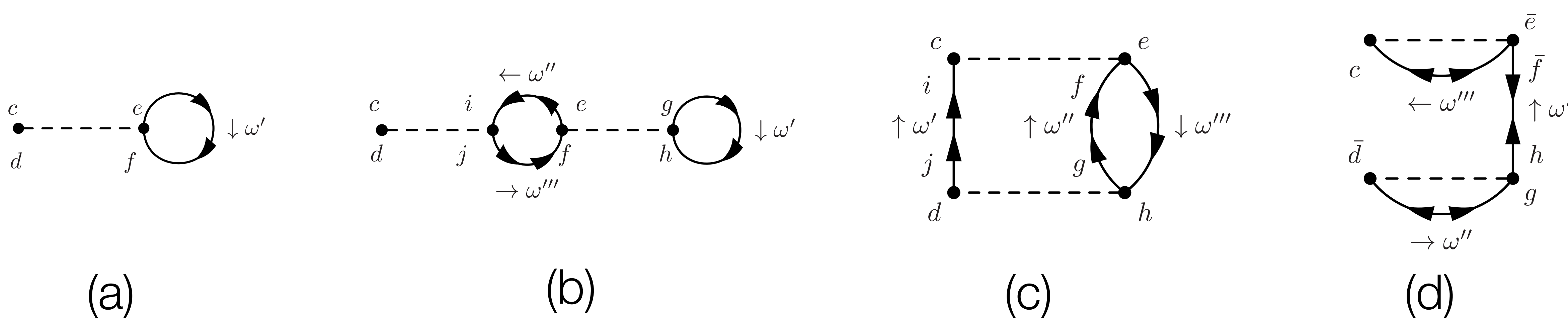


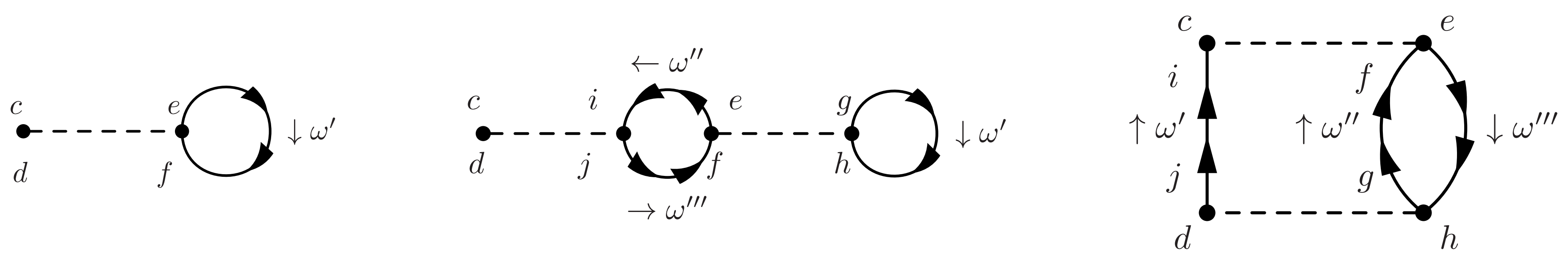
➟ Diagrams (a), (b) and (c) are irreducible

➟ Diagram (d) is reducible

Diagrammatic rules (3)

6 ▪ Derive the corresponding self-energy expansion by cutting external legs

7 ▪ Self-consistent schemes keep irreducible skeleton self-energy terms only



(a) (b) (c)

➟ Diagrams (a) and (c) are skeleton diagrams

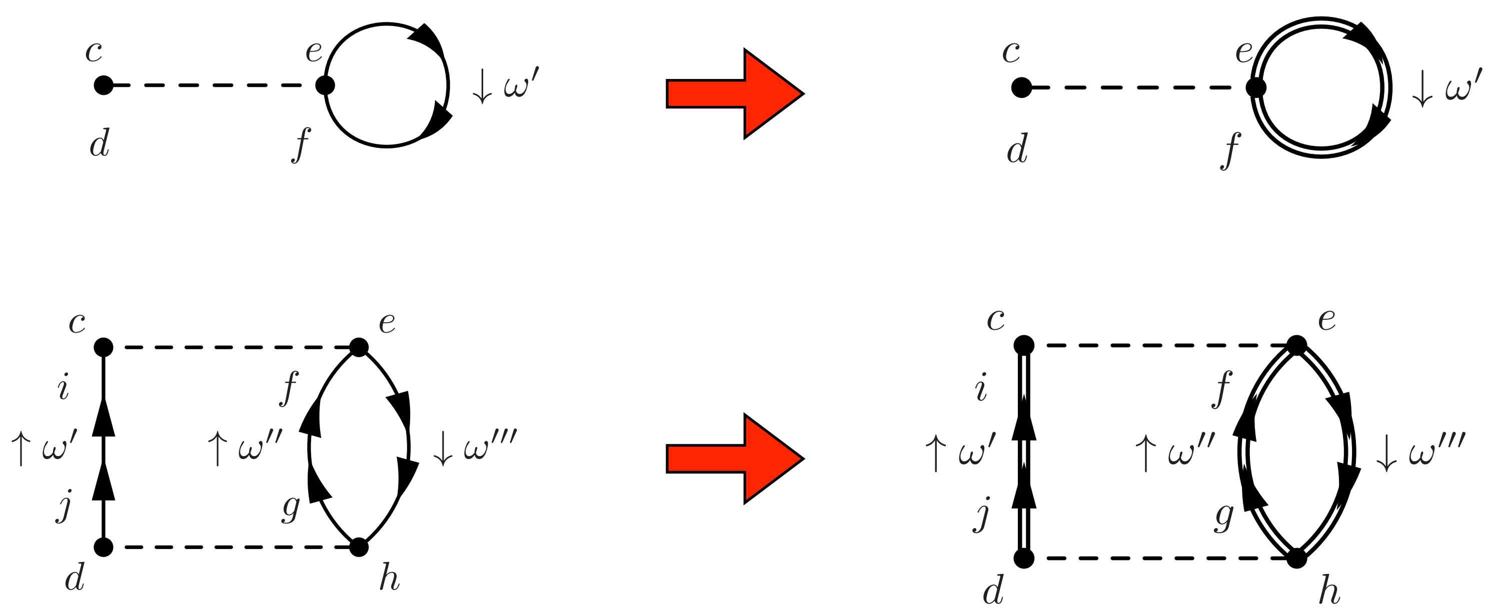
➟ Diagram (b) is a composed diagram

Diagrammatic rules (3)

6 ▪ Derive the corresponding self-energy expansion by cutting external legs

7 ▪ Self-consistent schemes keep irreducible skeleton self-energy terms only

8 ▪ Substitute all *unperturbed* propagators with *dressed* ones



...

Scaling

- Eigenvalue problem

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

- Numerical scaling

$$m_{p,1} \approx \binom{N_b}{3} \propto \frac{N_b^3}{6}$$

M_p, m_p, $2N_b$, N_b

h	$\tilde{h}$	C	$-D^\dagger$
$\tilde{h}^\dagger$	$-h$	$-D^\dagger$	C
$C^\dagger$	$-D$	E	0
$-D$	$C^\dagger$	0	$-E$

N_{tot}

N_b → dimension of the s.p. basis

n → number of iterations

$$N_{tot,1} = 2N_b + M_{p,1} \approx N_b^3$$

...

$$N_{tot,n} = 2N_b + M_{p,n} \approx N_b^{3n}$$

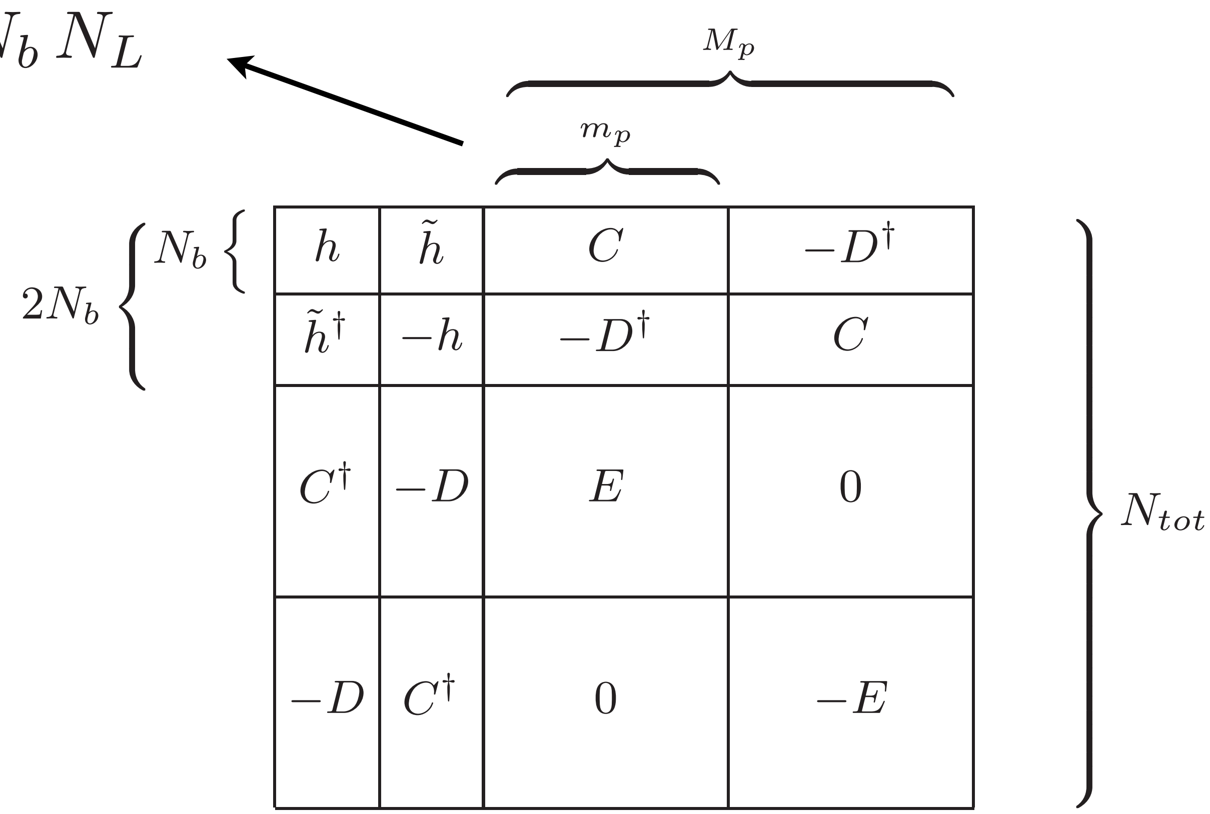
Lanczos algorithm

- Eigenvalue problem

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

- Numerical scaling with Lanczos

$$m'_p = 2\,N_b\,N_L$$



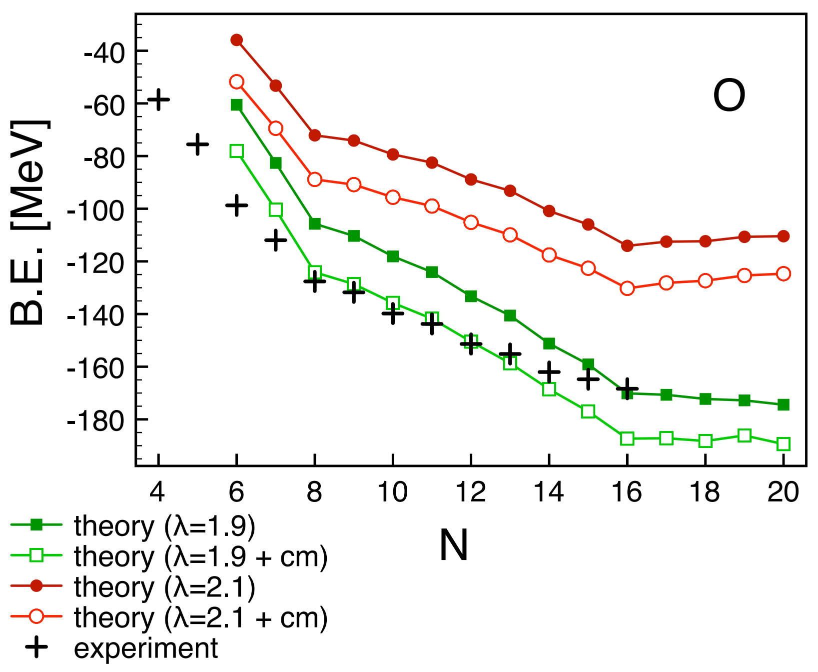
N_b → dimension of the s.p. basis

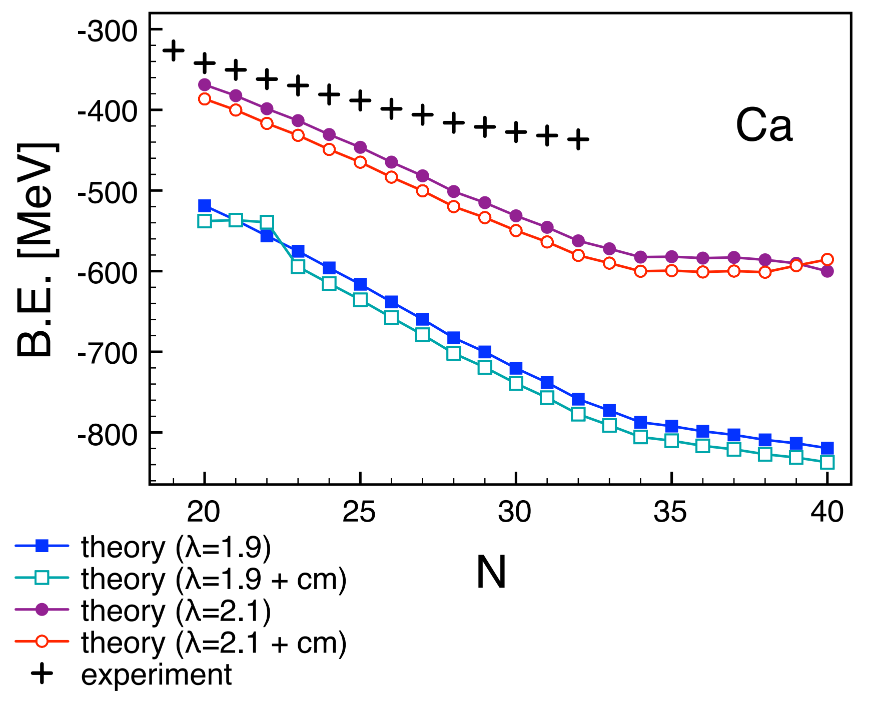
N_L → number of Lanczos iterations

$$N'_{tot} = 2N_b + 2\,m'_p = 2\,N_b(1+N_L)$$

Centre-of-mass correction

- Total binding energies





- Odd-even mass differences