# Self-consistent Gorkov Green's function theory for nuclei


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*Outline:*

1. Status of ab initio nuclear structure
2. Gorkov-Green's function theory
3. Results for open-shell nuclei

*In collaboration with*

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ESNT workshop

*Near-degenerate systems from ab initio many-body methods*

CEA Saclay, 1 April 2015

# Ab initio nuclear structure

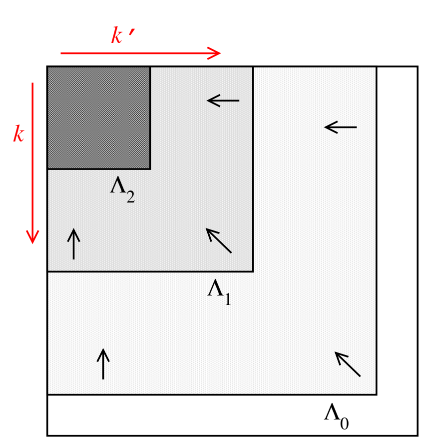
Long-term goal: predictive nuclear structure calculations

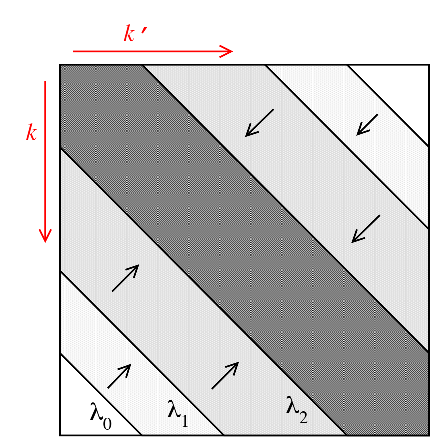
- ➟ Half of bound nuclei never observed, many poorly known
- ➟ Thorough quantification of theoretical errors (**Hamiltonian** & **many-body**)

Nuclear Hamiltonian not fixed

- ➟ **Traditional models**: strong repulsive core
- ➟ **Modern models**: softer core, towards a systematic expansion, consistent 3NF
- ➟ Major breakthrough: $\mathbf{V_{low\text{-}k}}$ or **SRG** of NN+3N interactions

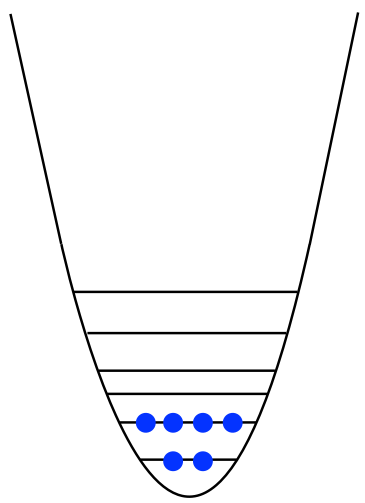
$V_{\text{low-k}}$



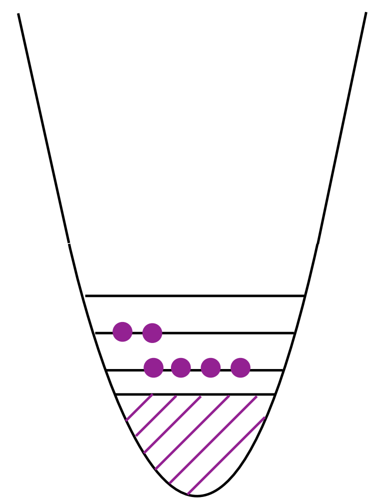

$V_{\text{SRG}}$

# Different nuclear ab initio strategies



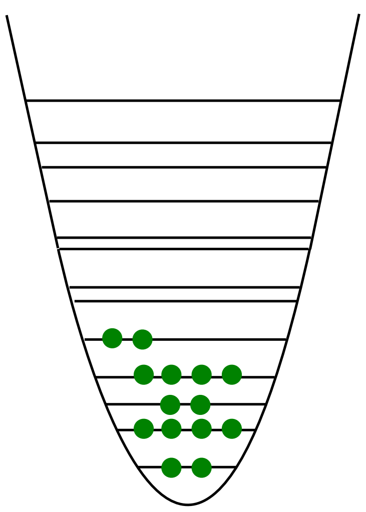
Virtually exact

NCSM, GFMC, ....



Valence space

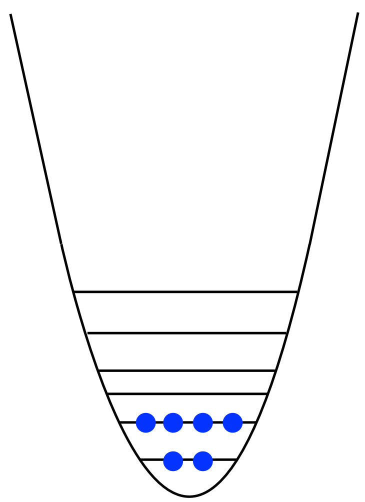
Shell model



Based on expansion

GF, CC, IM-SRG, ....

# Different nuclear ab initio strategies



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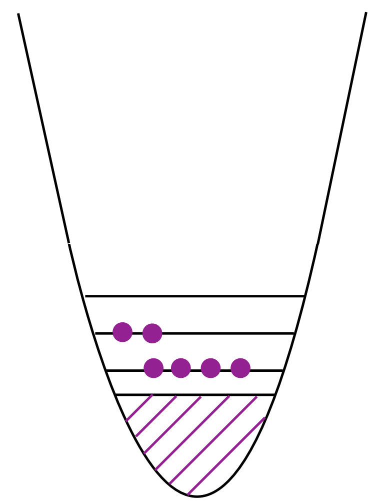
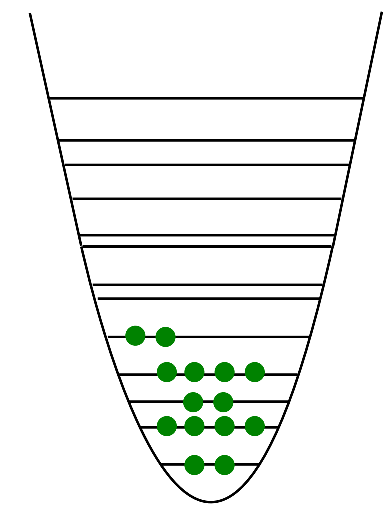


Valence space

Shell model



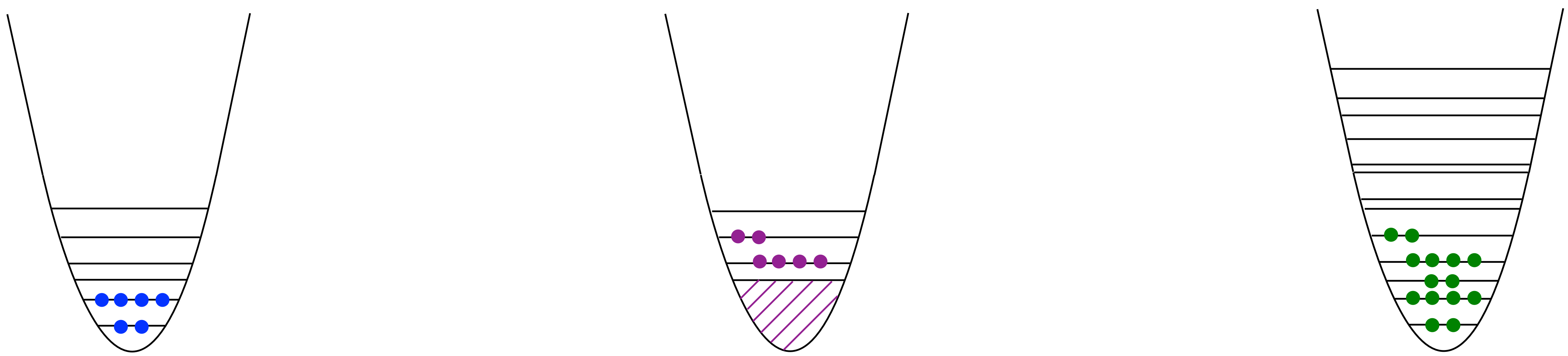
Based on expansion

GF, CC, IM-SRG, ....

**5-10 years ago**

- Hard repulsive core requires **large model spaces** to converge
- Open-shell: degeneracy w.r.t. particle-hole excitation → **expansion breaks down**

# Different nuclear ab initio strategies



Virtually exact | Valence space | Based on expansion
NCSM, GFMC, .... | Shell model | GF, CC, IM-SRG, ....

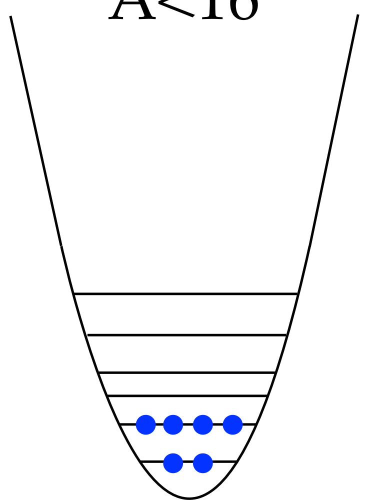
**Today**

- **Soft interactions** yield converged calculations in **smaller model spaces**
- Development of **new methods** allows to tackle **open-shell nuclei**

# Different nuclear ab initio strategies

### Light nuclei

A<16

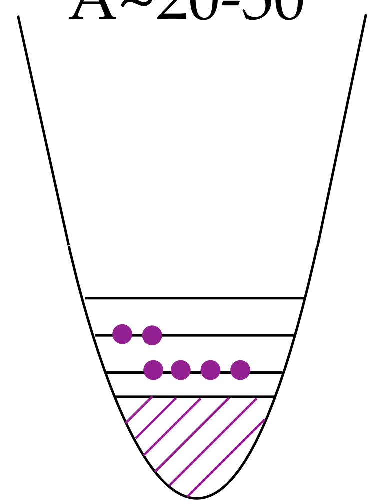


Virtually exact

NCSM, GFMC, ….

### Medium-mass nuclei

A~20-50

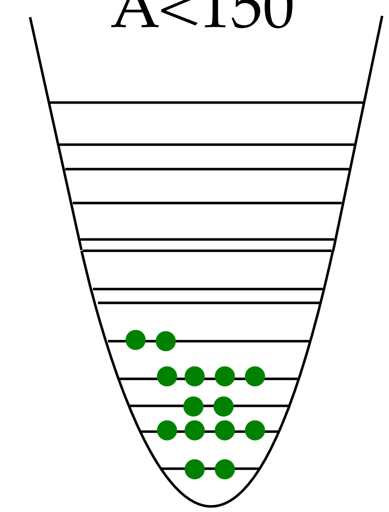


Valence space

**Ab initio** SM

### Mid/heavy nuclei

A<150



Based on expansion

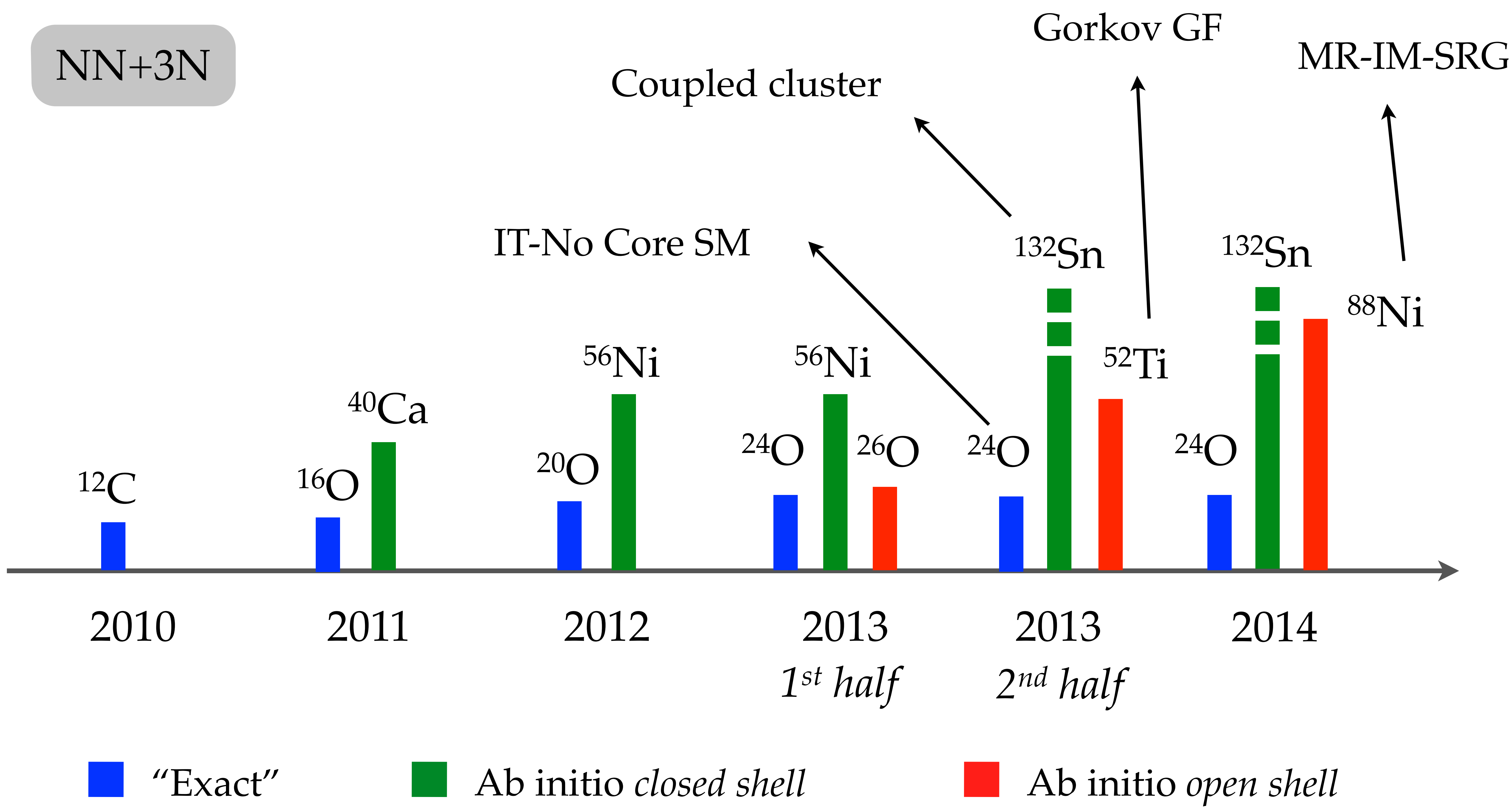
GF, CC, IM-SRG, ….

**Today**

- **Soft interactions** yield converged calculations in **smaller model spaces**
- Development of **new methods** allows to tackle **open-shell nuclei**

# Current limits / reach of nuclear ab initio calculations

➟ Heavier system computed in the different types of ab initio



# Gorkov framework

Idea: expand around an auxiliary many-body state

$$|\Psi_0\rangle \equiv \sum_A^{\text{even}} c_A \, |\psi_0^A\rangle$$

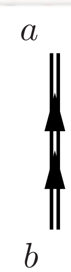
Breaks particle-number symmetry

- ➟ Introduce a "grand-canonical" potential $\Omega = H - \mu A$
- ➟ $|\Psi_0\rangle$ minimizes $\Omega_0 = \langle \Psi_0 | \Omega | \Psi_0 \rangle$ under the constraint $A = \langle \Psi_0 | A | \Psi_0 \rangle$
- ➟ Observables of the A-body system $\Omega_0 = \sum_{A'} |c_{A'}|^2 \, \Omega_0^{A'} \approx E_0^A - \mu A$

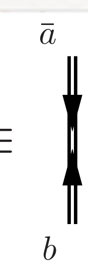
⬇ set of 4 propagators

[Gorkov 1958]

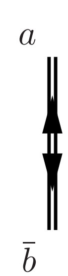
$$i\, G^{11}_{ab}(t,t') \equiv \langle \Psi_0 | T \left\{ a_a(t) a_b^\dagger(t') \right\} | \Psi_0 \rangle \equiv$$



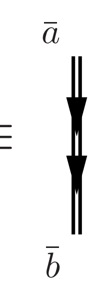

$$i\, G^{21}_{ab}(t,t') \equiv \langle \Psi_0 | T \left\{ \bar{a}_a^\dagger(t) a_b^\dagger(t') \right\} | \Psi_0 \rangle \equiv$$




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




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



# Gorkov equation & self-energy expansion

Many-body Schrödinger equation

$$H\Psi = E\Psi$$

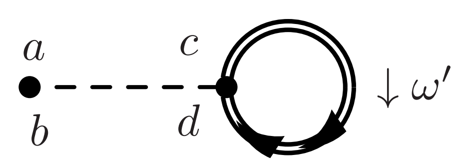
Dyson / Gorkov equation

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

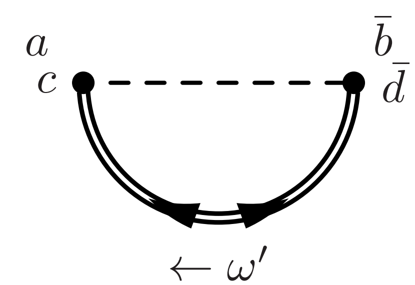
where $\mathbf{G}(\omega) = \begin{pmatrix} G^{11}(\omega) & G^{12}(\omega) \\ G^{21}(\omega) & G^{22}(\omega) \end{pmatrix}$

Current self-energy truncation: **first**- and **second-order** diagrams [Somà, Duguet & Barbieri 2011]

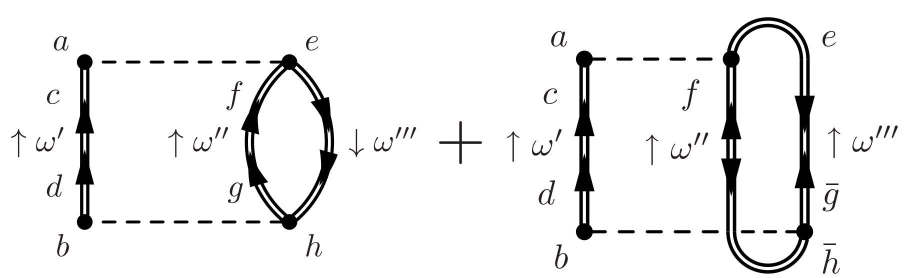
$\Sigma^{11\,(1)}_{ab} =$



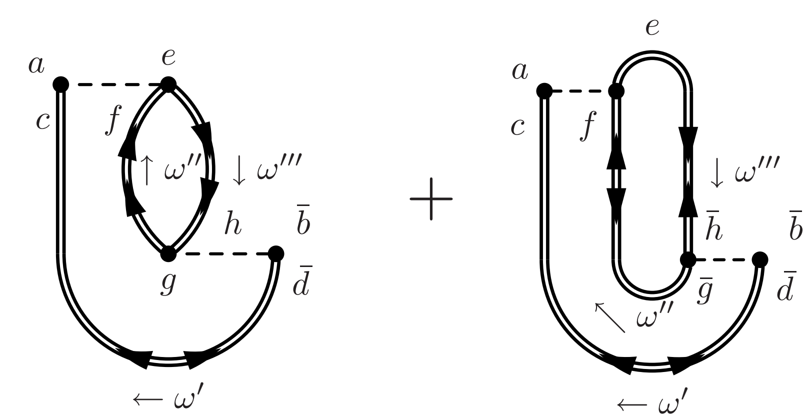

$\Sigma^{12\,(1)}_{ab} =$




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

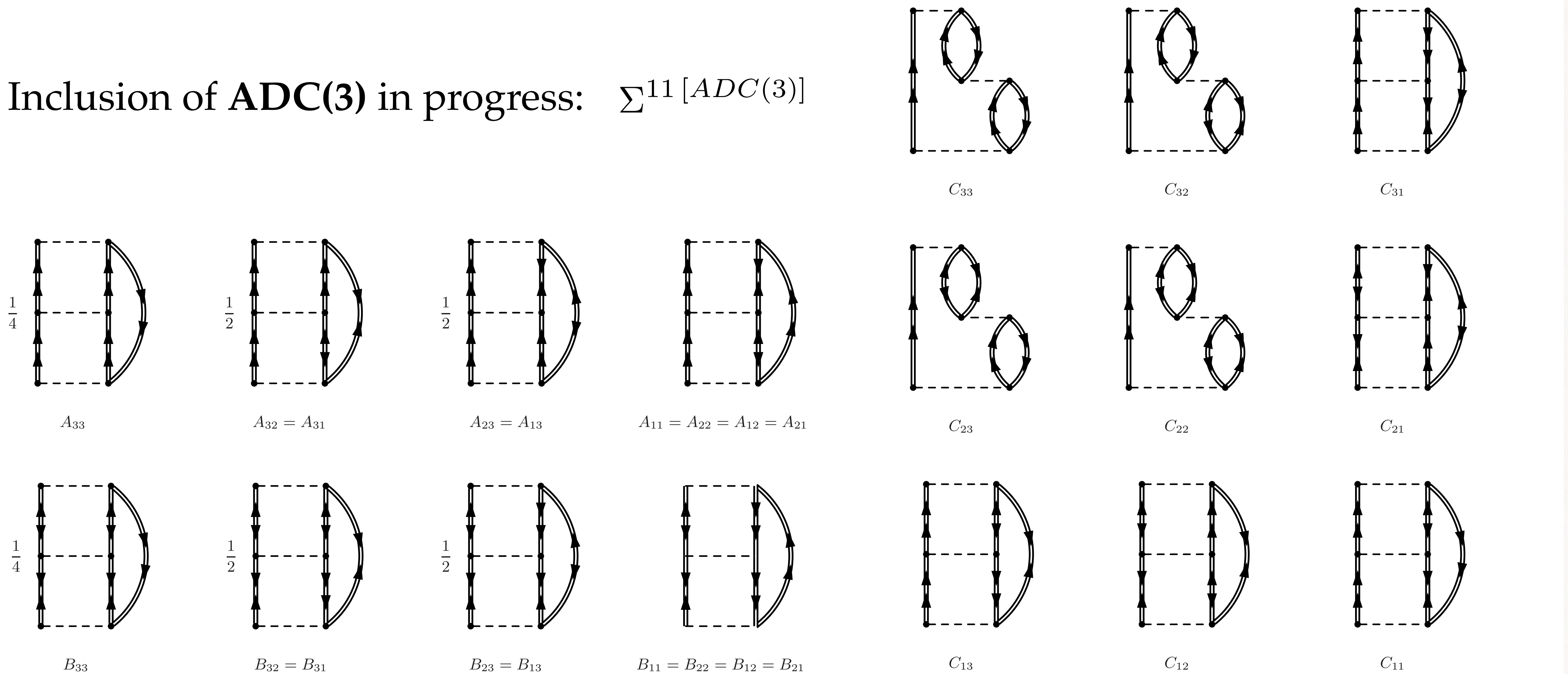



$\Sigma^{12\,(2)}_{ab}(\omega) =$



# Gorkov equation & self-energy expansion

Inclusion of **ADC(3)** in progress: $\Sigma^{11\,[ADC(3)]}$




***ADC(n)***
***# diagrams***

| *n* | **1** | **2** | **3** |
|---|---|---|---|
| Dyson | 1 | 1 | 2 |
| Gorkov | 2 | 4 | 34 |

[Barbieri, Duguet & Somà *in prep.*]

# Gorkov equation & self-energy expansion

**Many-body Schrödinger equation**

$$H\Psi = E\Psi$$

↓

**Dyson / Gorkov equation**

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

where

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

$$G^{12}_{ab}(\omega) = \sum_k \left\{ \frac{\mathcal{U}^k_a\, \mathcal{V}^{k*}_b}{\omega - \omega_k + \mathrm{i}\eta} + \frac{\bar{\mathcal{V}}^{k*}_a\, \bar{\mathcal{U}}^k_b}{\omega + \omega_k - \mathrm{i}\eta} \right\}$$

↓

**Energy *dependent* eigenvalue problem**

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

↓ [Schirmer & Angonoa 1989]

**Energy *independent* eigenvalue problem**

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

# Solution of Gorkov equation

Gorkov equation ⟶ energy *dependent* eigenvalue problem

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

energy *independent* eigenvalue problem

$\propto N_b^3$

typically ~$10^6$-$10^7$

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

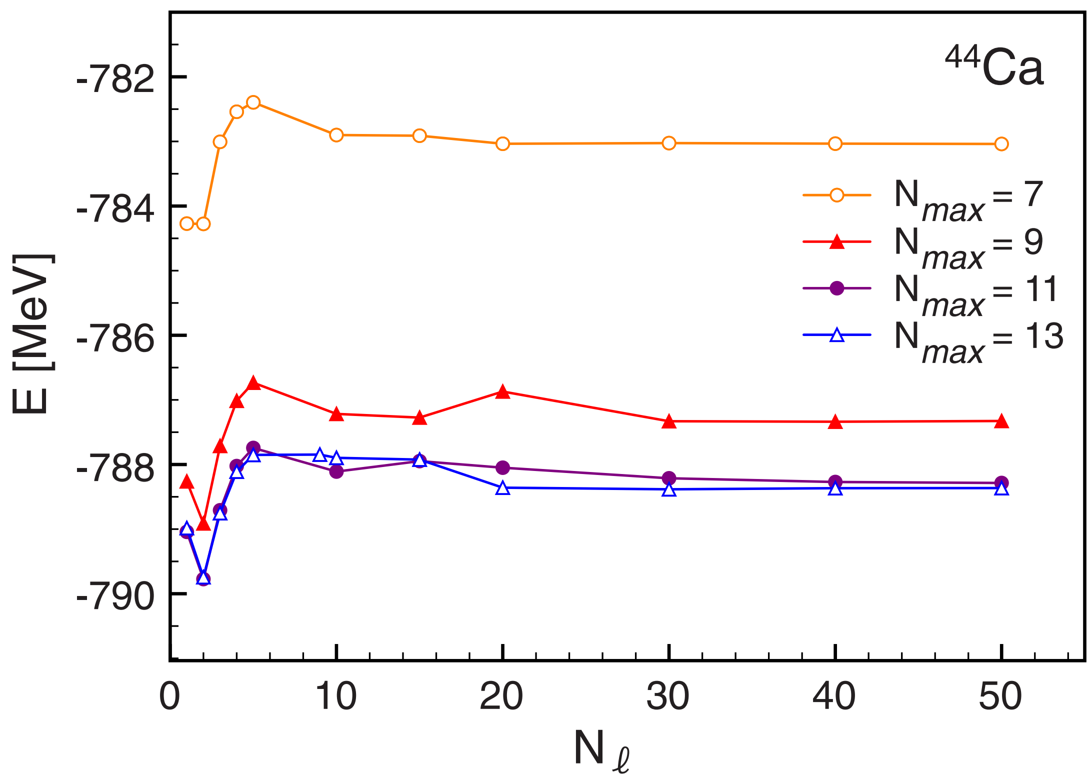
Krylov space eigenvalue problem

$\propto N_{\text{Lanczos}}$

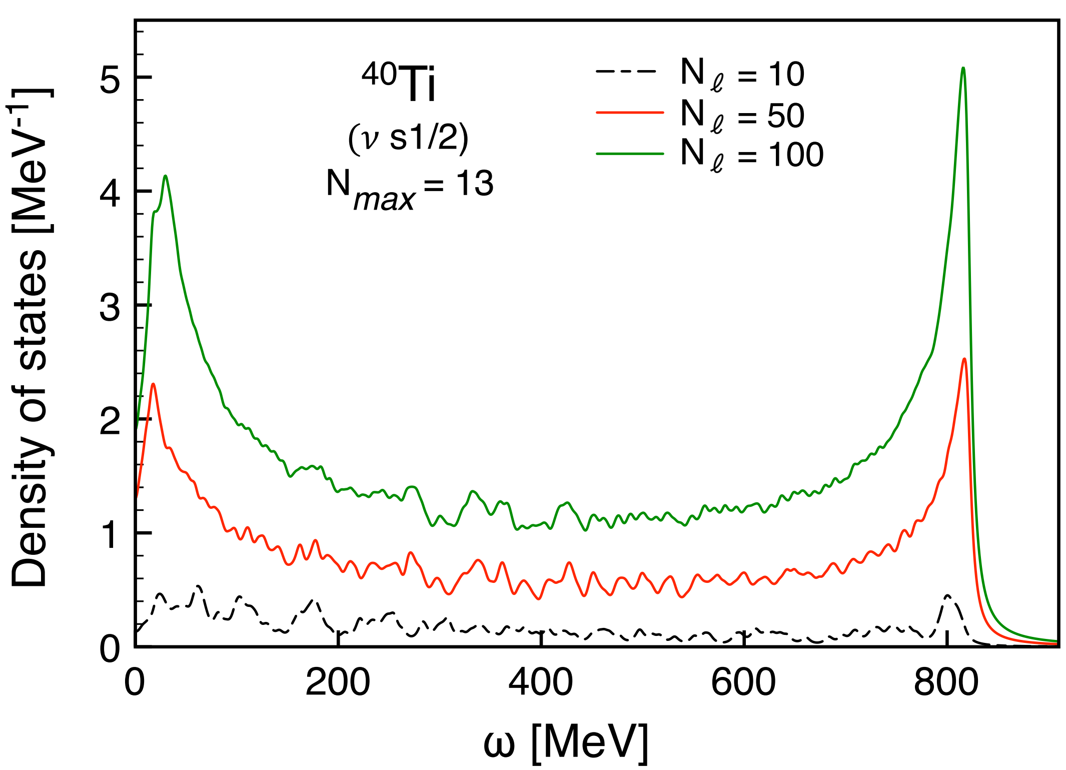
typically ~$10^2$-$10^3$

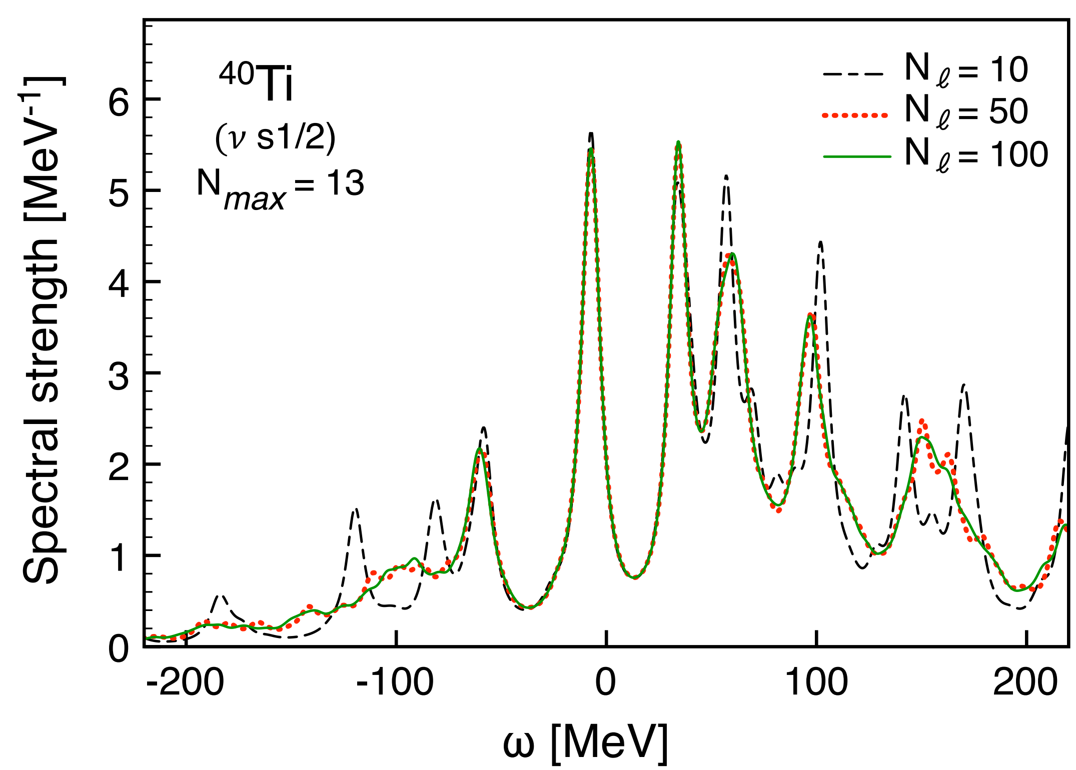
$$\begin{pmatrix} T-\mu+\Lambda & \tilde{h} & \mathcal{C} & -\mathcal{D}^\dagger \\ \tilde{h}^\dagger & -T+\mu-\Lambda & -\mathcal{D}^\dagger & \mathcal{C} \\ \mathcal{C}^\dagger & -\mathcal{D} & E & 0 \\ -\mathcal{D} & \mathcal{C}^\dagger & 0 & -E \end{pmatrix} \begin{pmatrix} \mathcal{U}^k \\ \mathcal{V}^k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

# Krylov projection




- ➟ Multi-pivot algorithm (# states ~ 10 $N_\ell$ )
- ➟ Well converged for $N_\ell$ ~ 50
- ➟ Independent of $N_{max}$
- ➟ Spectral strength quickly converges around the Fermi surface




[Somà, Barbieri & Duguet 2014]

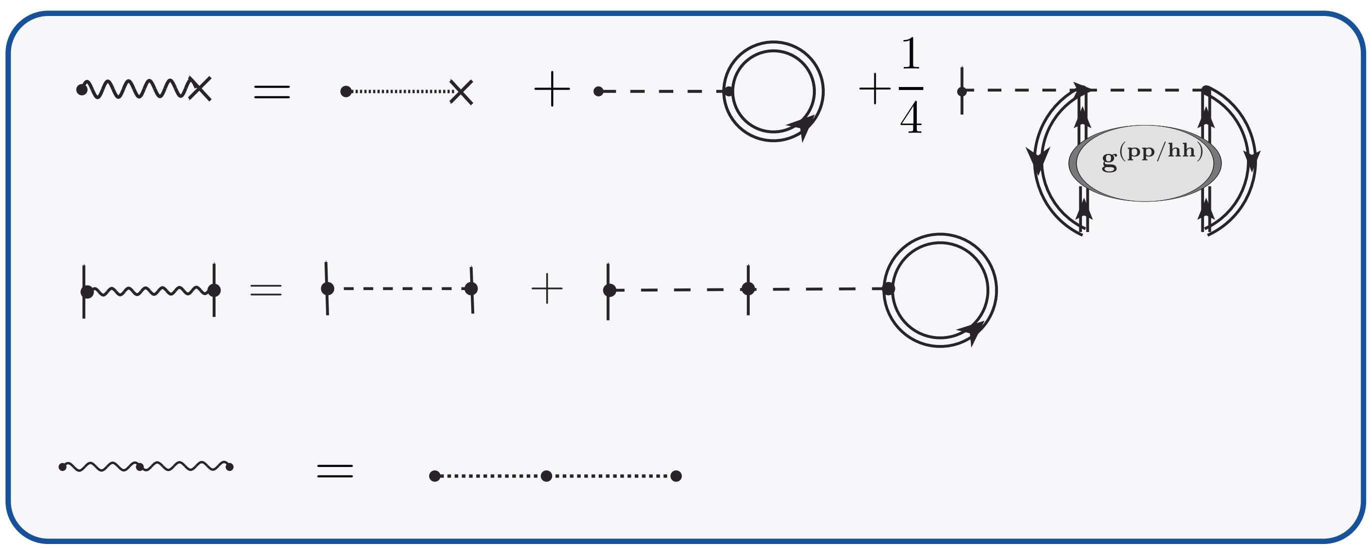
# Three-body forces

One- and two-body forces derived from the 3N part of the Hamiltonian

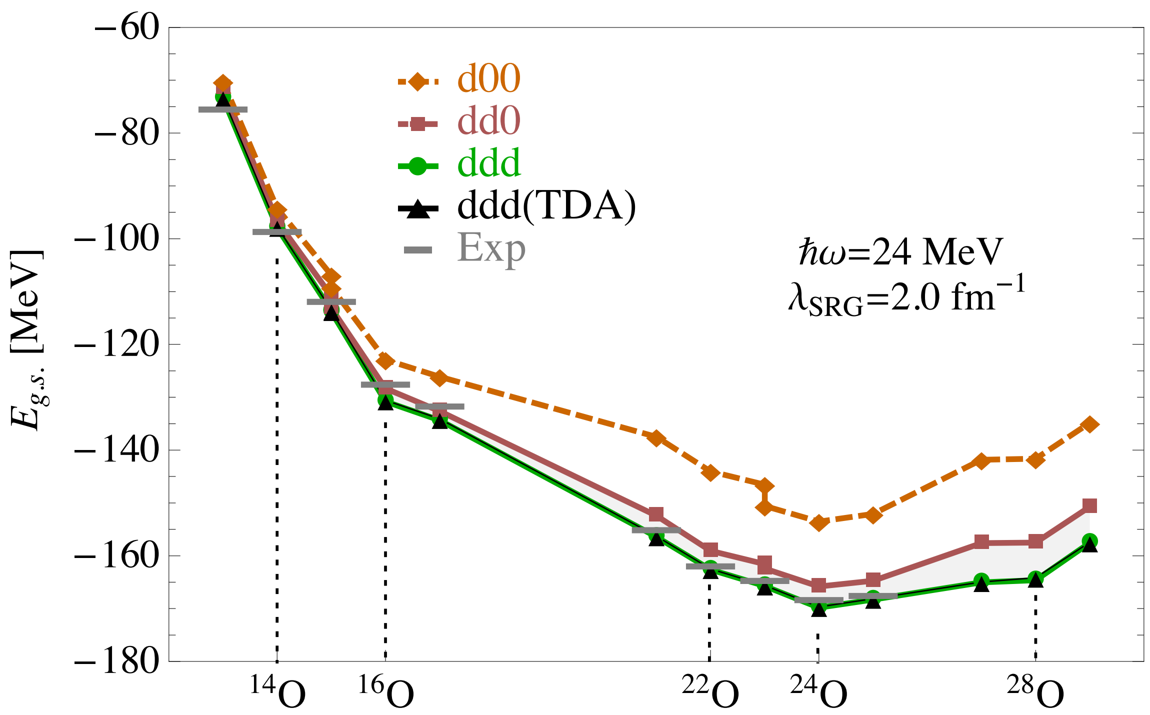
➟ Contractions with fully correlated density matrix

➟ Generalization of normal ordering

Galitskii-Koltun sum rule modified to account for 3N piece




[Carbone, Cipollone *et al.* 2013]




➟ Use of dressed propagators provides extra correlations

# Inside the Green's function

## 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***

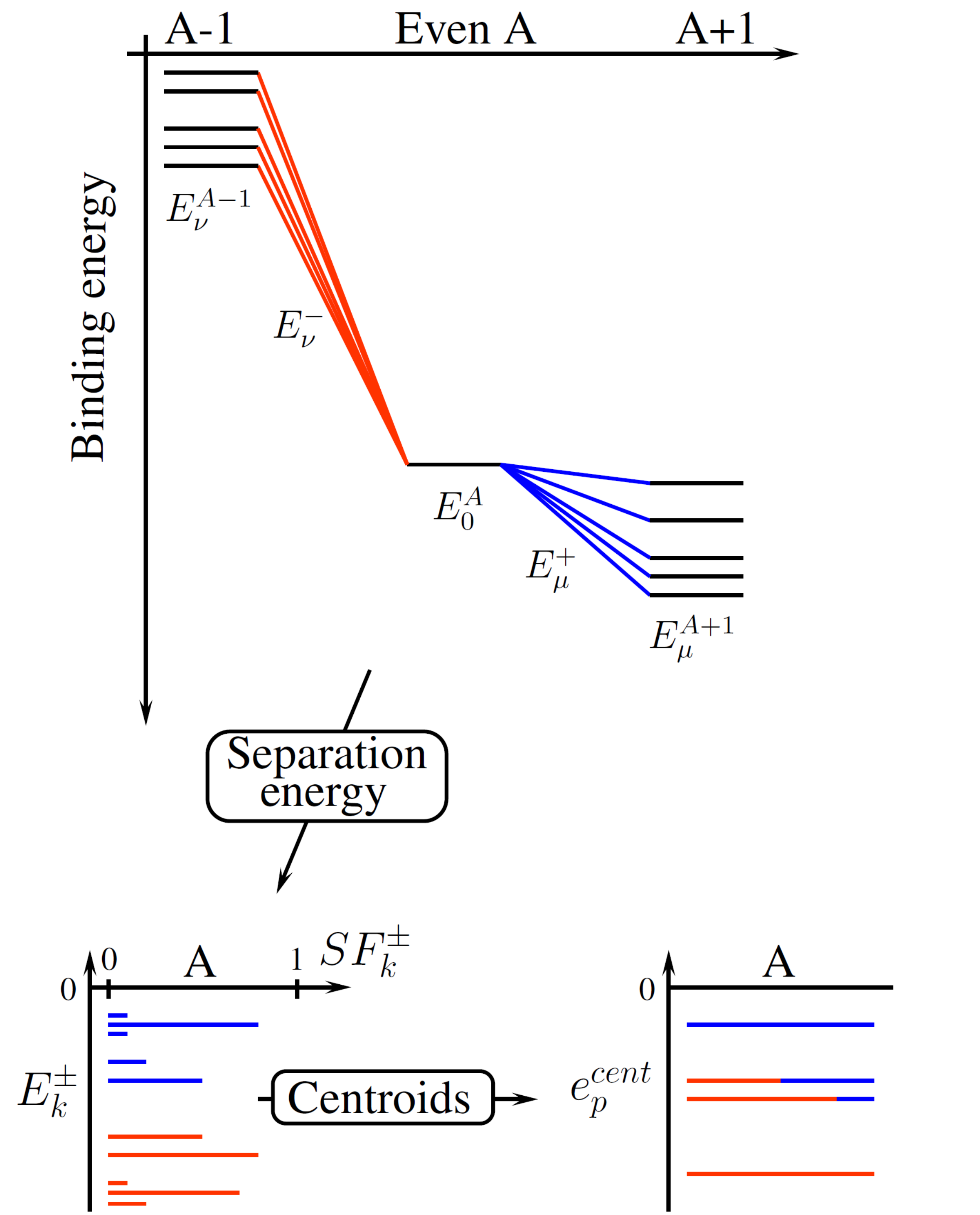
where
$$\begin{cases} \mathcal{U}^{k*}_a \equiv \langle \Psi_k | a^\dagger_a | \Psi_0 \rangle \\ \mathcal{V}^{k*}_a \equiv \langle \Psi_k | \bar{a}_a | \Psi_0 \rangle \end{cases}$$

and
$$\begin{cases} E^{+\,(A)}_k \equiv E^{A+1}_k - E^A_0 \equiv \mu + \omega_k \\ E^{-\,(A)}_k \equiv E^A_0 - E^{A-1}_k \equiv \mu - \omega_k \end{cases}$$

## Spectroscopic factors

$$SF^+_k \equiv \sum_{a \in \mathcal{H}_1} \left| \langle \psi_k | a^\dagger_a | \psi_0 \rangle \right|^2 = \sum_{a \in \mathcal{H}_1} \left| \mathcal{U}^k_a \right|^2$$

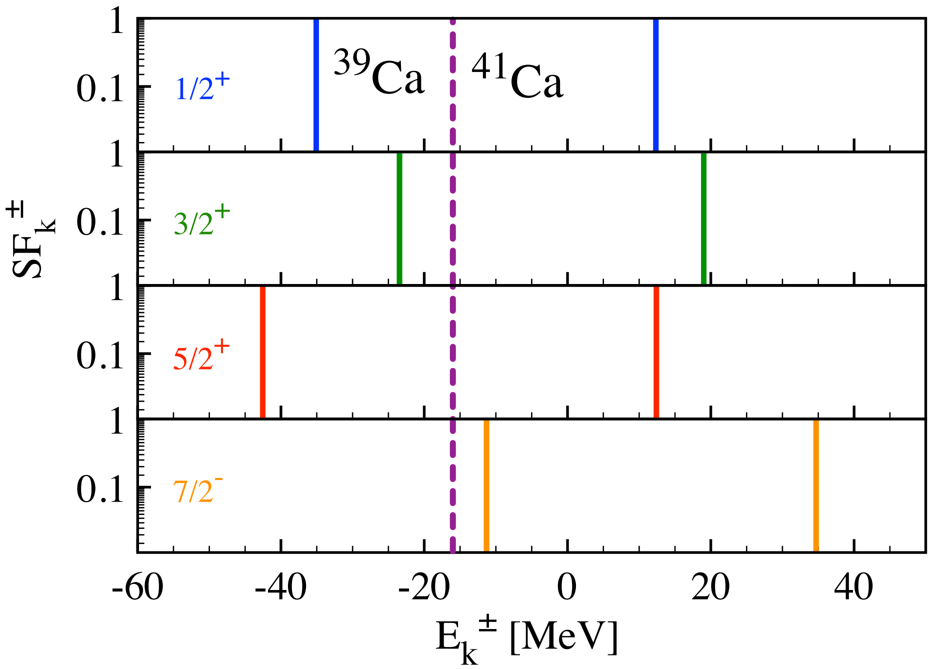
$$SF^-_k \equiv \sum_{a \in \mathcal{H}_1} \left| \langle \psi_k | a_a | \psi_0 \rangle \right|^2 = \sum_{a \in \mathcal{H}_1} \left| \mathcal{V}^k_a \right|^2$$



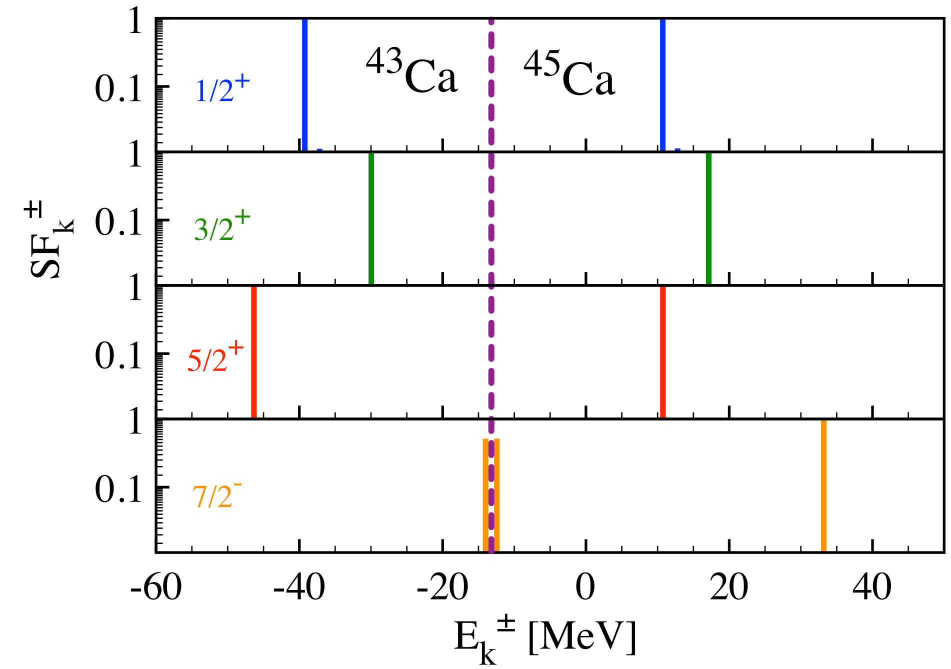

[figure from J. Sadoudi]

# Spectral strength distribution

Dyson 1st order (HF)




Gorkov 1st order (HFB)

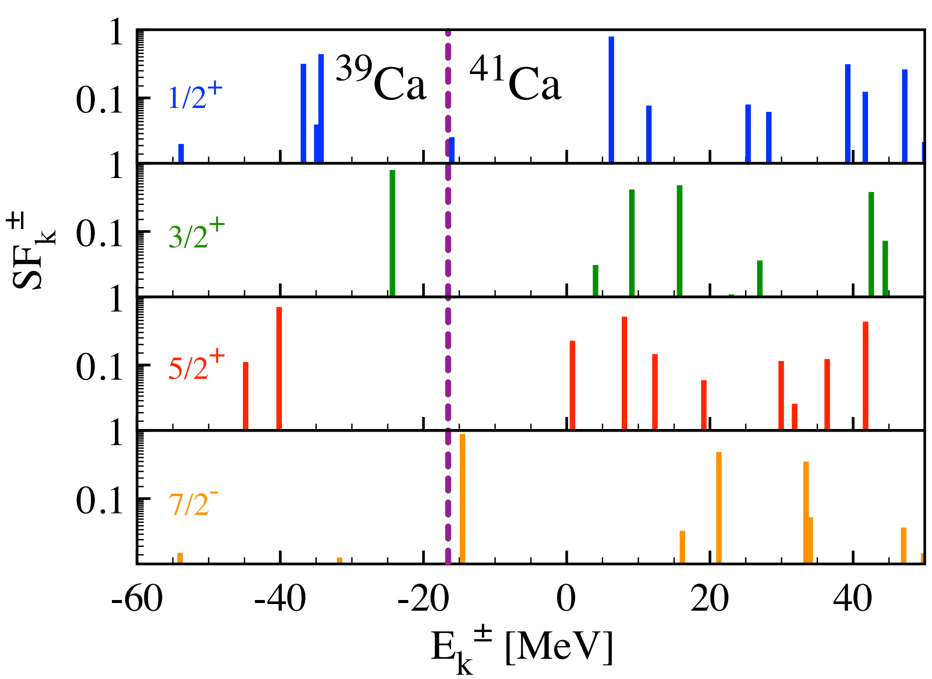



Fragmentation

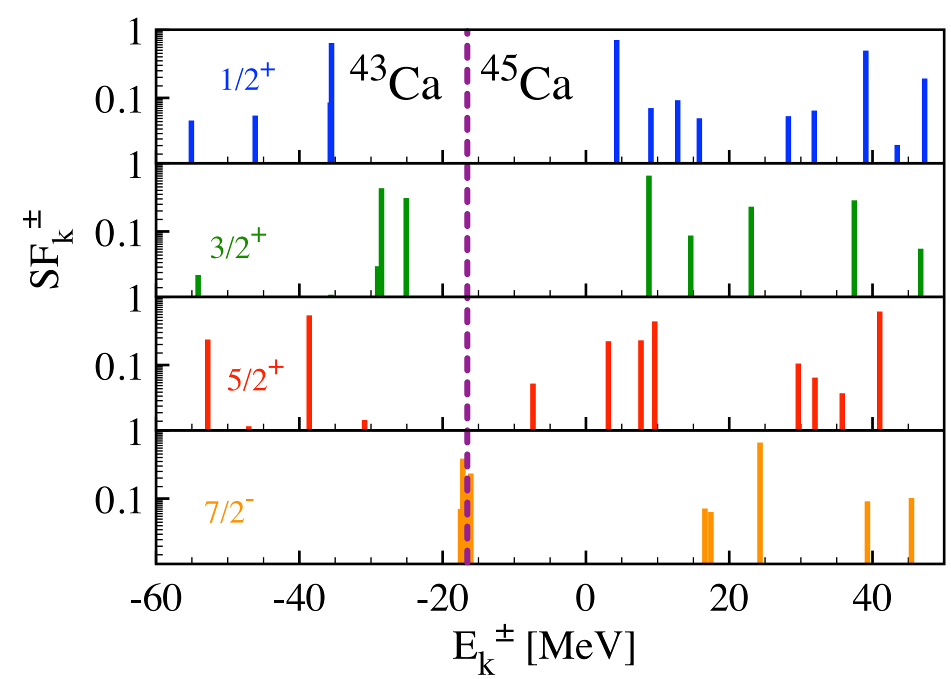
Static pairing

Dynamical fluctuations

Dyson 2nd order

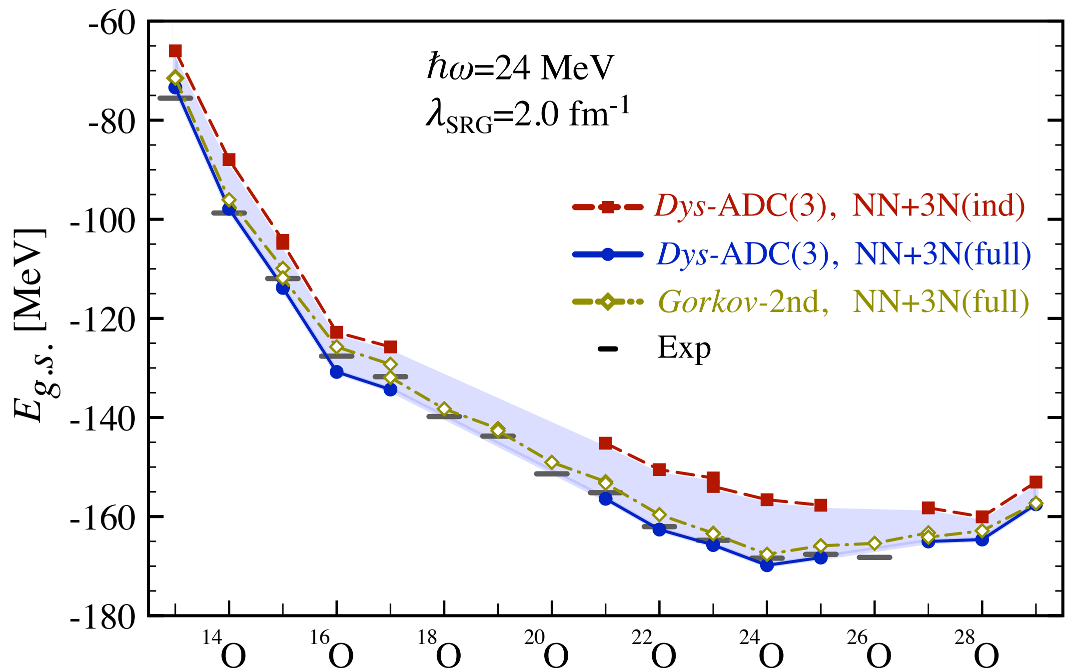



Gorkov 2nd order

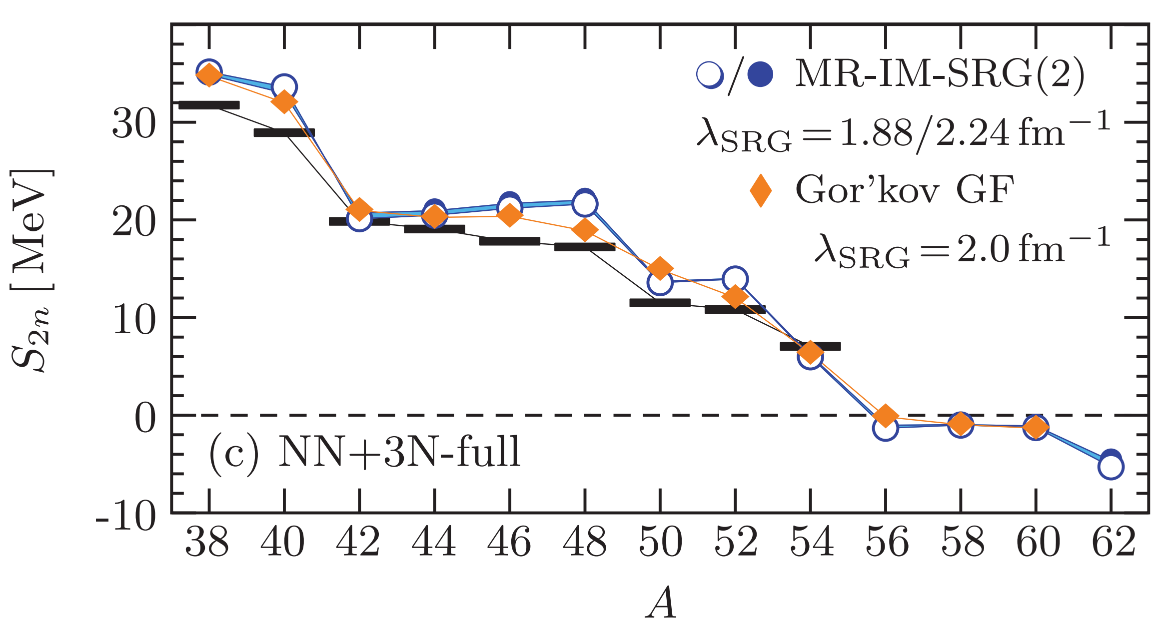


# Benchmarks

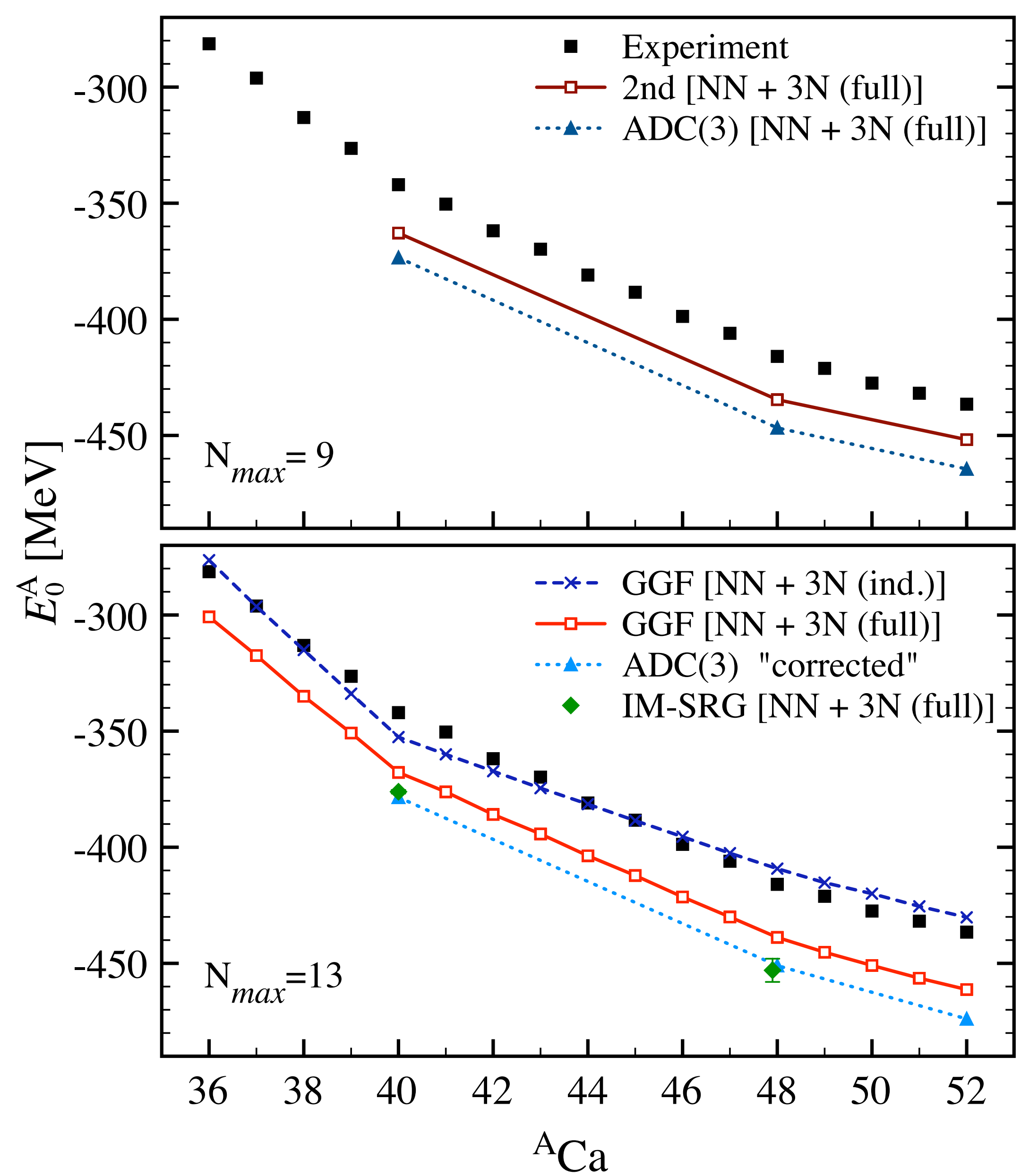
- ✪ Benchmarks between Gorkov GF, Dyson GF & IM-SRG
  - ➟ Solidity of many-body machinery




[Cipollone, Barbieri, Navrátil 2014]

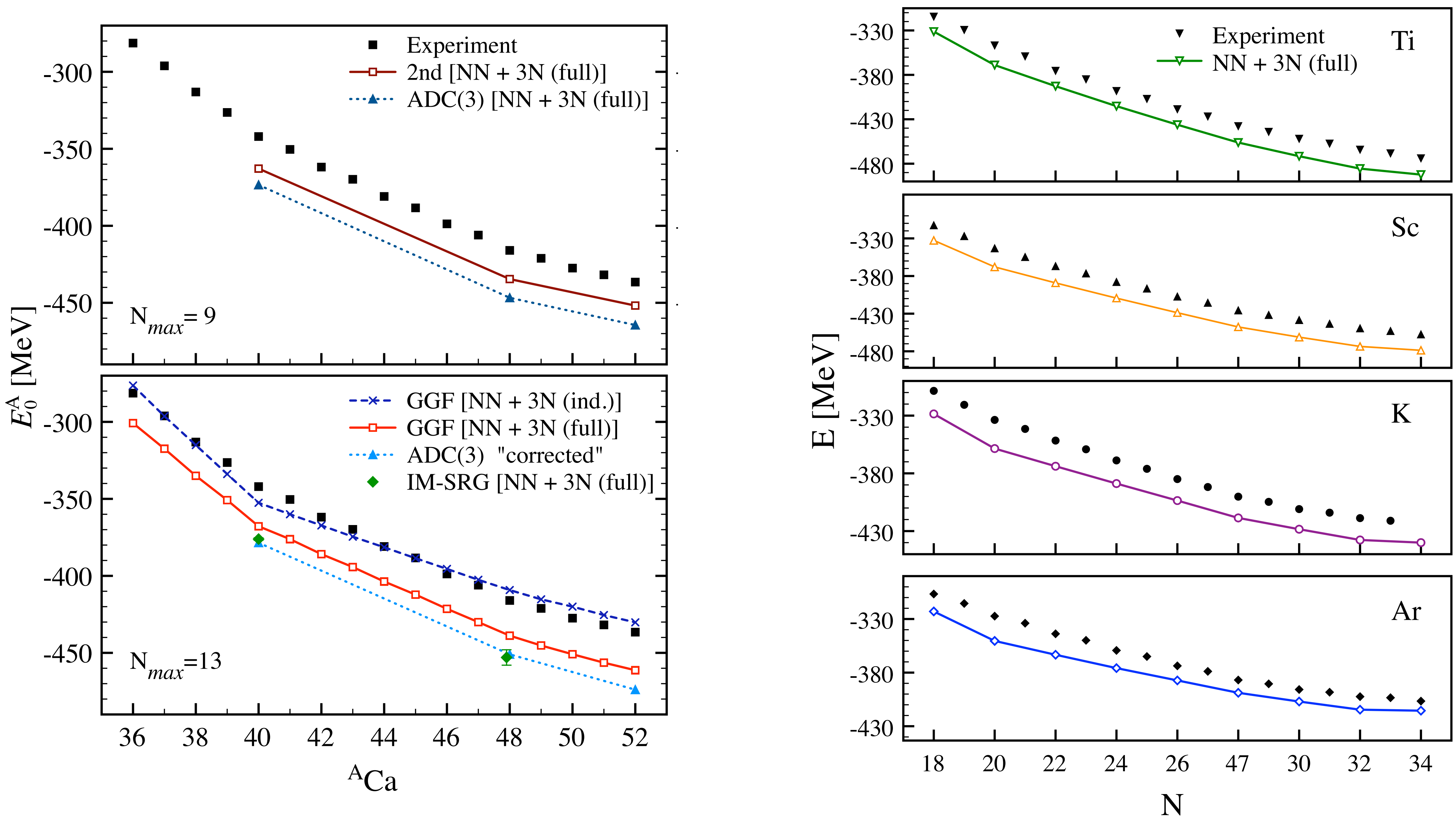



[Hergert *et al.* 2014]




[Somà *et al.* 2014]

# Binding energies around Ca



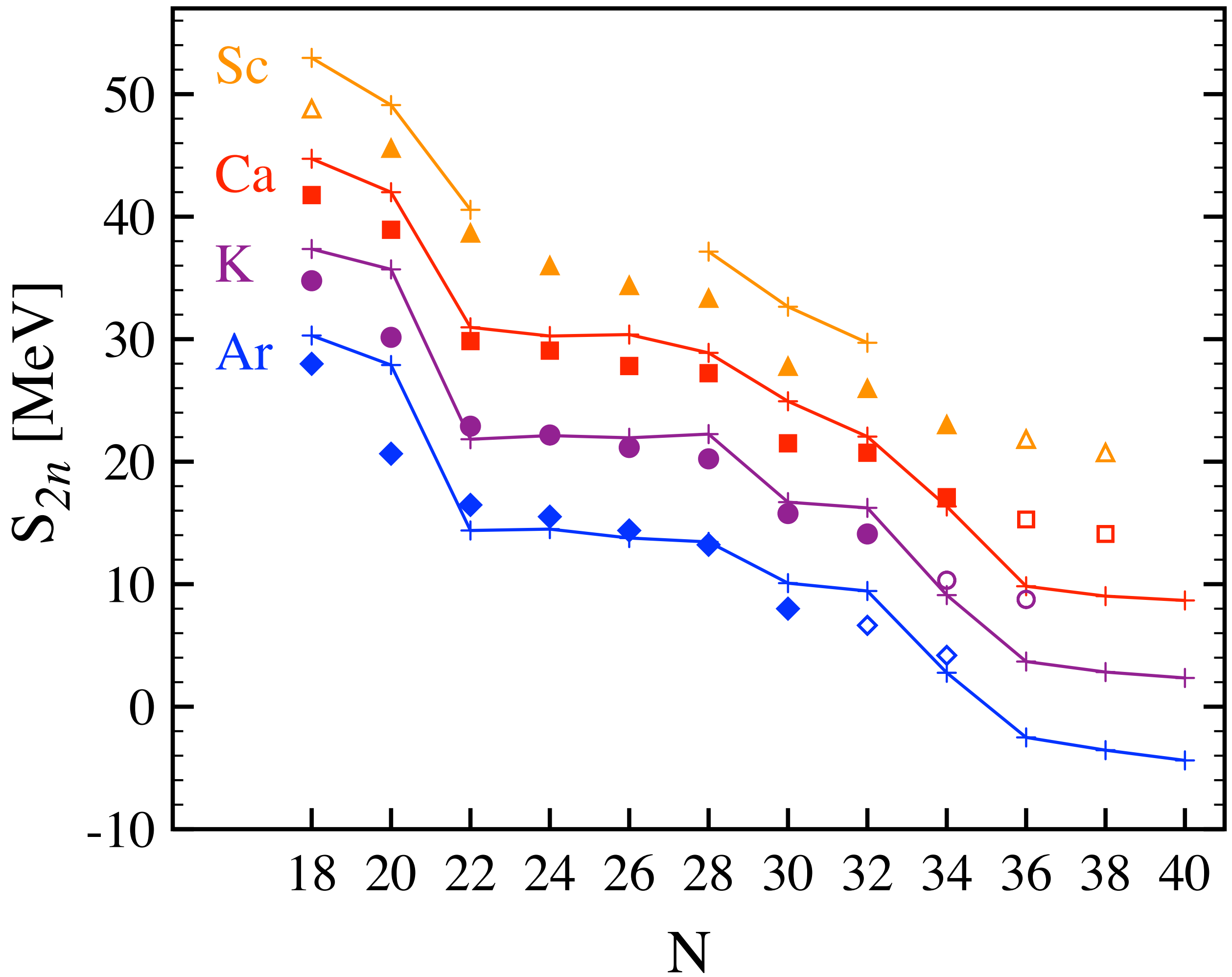

[Somà *et al.* 2014]

✪ Access to **several neighbouring isotopic chains** (here $Z = 18 \rightarrow 22$)

✪ Can not go "too far" from **singly-magic** nuclei

➟ Would require additional breaking of SU(2) rotational → see BCC [Signoracci *et al.* ]

# Two-neutron separation energies around Ca




Two-neutron separation energies

$$S_{2n} \equiv E_0^{Z,N} - E_0^{Z,N-2}$$

[Somà *et al., update on* PRC 89 061301]

✪ A number of new experiments target neutron-rich isotopes in this mass region

✪ Calculations reveal deficiencies of employed chiral interactions

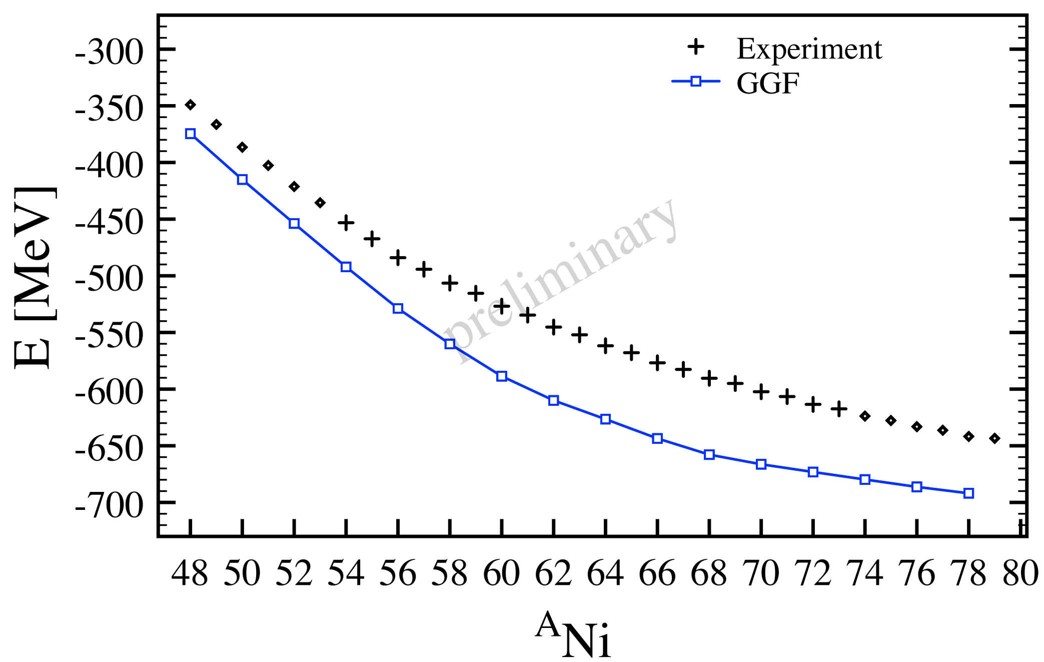
➟ Systematic overbinding & too small radii

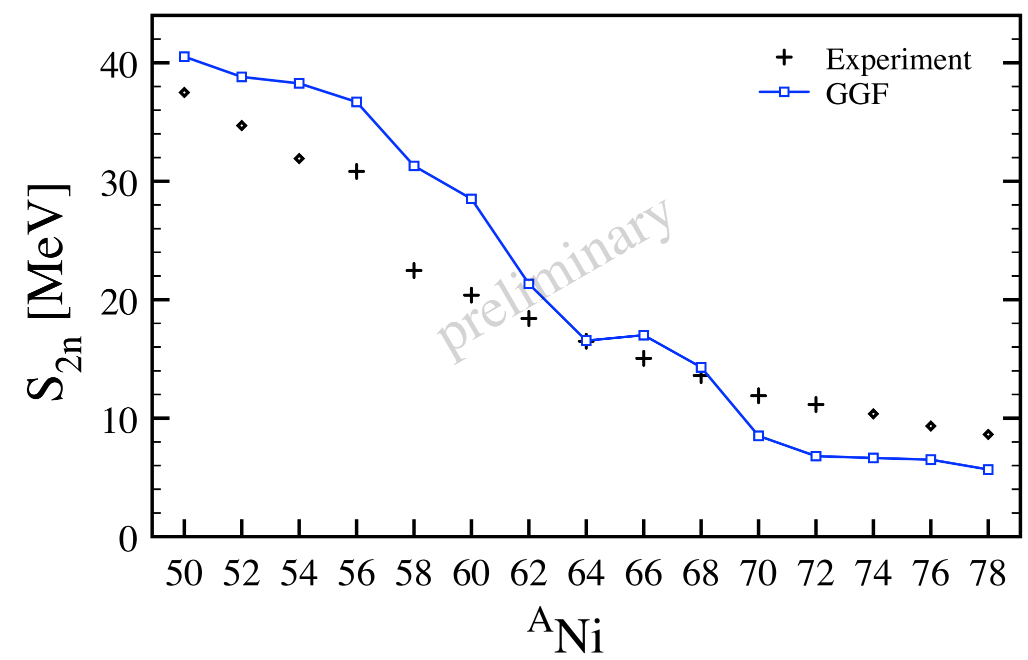
➟ Overestimation of N=20 gap traced back to spectrum too spread out

# Towards heavier systems

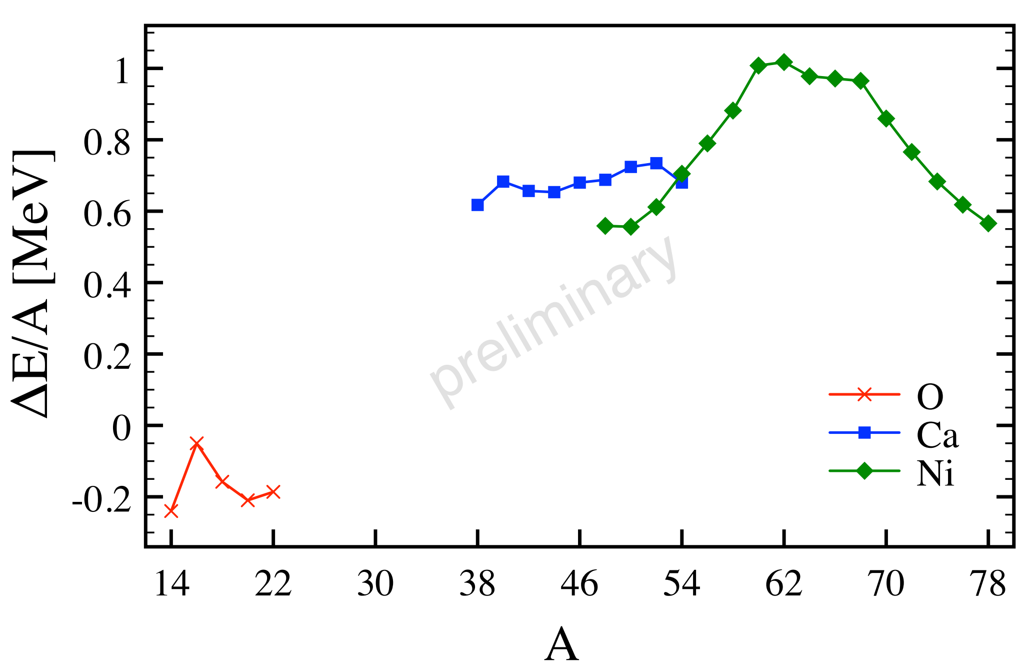
✪ Ab initio calculations being pushed towards A=100 and above

➟ Extended **testing ground** for nuclear Hamiltonians




[Somà *et al.*, in preparation]




➟ Confirmed by different ab initio methods

[Binder *et al.* 2014, Hergert *et al.* 2014]

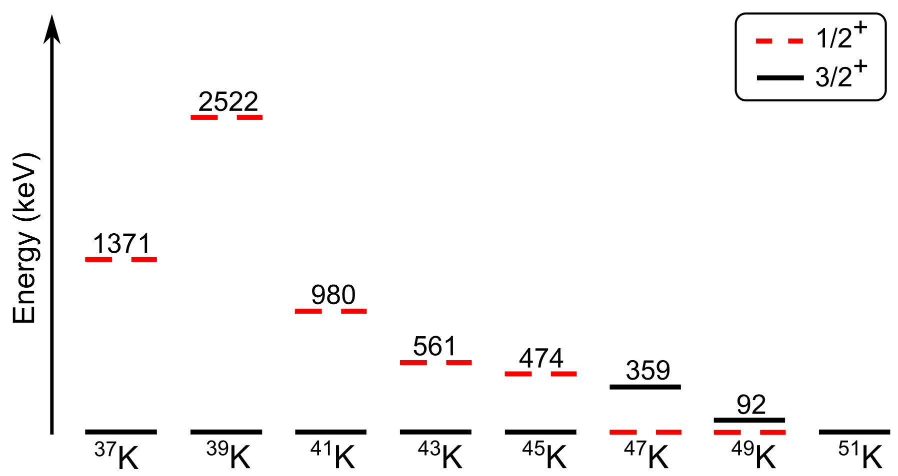
➟ Saturation at too high density?

➟ Consistent NM calculations?

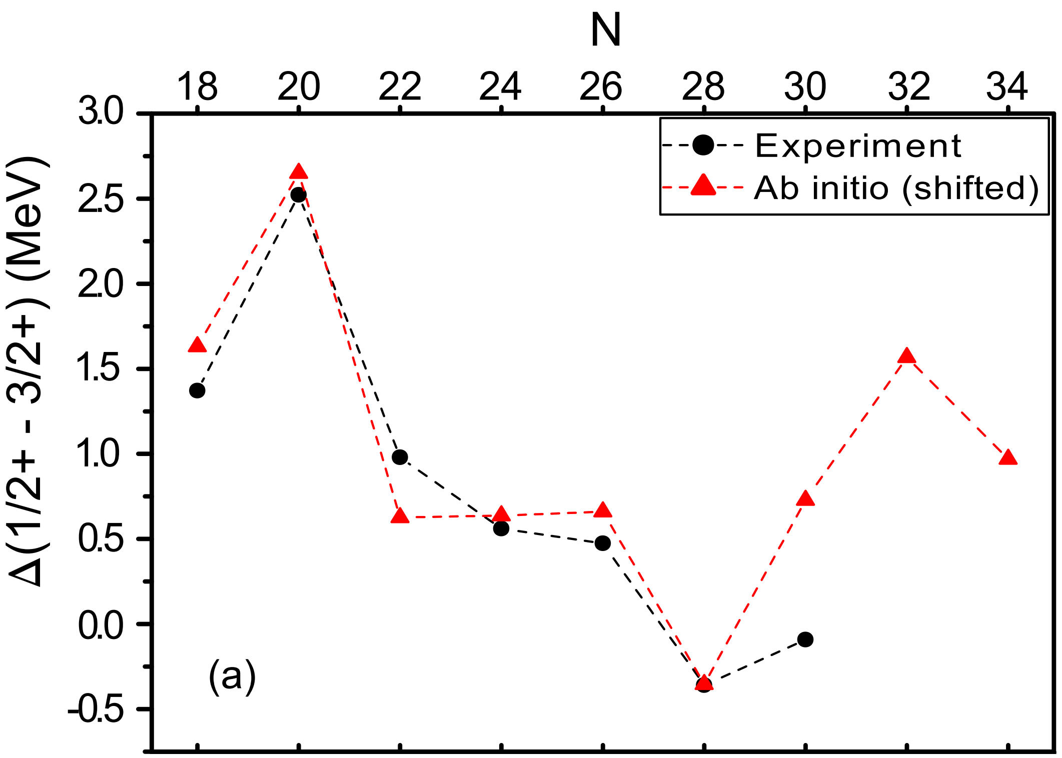
# Potassium ground states (re)inversion

✪ Ground-state spin inversion & re-inversion recently established

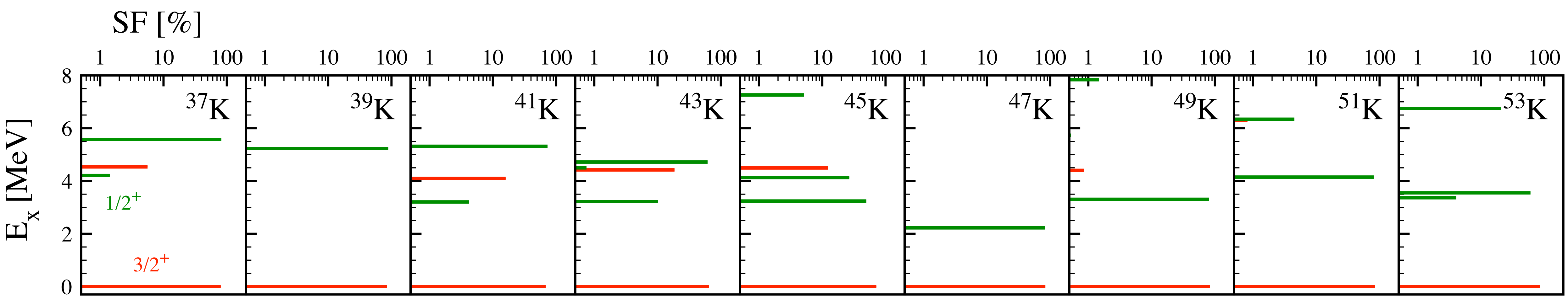
➟ Laser spectroscopy @ ISOLDE




[Papuga *et al.* 2014]




➟ GGF calculations of K spectra



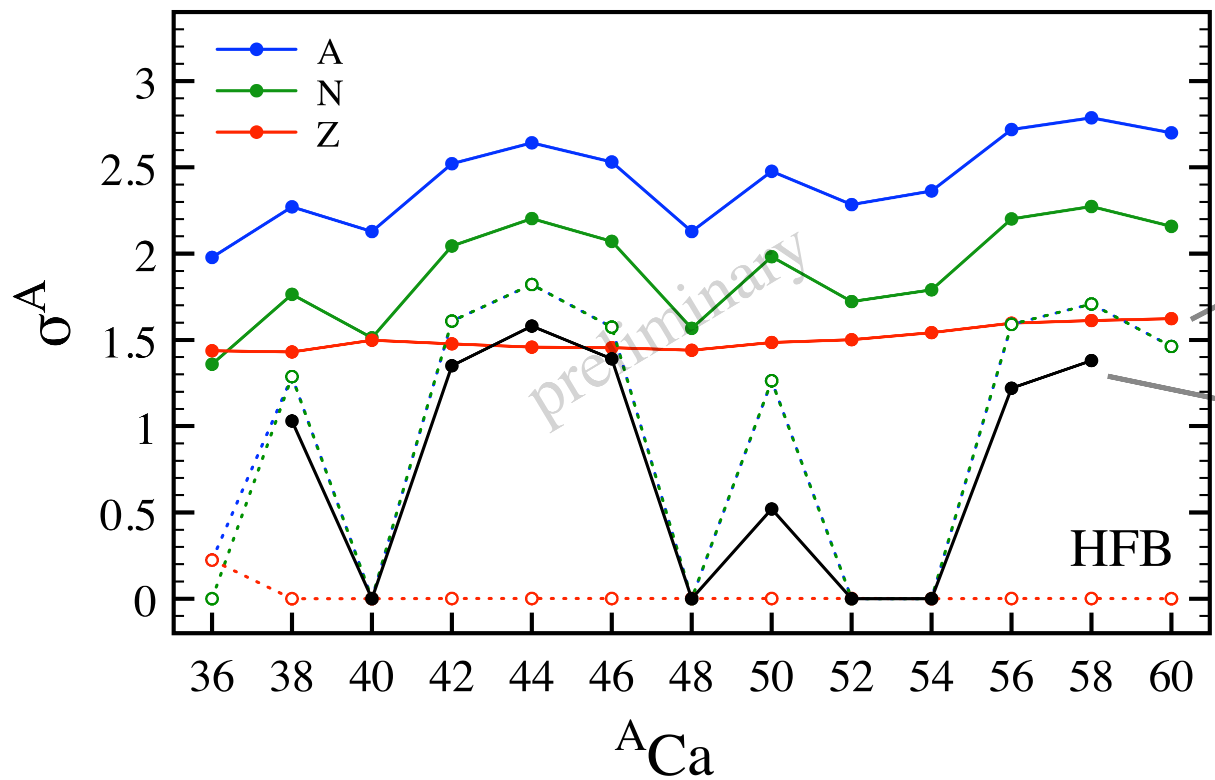
# Particle-number variance

✪ Gorkov GF calculations break particle number symmetry ⟶ $\sigma_A = \sqrt{\langle \hat{A}^2 \rangle - \langle \hat{A} \rangle^2}$

✪ Breaking has two sources:

1) Reference state mixes different $A$

2) Green's function formalism itself explores Fock space




GF breaking evident in protons

After subtracting GF part

# Particle-number variance

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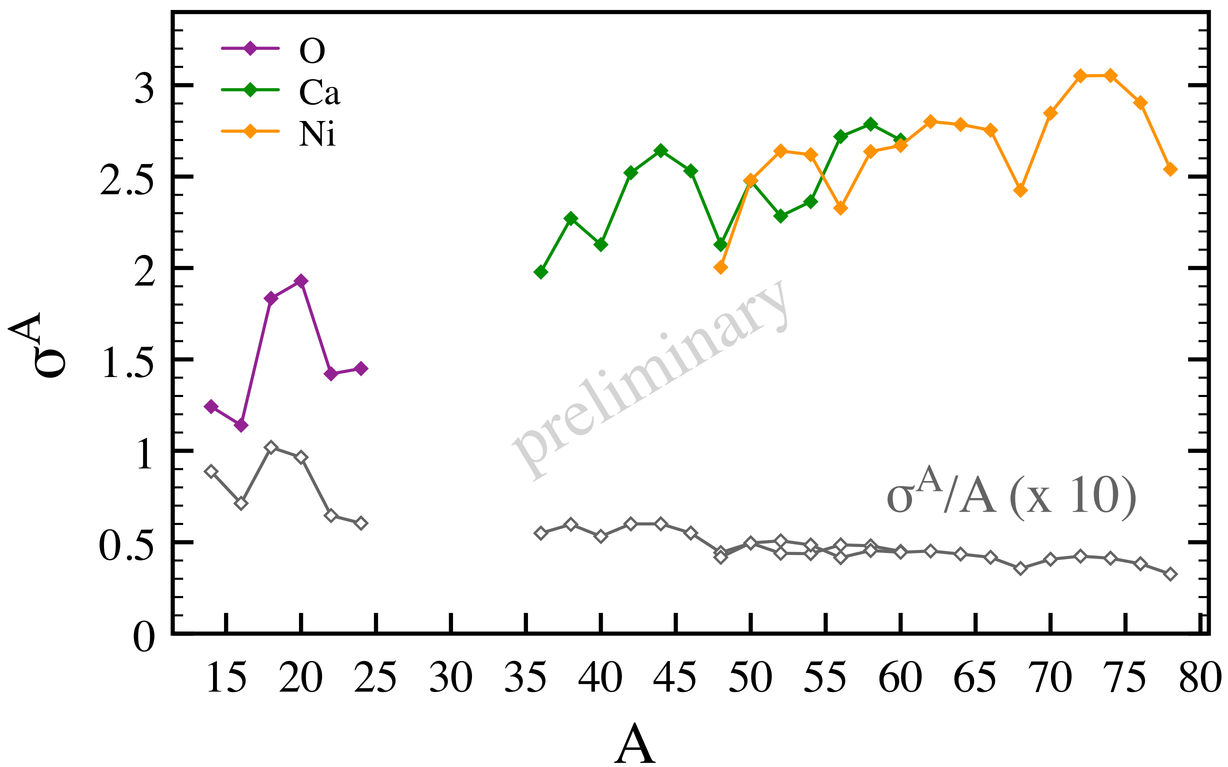


➟ Need to go beyond approximation $\rho^{(2)} \sim \rho^{(1)}\rho^{(1)}$

➟ To be further investigated at next order in GF expansion

➟ Calls for restoration of symmetry

# Conclusions

- ✪ Considerable advances in ab initio nuclear structure
  - ○ **SRG**-ed Hamiltonian extend domain of applicability
  - ○ new approaches allow to go **beyond closed-shell** limitations

- ✪ **Gorkov**-Green's function theory
  - ○ combines richness of GF with symmetry breaking techniques
  - ○ reaching state-of-the-art of nuclear many-body → **ADC(3)**

- ✪ Breaking of symmetries viable way to tackle near-degenerate systems
  - ○ case of U(1) crucial to treat **pairing** correlations
  - ○ **symmetry restoration** must be addressed