

***Self-consistent Green's function in Finite Nuclei and related things...***

-

***Lectures VI***

***The Gorkov-SCGF formalism for open shell nuclei;  
Applications to medium-mass nuclei***



# Adding 3-nucleon forces

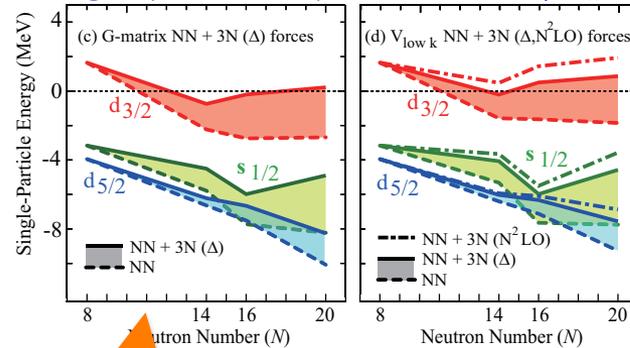
# Modern realistic nuclear forces

## Chiral EFT for nuclear forces:

	2N forces	3N forces	4N forces
LO $\mathcal{O}\left(\frac{Q^0}{\Lambda^0}\right)$			
NLO $\mathcal{O}\left(\frac{Q^2}{\Lambda^2}\right)$			
N <sup>2</sup> LO $\mathcal{O}\left(\frac{Q^3}{\Lambda^3}\right)$			
N <sup>3</sup> LO $\mathcal{O}\left(\frac{Q^4}{\Lambda^4}\right)$			

(3NFs arise naturally at N2LO)

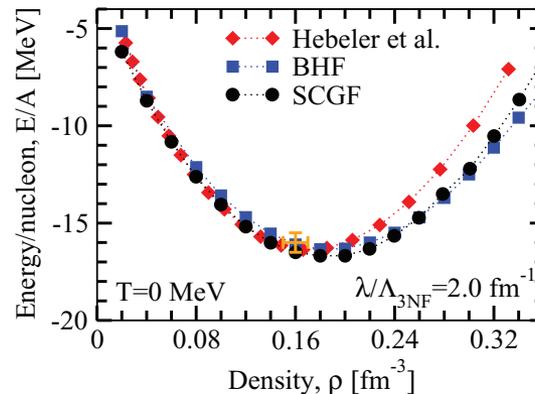
## Single particle spectrum at $E_{\text{fermi}}$ :



[T. Otsuka et al., Phys Rev. Lett **105**, 032501 (2010)]

Need at LEAST 3NF!!!  
("cannot" do RNB physics without...)

## Saturation of nuclear matter:

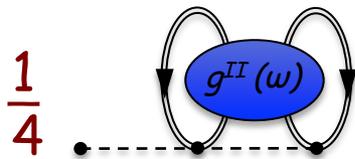


[A. Carbone et al., Phys. Rev. C **88**, 044302 (2013)]

# Inclusion of NNN forces

A. Carbone, CB, et al., Phys. Rev. C88, 054326 (2013)

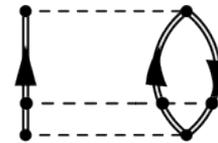
\* NNN forces can enter diagrams in three different ways:



Correction to external  
1-Body interaction



Correction to  
non-contracted  
2-Body interaction



pure 3-Body  
contribution

- Contractions are with fully correlated density matrices (BEYOND a normal ordering...)



# Inclusion of NNN forces

A. Carbone, CB, et al., Phys. Rev. C88, 054326 (2013)

\* NNN forces can enter diagrams in three different ways:

→ Define new 1- and 2-body interactions and use only interaction-irreducible diagrams

$$\tilde{U} = \sum_{\alpha\beta} \left[ -U_{\alpha\beta} - i\hbar \sum_{\delta\gamma} v_{\alpha\gamma,\beta\delta} g_{\delta\gamma}(\tau = 0^-) + \frac{i\hbar}{4} \sum_{\gamma\delta\mu\nu} g_{\mu\nu,\gamma\delta}^{II}(\tau = 0^-) w_{\alpha\gamma\delta,\beta\mu\nu} \right] a_{\alpha}^{\dagger} a_{\beta}$$

$$\tilde{V} = \sum_{\alpha\beta} \frac{1}{4} \left[ v_{\alpha\beta,\gamma\delta} - i\hbar \sum_{\mu\nu} w_{\alpha\beta\mu,\gamma\delta\nu} g_{\nu\mu}(\tau = 0^-) \right] a_{\alpha}^{\dagger} a_{\beta}^{\dagger} a_{\delta} a_{\gamma}$$

$$W = \bullet \text{---} \bullet \text{---} \bullet \quad \equiv \quad W_{\alpha\beta\gamma,\mu\nu\lambda} a_{\alpha}^{\dagger} a_{\beta}^{\dagger} a_{\gamma}^{\dagger} a_{\lambda} a_{\nu} a_{\mu}$$

- Contractions are with fully correlated density matrices (BEYOND a normal ordering...)

# Inclusion of NNN forces

A. Carbone, CB, et al., *Phys. Rev. C* **88**, 054326 (2013)

- Second order PT  
diagrams with 3BFs:

effectively:

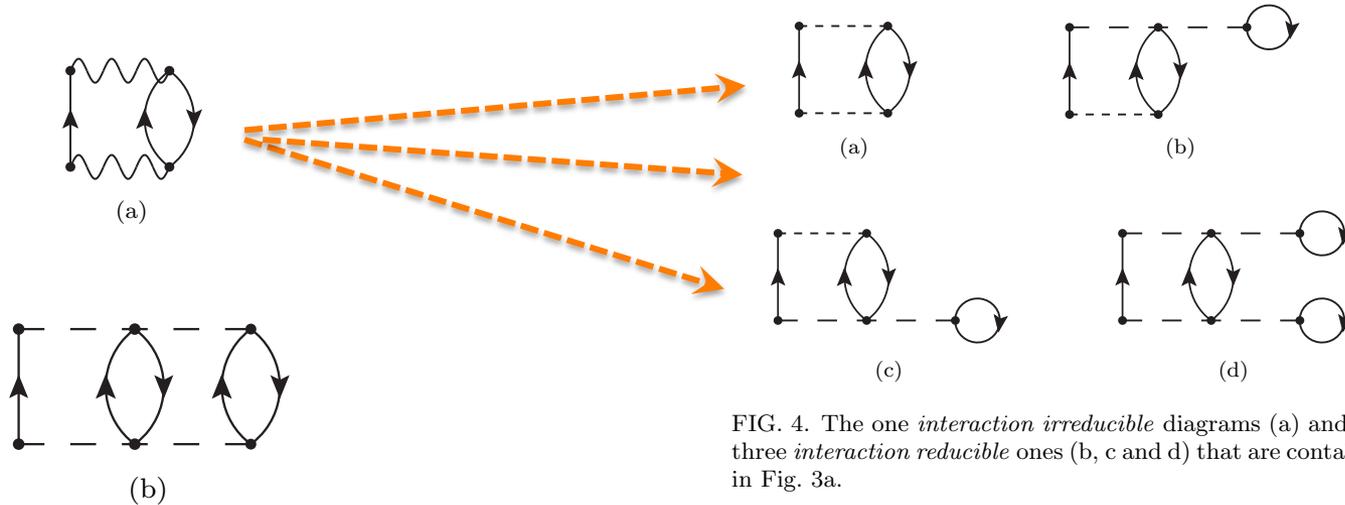
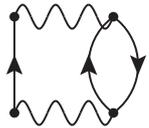


FIG. 4. The one *interaction irreducible* diagrams (a) and the three *interaction reducible* ones (b, c and d) that are contained in Fig. 3a.

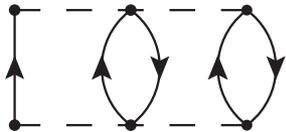
# Inclusion of NNN forces

A. Carbone, CB, et al., Phys. Rev. C88, 054326 (2013)

- Second order PT diagrams with 3BFs:



(a)

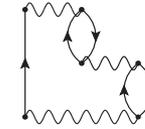


(b)

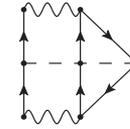
- Third order PT diagrams with 3BFs:



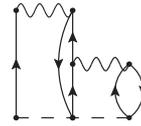
(a)



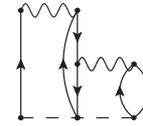
(b)



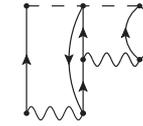
(c)



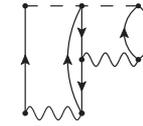
(d)



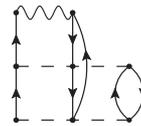
(e)



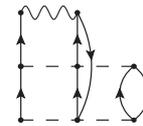
(f)



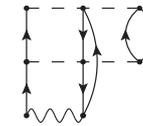
(g)



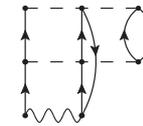
(h)



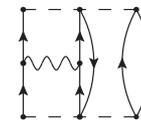
(i)



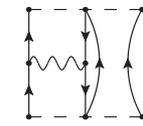
(j)



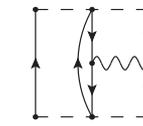
(k)



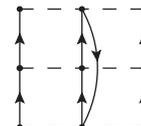
(l)



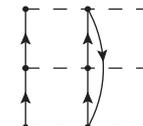
(m)



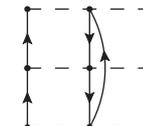
(n)



(o)



(p)



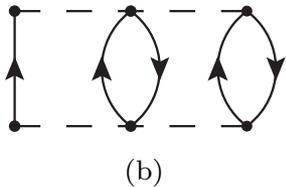
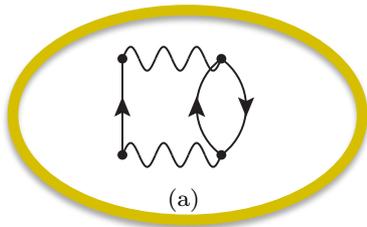
(q)

FIG. 5. 1PI, skeleton and interaction irreducible self-energy diagrams appearing at  $3^{\text{rd}}$ -order in perturbative expansion (7), making use of the effective hamiltonian of Eq. (9).

# Inclusion of NNN forces

A. Carbone, CB, et al., Phys. Rev. C88, 054326 (2013)

- Second order PT diagrams with 3BFs:



- Third order PT diagrams with 3BFs:

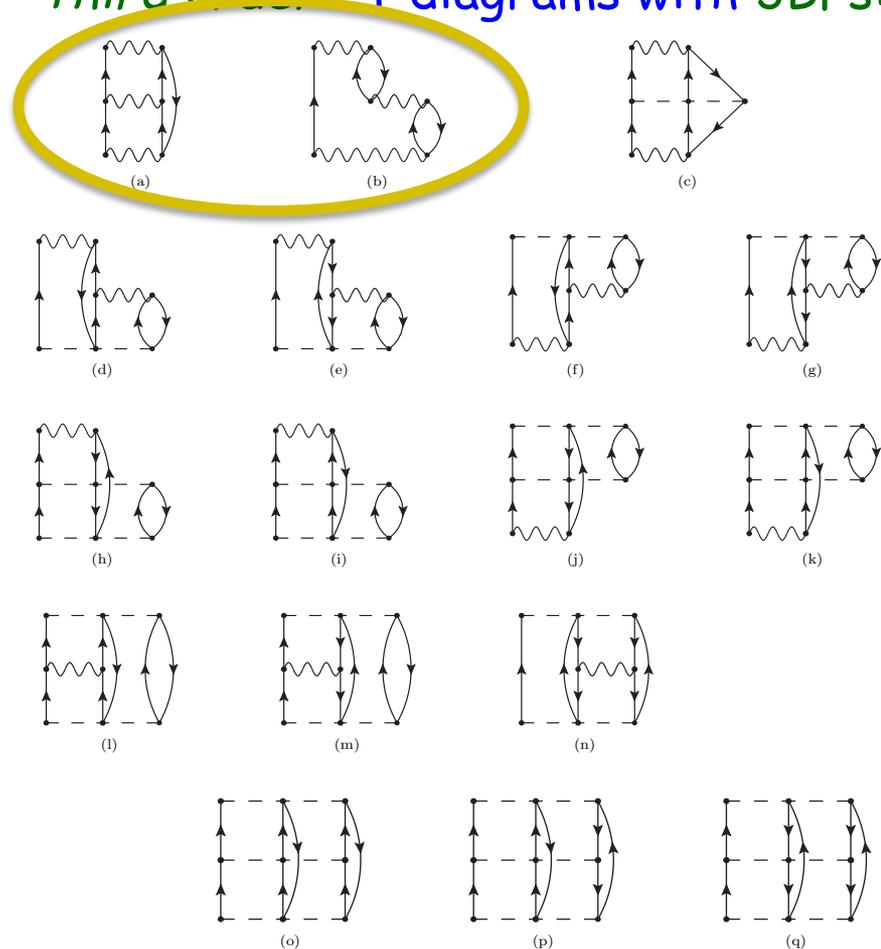
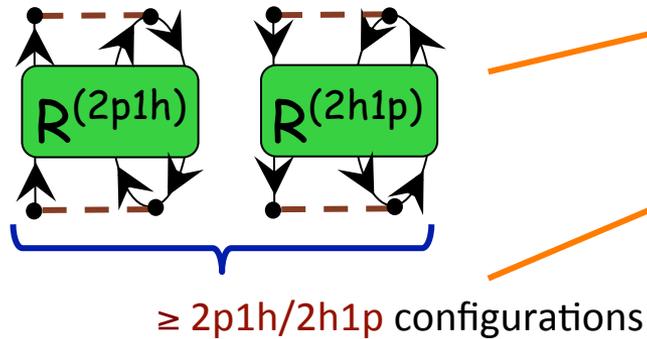
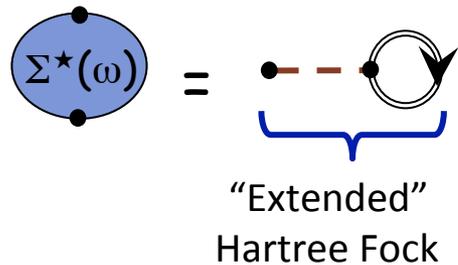


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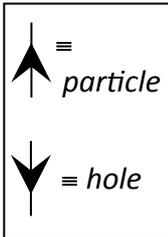
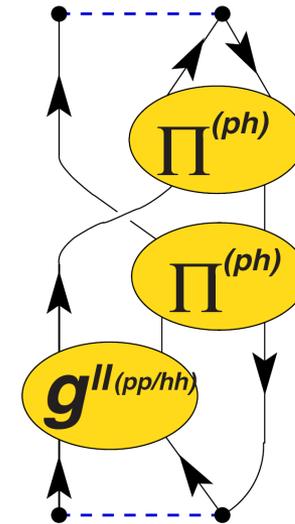
# *Gorkov method for the open-shells*

# Faddeev-RPA in two words...

Self-energy  
(optical potential):



Faddeev-RPA:



- A complete expansion requires all types of particle-vibration coupling:
  - ✓  $g^{II}(\omega) \rightarrow$  pairing effects, two-nucleon transfer
  - ✓  $\Pi^{(ph)}(\omega) \rightarrow$  collective motion, using RPA or beyond
  - ✓ Pauli exchange effects
- The Self-energy  $\Sigma^*(\omega)$  yields *both* single-particle states and scattering
- Finite nuclei:  $\rightarrow$  require high-performance computing

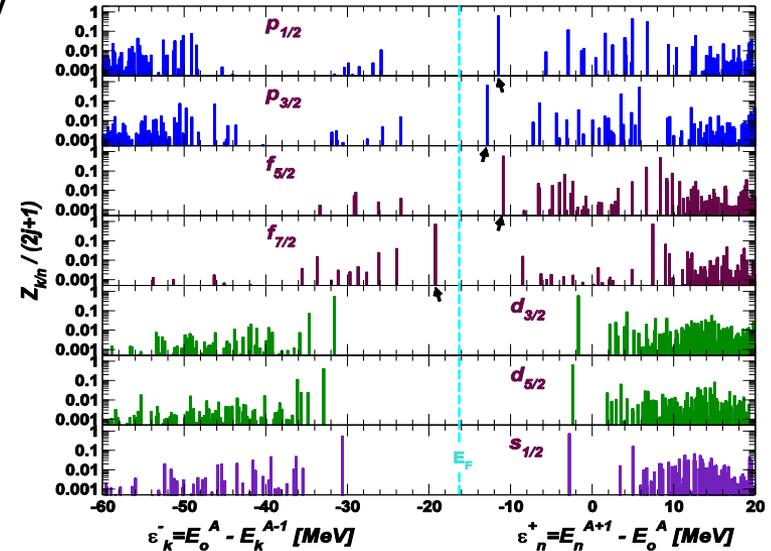
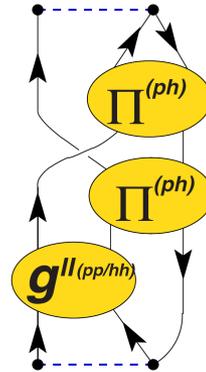


# Applications to doubly-magic nuclei

✱ Faddeev-RPA approximation for the self-energy

↓  
 ↓  
 collective vibrations  
 particle-vibration coupling

[C.B. *et al.* 2001-2011]



✱ Successful in medium-mass doubly-magic systems

↪ Expansion breaks down when pairing instabilities appear



Explicit configuration mixing

Single-reference: Bogoliubov (Gorkov)

# Going to open-shells: Gorkov ansatz

[V. Somà, T. Duguet, CB, Pys. Rev. C84, 046317 (2011) ]

✱ Ansatz

$$\dots \approx E_0^{N+2} - E_0^N \approx E_0^N - E_0^{N-2} \approx \dots \approx 2\mu$$

✱ 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  $N = \langle \Psi_0 | N | \Psi_0 \rangle$

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

# Gorkov Green's functions and equations

[V. Somà, T. Duguet, CB, Pys. Rev. C84, 046317 (2011) ]

✱ Set of 4 Green's functions

$i G_{ab}^{11}(t, t') \equiv \langle \Psi_0   T \{ a_a(t) a_b^\dagger(t') \}   \Psi_0 \rangle \equiv$ 	$i G_{ab}^{21}(t, t') \equiv \langle \Psi_0   T \{ \bar{a}_a^\dagger(t) a_b^\dagger(t') \}   \Psi_0 \rangle \equiv$ 
$i G_{ab}^{12}(t, t') \equiv \langle \Psi_0   T \{ a_a(t) \bar{a}_b(t') \}   \Psi_0 \rangle \equiv$ 	$i G_{ab}^{22}(t, t') \equiv \langle \Psi_0   T \{ \bar{a}_a^\dagger(t) \bar{a}_b(t') \}   \Psi_0 \rangle \equiv$ 

[Gorkov 1958]



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

Gorkov equations

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

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

# Open-shells: 1st & 2nd order Gorkov diagrams

V. Somà, CB, T. Duguet, , Phys. Rev. C **89**, 024323 (2014)

V. Somà, CB, T. Duguet, Phys. Rev. C **87**, 011303R (2013)

V. Somà, T. Duguet, CB, Phys. Rev. C **84**, 064317 (2011)

✱ 1<sup>st</sup> order  $\Rightarrow$  energy-independent self-energy

$$\Sigma_{ab}^{11(1)} = \text{diagram: } a \text{---} b \text{---} c \text{---} d \text{---} a \text{ (loop)} \downarrow \omega'$$

$$\Sigma_{ab}^{12(1)} = \text{diagram: } a \text{---} c \text{---} b \text{---} d \text{---} a \text{ (loop)} \leftarrow \omega'$$

✱ 2<sup>nd</sup> order  $\Rightarrow$  energy-dependent self-energy

$$\Sigma_{ab}^{11(2)}(\omega) = \text{diagram 1} + \text{diagram 2}$$

$$\Sigma_{ab}^{12(2)}(\omega) = \text{diagram 3} + \text{diagram 4}$$

✱ Gorkov equations



eigenvalue problem

$$\sum_b \begin{pmatrix} t_{ab} - \mu_{ab} + \Sigma_{ab}^{11}(\omega) & \Sigma_{ab}^{12}(\omega) \\ \Sigma_{ab}^{21}(\omega) & -t_{ab} + \mu_{ab} + \Sigma_{ab}^{22}(\omega) \end{pmatrix} \Big|_{\omega_k} \begin{pmatrix} \mathcal{U}_b^k \\ \mathcal{V}_b^k \end{pmatrix} = \omega_k \begin{pmatrix} \mathcal{U}_a^k \\ \mathcal{V}_a^k \end{pmatrix}$$

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

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

# Expressions for 1st & 2nd order diagrams

$$G_{ab}^{11}(\omega) \equiv \begin{array}{c} \uparrow \omega \\ | \\ a \\ | \\ b \end{array} \quad (B5a)$$

$$G_{ab}^{12}(\omega) \equiv \begin{array}{c} \uparrow \omega \\ | \\ a \\ | \\ b \\ | \\ a \\ | \\ a \end{array} \quad (B5b)$$

V. SOMÀ, T. DUGUET, AND C. BARBIERI

It is interesting to note that the first-order  $a$  with a  $J = 0$  many-body state. The other:

$$\begin{aligned} \Sigma_{ab}^{21(1)} &= \frac{1}{2} \sum_{cd,k} \tilde{V}_{cdab} \tilde{U} \\ &= -\frac{1}{2} \sum_{n_1, n_2, n_3} \sum_{\gamma} \\ &= \delta_{a\beta} \delta_{m_1 m_2} \frac{1}{2} \cdot \\ &\equiv \delta_{a\beta} \delta_{m_1 m_2} \Sigma_{n_1 n_2}^{21} \\ &= \delta_{a\beta} \delta_{m_1 m_2} \tilde{F}_{n_1 n_2}^{(a)} \end{aligned}$$

Ab INITIO SELF-CONSISTENT GORKOV-GREEN'S ...

## 5. Block-diagonal structure

a. First order

The goal of this subsection is to discuss how the block-diagonals reflects in the various self-energy contributions, starting with the first and (C19) into Eq. (B7), and introducing the factor

$$f_{a\beta\gamma\delta}^{n_1 n_2 n_3 n_4} \equiv \sqrt{1 + \delta_{a\beta} \delta_{n_1 n_2}}$$

one obtains

$$\begin{aligned} \Sigma_{ab}^{11(1)} &= \sum_{cd,k} \tilde{V}_{abcd} \tilde{V}_d^* \tilde{V}_c^* \\ &= \sum_{n_1, n_2, n_3} \sum_{\gamma} \sum_{JM} f_{a\beta\gamma\gamma}^{n_1 n_2 n_3 n_4} C_{JM}^{JM} \\ &= \delta_{a\beta} \delta_{m_1 m_2} \sum_{n_1, n_2} \sum_{\gamma} \sum_{JM} f_{a\beta\gamma\gamma}^{n_1 n_2 n_3 n_4} \frac{1}{2} \\ &\equiv \delta_{a\beta} \delta_{m_1 m_2} \Sigma_{n_1 n_2}^{11(1)} \\ &\equiv \delta_{a\beta} \delta_{m_1 m_2} \Lambda_{n_1 n_2}^{(1)} \end{aligned}$$

where the block-diagonal normal density matrix is introduced through

$$\rho_{n_1 n_2}^{(a)} = \sum_{n_3} \mathcal{V}_{n_3 | a}^{(a)}$$

and properties of Clebsch-Gordan coefficients has been used. The  $\delta_{n_1 n_2}$  and  $\delta_{k_1 k_2}$ , leading to  $\delta_{a\beta} = \delta_{j_1 j_2} \delta_{m_1 m_2} \delta_{k_1 k_2}$ . Similarly, for  $\Sigma^{22(1)}$

$$\begin{aligned} \Sigma_{ab}^{22(1)} &= -\sum_{cd,k} \tilde{V}_{abcd} \tilde{V}_d^* \tilde{V}_c^* \\ &= -\delta_{a\beta} \delta_{m_1 m_2} \sum_{n_1, n_2} \sum_{\gamma} \sum_{JM} f_{a\beta}^{n_1 n_2} \\ &\equiv \delta_{a\beta} \delta_{m_1 m_2} \Sigma_{n_1 n_2}^{22(1)} \\ &= -\delta_{a\beta} \delta_{m_1 m_2} \Lambda_{n_1 n_2}^{(2)} \\ &= -\delta_{a\beta} \delta_{m_1 m_2} [\Lambda_{n_1 n_2}^{(2)}]^* \end{aligned}$$

Let us consider the anomalous contributions to the first-order self-energy derives

$$\begin{aligned} \Sigma_{ab}^{21(1)} &= \frac{1}{2} \sum_{cd,k} \tilde{V}_{abcd} \tilde{V}_d^* \tilde{U}_c^* \\ &= -\frac{1}{2} \sum_{n_1, n_2, n_3} \sum_{\gamma} \sum_{JM} \sum_{M'} f_{a\beta\gamma\gamma}^{n_1 n_2 n_3 n_4} \eta_a \eta_b C_{JM}^{JM'} \\ &= -\frac{1}{2} \sum_{n_1, n_2, n_3} \sum_{\gamma} \sum_{JM} f_{a\beta\gamma\gamma}^{n_1 n_2 n_3 n_4} \eta_a \eta_b C_{JM}^{JM} \\ &= -\frac{1}{2} \sum_{n_1, n_2, n_3} \sum_{\gamma} f_{a\beta\gamma\gamma}^{n_1 n_2 n_3 n_4} \eta_a \eta_b (-1)^{j_1} C_{JM}^{00} \\ &= \delta_{a\beta} \delta_{m_1 m_2} \frac{1}{2} \sum_{n_1, n_2} \sum_{JM} f_{a\beta\gamma\gamma}^{n_1 n_2 n_3 n_4} \pi_a \pi_b (-) \\ &\equiv \delta_{a\beta} \delta_{m_1 m_2} \Sigma_{n_1 n_2}^{21(1)} \\ &\equiv \delta_{a\beta} \delta_{m_1 m_2} \tilde{F}_{n_1 n_2}^{(a)} \end{aligned}$$

where the block-diagonal anomalous density matrix is introduced through

$$\tilde{F}_{n_1 n_2}^{(a)} = \sum_{n_3} \tilde{U}_{n_3 | a}^{(a)}$$

$$-i \int_{C_1} \frac{d\omega'}{2\pi} \sum_{cd,k} \tilde{V}_{abcd} \frac{\mathcal{V}_d^*}{\omega' + \omega}$$

$$C_{n_1 n_2 n_3 n_4}^{n_1 n_2 n_3 n_4} J_c \equiv \frac{1}{\sqrt{6}} [\mathcal{M}_{n_1 n_2 n_3 n_4}^{n_1 n_2 n_3 n_4} J_c - \mathcal{P}_{n_1 n_2 n_3 n_4}^{n_1 n_2 n_3 n_4} J_c - \mathcal{R}_{n_1 n_2 n_3 n_4}^{n_1 n_2 n_3 n_4} J_c], \quad (C43a)$$

## [V. Somà, T. Duguet, CB, Pys. Rev. C84, 046317 (2011)]

$$\Sigma_{n_1 n_2}^{11(2)} = \sum_{n_3, n_4} \sum_{J_c} \sum_{k_1, k_2} \left\{ \frac{C_{n_1 n_2 n_3 n_4}^{n_1 n_2 n_3 n_4} (C_{n_1 n_2 n_3 n_4}^{n_1 n_2 n_3 n_4} J_c)^*}{\omega - (\omega_{k_1} + \omega_{k_2} + \omega_{k_3}) + i\eta} + \frac{(D_{n_1 n_2 n_3 n_4}^{n_1 n_2 n_3 n_4} J_c)^* D_{n_1 n_2 n_3 n_4}^{n_1 n_2 n_3 n_4} J_c}{\omega + (\omega_{k_1} + \omega_{k_2} + \omega_{k_3}) - i\eta} \right\}, \quad (C44a)$$

$$\Sigma_{n_1 n_2}^{12(2)} = \sum_{n_3, n_4} \sum_{J_c} \sum_{k_1, k_2} \left\{ \frac{C_{n_1 n_2 n_3 n_4}^{n_1 n_2 n_3 n_4} (D_{n_1 n_2 n_3 n_4}^{n_1 n_2 n_3 n_4} J_c)^*}{\omega - (\omega_{k_1} + \omega_{k_2} + \omega_{k_3}) + i\eta} + \frac{(D_{n_1 n_2 n_3 n_4}^{n_1 n_2 n_3 n_4} J_c)^* C_{n_1 n_2 n_3 n_4}^{n_1 n_2 n_3 n_4} J_c}{\omega + (\omega_{k_1} + \omega_{k_2} + \omega_{k_3}) - i\eta} \right\}, \quad (C44b)$$

$$\Sigma_{n_1 n_2}^{21(2)} = \sum_{n_3, n_4} \sum_{J_c} \sum_{k_1, k_2} \left\{ \frac{D_{n_1 n_2 n_3 n_4}^{n_1 n_2 n_3 n_4} (C_{n_1 n_2 n_3 n_4}^{n_1 n_2 n_3 n_4} J_c)^*}{\omega - (\omega_{k_1} + \omega_{k_2} + \omega_{k_3}) + i\eta} + \frac{(C_{n_1 n_2 n_3 n_4}^{n_1 n_2 n_3 n_4} J_c)^* D_{n_1 n_2 n_3 n_4}^{n_1 n_2 n_3 n_4} J_c}{\omega + (\omega_{k_1} + \omega_{k_2} + \omega_{k_3}) - i\eta} \right\}, \quad (C44c)$$

$$\Sigma_{n_1 n_2}^{22(2)} = \sum_{n_3, n_4} \sum_{J_c} \sum_{k_1, k_2} \left\{ \frac{D_{n_1 n_2 n_3 n_4}^{n_1 n_2 n_3 n_4} (D_{n_1 n_2 n_3 n_4}^{n_1 n_2 n_3 n_4} J_c)^*}{\omega - (\omega_{k_1} + \omega_{k_2} + \omega_{k_3}) + i\eta} + \frac{(D_{n_1 n_2 n_3 n_4}^{n_1 n_2 n_3 n_4} J_c)^* C_{n_1 n_2 n_3 n_4}^{n_1 n_2 n_3 n_4} J_c}{\omega + (\omega_{k_1} + \omega_{k_2} + \omega_{k_3}) - i\eta} \right\}, \quad (C44d)$$

which recovers relation (72a). The remaining quantum  $\{k_1, k_2, k_3\}$  indices and can be obtained from Eqs. (C43) to  $J_{bc}$  and  $J_c$  as follows:

$$\begin{aligned} \mathcal{P}_{a(J_c, J_{bc})}^{k_1 k_2 k_3} &= \sum_{J_c} (-1)^{j_1 + j_2 + j_3 + j_4} \sqrt{2J_c} \\ &= -\delta_{J_{bc}, J_c} \delta_{M_{bc}, -m_c} \sum_{n_1, n_2, n_3} \sum_{J_c} \pi_c \\ &\quad \times \tilde{V}_{J_c [a(k_1 k_2 k_3)]}^{n_1 n_2 n_3} \mathcal{U}_{n_1 n_2 n_3}^{n_1 n_2 n_3} \\ &\equiv \delta_{J_{bc}, J_c} \delta_{M_{bc}, -m_c} \mathcal{P}_{n_1 n_2 n_3}^{n_1 n_2 n_3} J_c, \end{aligned}$$

$$\begin{aligned} \mathcal{Q}_{a(J_c, J_{bc})}^{k_1 k_2 k_3} &= \sum_{J_c} (-1)^{j_1 + j_2 + j_3 + j_4} \sqrt{2J_c} \\ &= \delta_{J_{bc}, J_c} \delta_{M_{bc}, m_c} \sum_{n_1, n_2, n_3} \sum_{J_c} \pi_c \\ &\quad \times \tilde{V}_{J_c [a(k_1 k_2 k_3)]}^{n_1 n_2 n_3} \mathcal{U}_{n_1 n_2 n_3}^{n_1 n_2 n_3} \\ &\equiv \delta_{J_{bc}, J_c} \delta_{M_{bc}, m_c} \mathcal{Q}_{n_1 n_2 n_3}^{n_1 n_2 n_3} J_c, \end{aligned}$$

$$\begin{aligned} \mathcal{R}_{a(J_c, J_{bc})}^{k_1 k_2 k_3} &= \sum_{J_c} (-1)^{j_1 + j_2 + 2j_3} \sqrt{2J_c} + 1 \\ &= -\delta_{J_{bc}, J_c} \delta_{M_{bc}, m_c} \sum_{n_1, n_2, n_3} \sum_{J_c} \pi_c \\ &\quad \times \tilde{V}_{J_c [a(k_1 k_2 k_3)]}^{n_1 n_2 n_3} \mathcal{U}_{n_1 n_2 n_3}^{n_1 n_2 n_3} \\ &\equiv \delta_{J_{bc}, J_c} \delta_{M_{bc}, m_c} \mathcal{R}_{n_1 n_2 n_3}^{n_1 n_2 n_3} J_c, \end{aligned}$$

$$\begin{aligned} \mathcal{S}_{a(J_c, J_{bc})}^{k_1 k_2 k_3} &= \sum_{J_c} (-1)^{j_1 + j_2 + 2j_3} \sqrt{2J_c} + 1 \\ &= \delta_{J_{bc}, J_c} \delta_{M_{bc}, m_c} \sum_{n_1, n_2, n_3} \sum_{J_c} \pi_c \\ &\quad \times \tilde{V}_{J_c [a(k_1 k_2 k_3)]}^{n_1 n_2 n_3} \mathcal{V}_{n_1 n_2 n_3}^{n_1 n_2 n_3} \\ &\equiv \delta_{J_{bc}, J_c} \delta_{M_{bc}, m_c} \mathcal{S}_{n_1 n_2 n_3}^{n_1 n_2 n_3} J_c, \end{aligned}$$

where general properties of Clebsch-Gordan

$$\begin{aligned} \Lambda_{a(J_c, J_{bc})}^{k_1 k_2 k_3} &= \delta_{J_{bc}, J_c} \delta_{M_{bc}, m_c} \sum_{n_1, n_2} \\ &\equiv \delta_{J_{bc}, J_c} \delta_{M_{bc}, m_c} \mathcal{N}_{n_1 n_2}^{n_1 n_2} \end{aligned}$$

One can show that the same result is obtained

$$\begin{aligned} \tilde{\mathcal{N}}_{a(J_c, J_{bc})}^{k_1 k_2 k_3} &= \sum_{m_1, m_2, m_3, M_c} C_{J_1 M_1}^{J_c M_c} C_{J_2 M_2}^{J_c M_c} C_{J_3 M_3}^{J_c M_c} \\ &= \sum_{m_1, m_2, m_3, M_c} C_{J_1 M_1}^{J_c M_c} C_{J_2 M_2}^{J_c M_c} C_{J_3 M_3}^{J_c M_c} \\ &= \sum_{m_1, m_2, m_3, M_c} \sum_{J_c} \delta_{k_1, 0} \delta_{m_1, -m_c} \delta_{k_2, 0} \delta_{m_2, -m_c} \delta_{k_3, 0} \delta_{m_3, m_c} \eta_a \eta_b f_{a\beta\gamma\gamma}^{n_1 n_2 n_3 n_4} \\ &\quad \times C_{J_1 M_1}^{J_c M_c} C_{J_2 M_2}^{J_c M_c} C_{J_3 M_3}^{J_c M_c} C_{J_c M_c}^{J_c M_c} \mathcal{V}_{n_1 n_2 n_3}^{n_1 n_2 n_3} \mathcal{U}_{n_1 n_2 n_3}^{n_1 n_2 n_3} \mathcal{U}_{n_1 n_2 n_3}^{n_1 n_2 n_3} \end{aligned}$$

## 6. Block-diagonal structure of Gorkov's equations

In the previous subsections it has been proven that all single-particle Green's functions and all self-energy contributions entering Gorkov's equations display the same block-diagonal structure if the systems is in a  $0^+$  state. Defining

$$T_{ab} - \mu \delta_{ab} \equiv \delta_{a\beta} \delta_{m_1 m_2} [T_{n_1 n_2}^{(a)} - \mu^{(a)} \delta_{n_1 n_2}], \quad (C45)$$

introducing block-diagonal forms for amplitudes  $\mathcal{W}$  and  $\mathcal{Z}$  through

$$\mathcal{W}_{k(J_c, J_{bc})}^{k_1 k_2 k_3} \equiv \delta_{J_{bc}, J_c} \delta_{M_{bc}, m_c} \mathcal{W}_{n_1 n_2 n_3}^{n_1 n_2 n_3} J_c, \quad (C46a)$$

$$\mathcal{Z}_{k(J_c, J_{bc})}^{k_1 k_2 k_3} \equiv -\delta_{J_{bc}, J_c} \delta_{M_{bc}, -m_c} \eta_c \mathcal{Z}_{n_1 n_2 n_3}^{n_1 n_2 n_3} J_c, \quad (C46b)$$

with

$$(\omega_k - E_{k_1 k_2 k_3}) \mathcal{W}_{n_1 n_2 n_3}^{n_1 n_2 n_3} J_c \equiv \sum_{n_4} [(T_{n_1 n_2 n_3 n_4}^{n_1 n_2 n_3 n_4} J_c)^* \mathcal{U}_{n_4 | a}^{(a)} + (D_{n_1 n_2 n_3 n_4}^{n_1 n_2 n_3 n_4} J_c)^* \mathcal{V}_{n_4 | a}^{(a)}], \quad (C47a)$$

$$(\omega_k + E_{k_1 k_2 k_3}) \mathcal{Z}_{n_1 n_2 n_3}^{n_1 n_2 n_3} J_c \equiv \sum_{n_4} [D_{n_1 n_2 n_3 n_4}^{n_1 n_2 n_3 n_4} J_c \mathcal{U}_{n_4 | a}^{(a)} + C_{n_1 n_2 n_3 n_4}^{n_1 n_2 n_3 n_4} J_c \mathcal{V}_{n_4 | a}^{(a)}], \quad (C47b)$$

and using Eqs. (C29), (C31), (C32), (C34), and (C44), one finally writes Eqs. (81) as

$$\begin{aligned} \omega_k \mathcal{U}_{n_1 n_2}^{n_1 n_2} |a\rangle &= \sum_{n_3} [(T_{n_1 n_2 n_3}^{n_1 n_2 n_3} |a\rangle - \mu^{(a)} \delta_{n_1 n_2} |a\rangle) \mathcal{U}_{n_3 | a}^{(a)} + \Lambda_{n_1 n_2}^{(a)*} \mathcal{V}_{n_3 | a}^{(a)} |a\rangle] \\ &\quad + \sum_{n_3, n_4} \sum_{J_c} [C_{n_1 n_2 n_3 n_4}^{n_1 n_2 n_3 n_4} J_c \mathcal{W}_{n_3 n_4}^{n_1 n_2 n_3 n_4} J_c + (D_{n_1 n_2 n_3 n_4}^{n_1 n_2 n_3 n_4} J_c)^* \mathcal{Z}_{n_3 n_4}^{n_1 n_2 n_3 n_4} J_c], \end{aligned} \quad (C48a)$$

$$\begin{aligned} \omega_k \mathcal{V}_{n_1 n_2}^{n_1 n_2} |a\rangle &= \sum_{n_3} [-(T_{n_1 n_2 n_3}^{n_1 n_2 n_3} |a\rangle - \mu^{(a)} \delta_{n_1 n_2} |a\rangle) \mathcal{V}_{n_3 | a}^{(a)} + \tilde{F}_{n_1 n_2}^{(a)} \mathcal{U}_{n_3 | a}^{(a)} |a\rangle] \\ &\quad + \sum_{n_3, n_4} \sum_{J_c} [D_{n_1 n_2 n_3 n_4}^{n_1 n_2 n_3 n_4} J_c \mathcal{W}_{n_3 n_4}^{n_1 n_2 n_3 n_4} J_c + (C_{n_1 n_2 n_3 n_4}^{n_1 n_2 n_3 n_4} J_c)^* \mathcal{Z}_{n_3 n_4}^{n_1 n_2 n_3 n_4} J_c]. \end{aligned} \quad (C48b)$$

064317-30

These terms are finally put together to form the different contributions to second-order self-energies. Let us consider  $\Sigma_{ab}^{21(2)}$  as an example (see Eq. (75)). By inserting Eqs. (C35) and (C36) and summing over all possible total and intermediate angular momenta, one has

$$\Sigma_{ab}^{21(2)} = \frac{1}{2} \sum_{m_1, m_2, m_3, k_1, k_2, k_3} \left\{ \frac{\mathcal{M}_{a(J_c, J_{bc})}^{k_1 k_2 k_3} (\mathcal{M}_{b(J_c, J_{bc})}^{k_1 k_2 k_3})^*}{\omega - (\omega_{k_1} + \omega_{k_2} + \omega_{k_3}) + i\eta} + \frac{\Lambda_{a(J_c, J_{bc})}^{k_1 k_2 k_3} (\Lambda_{b(J_c, J_{bc})}^{k_1 k_2 k_3})^*}{\omega + (\omega_{k_1} + \omega_{k_2} + \omega_{k_3}) - i\eta} \right\}$$

064317-29

$$\begin{array}{c} \uparrow \omega'' \\ | \\ e \\ | \\ \circlearrowleft \\ | \\ f \\ | \\ h \\ | \\ \downarrow \omega'' \end{array} \quad (B31)$$

$$\begin{aligned} &\frac{1}{2} \sum_{cdefgh} G_{cd}^{11}(\omega'') G_{ef}^{11}(\omega'') G_{gh}^{11}(\omega'') \\ &- \frac{1}{2} \sum_{cdefgh, k_1 k_2 k_3} \tilde{V}_{cdefgh} \left\{ \frac{\mathcal{V}_c^* \mathcal{U}_d^* \mathcal{U}_e^* \mathcal{U}_f^* \mathcal{U}_g^* \mathcal{V}_h^*}{\omega - (\omega_{k_1} + \omega_{k_2} + \omega_{k_3}) + i\eta} + \frac{\tilde{U}_c^* \mathcal{V}_d^* \mathcal{V}_e^* \mathcal{U}_f^* \mathcal{U}_g^* \mathcal{U}_h^*}{\omega + (\omega_{k_1} + \omega_{k_2} + \omega_{k_3}) - i\eta} \right\}. \end{aligned} \quad (B32)$$

064317-28

(C45)

064317-23

# Gorkov equations

[V. Somà, T. Duguet, CB, Pys. Rev. C84, 046317 (2011) ]

$$\sum_b \begin{pmatrix} t_{ab} - \mu_{ab} + \Sigma_{ab}^{11}(\omega) & \Sigma_{ab}^{12}(\omega) \\ \Sigma_{ab}^{21}(\omega) & -t_{ab} + \mu_{ab} + \Sigma_{ab}^{22}(\omega) \end{pmatrix} \Big|_{\omega_k} \begin{pmatrix} \mathcal{U}_b^k \\ \mathcal{V}_b^k \end{pmatrix} = \omega_k \begin{pmatrix} \mathcal{U}_a^k \\ \mathcal{V}_a^k \end{pmatrix}$$



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

Energy independent eigenvalue problem

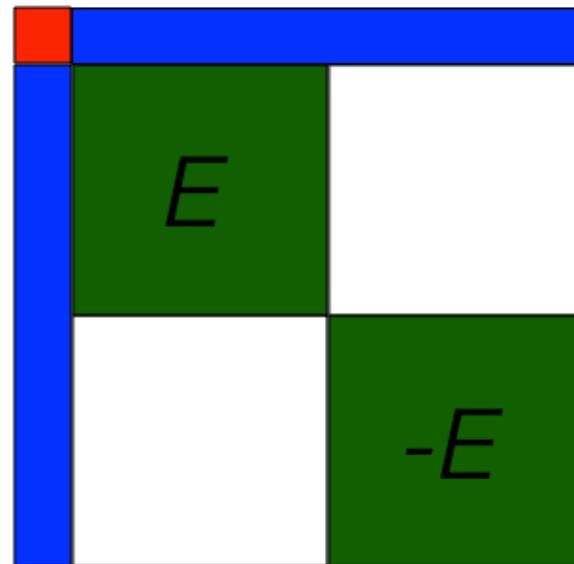
with the normalization condition 
$$\sum_a \left[ |\mathcal{U}_a^k|^2 + |\mathcal{V}_a^k|^2 \right] + \sum_{k_1 k_2 k_3} \left[ |\mathcal{W}_k^{k_1 k_2 k_3}|^2 + |\mathcal{Z}_k^{k_1 k_2 k_3}|^2 \right] = 1$$

# Lanczos reduction of self-energy

V. Somà, CB, T. Duguet, , Phys. Rev. C **89**, 024323 (2014)

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

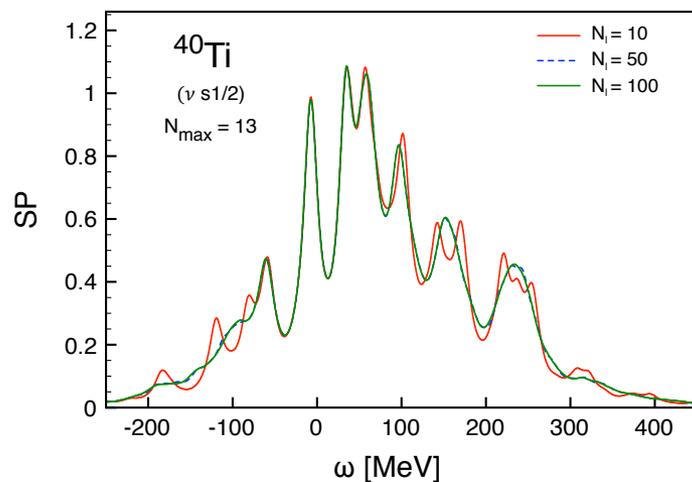
HFB



→ Conserves moments of spectral functions

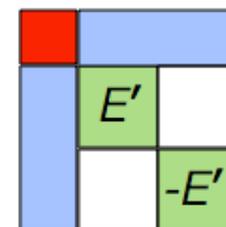
→ Equivalent to exact diagonalization for  $N_L \rightarrow \dim(E)$

## Spectral strength



Lanczos

HFB



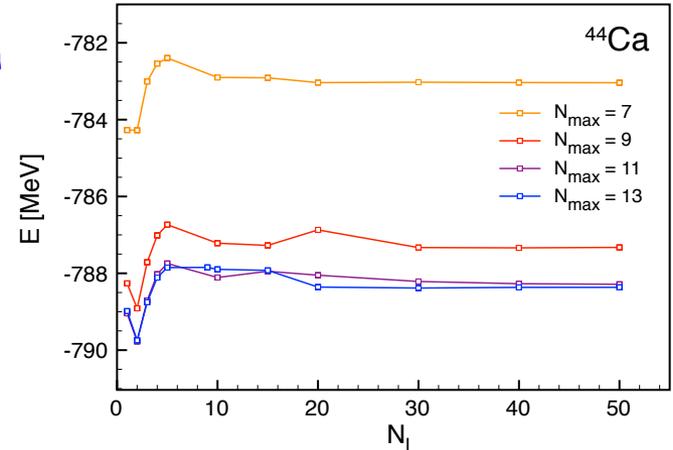
# Testing Krylov projection

V. Somà, CB, T. Duguet, , Phys. Rev. C **89**, 024323 (2014)

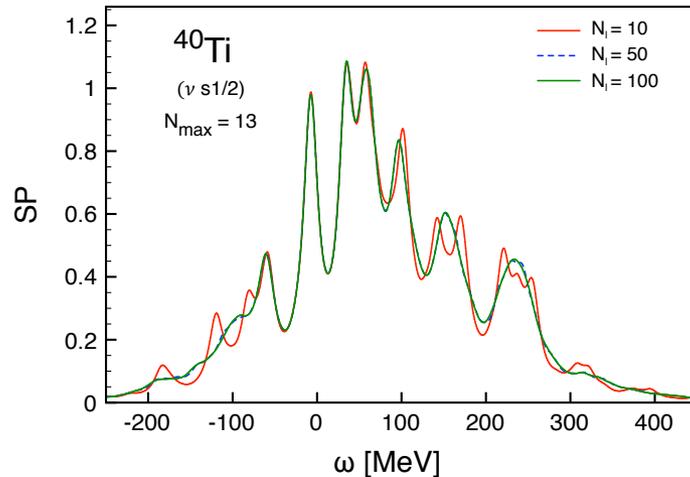
- Energy and spectra independent of the projection
- Same behavior for all model spaces



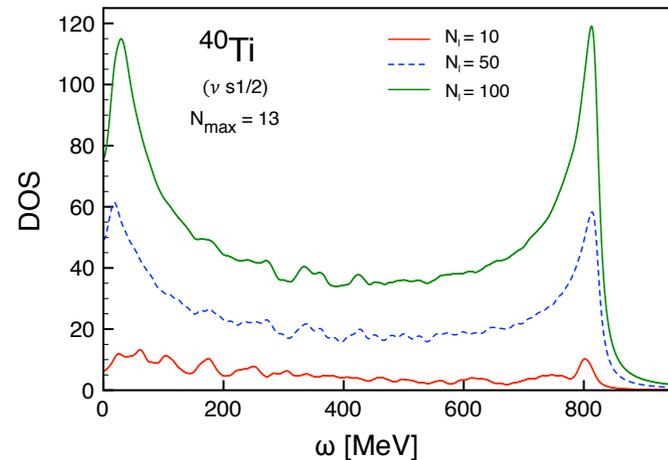
**Favourable scaling**



**Spectral strength**

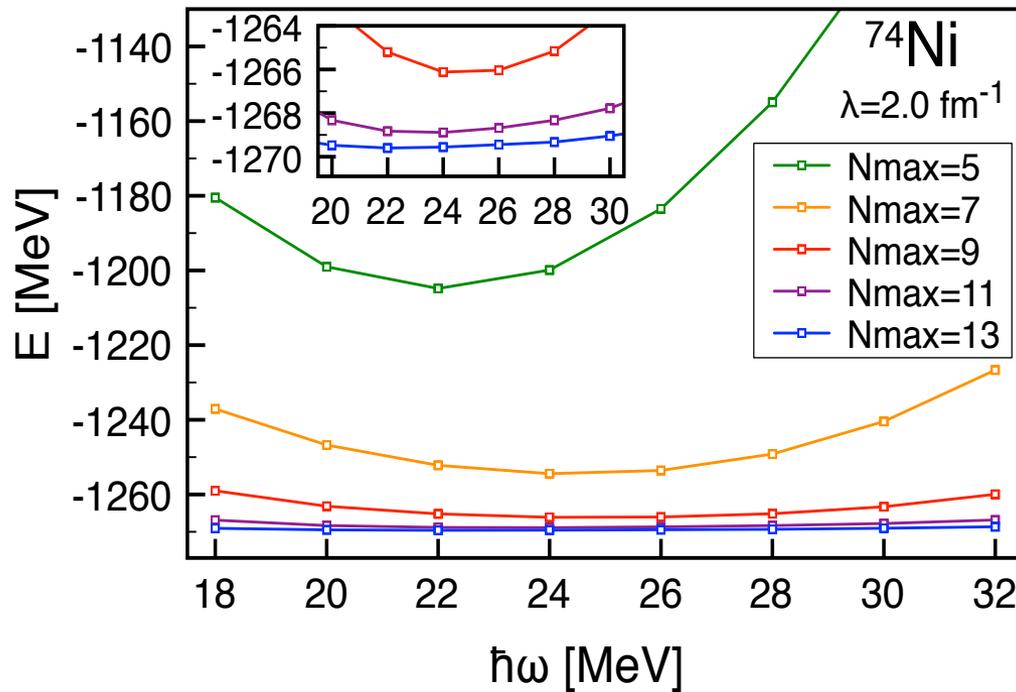


**Density of states**



# Binding energies

Somà, CB, Duguet, Phys. Rev. C **87**, 011303 (2013)



⇒ NN interaction:  
chiral  $N^3\text{LO}$  SRG-evolved to  $2.0 \text{ fm}^{-1}$

[Entem and Machleidt 2003]

⇒ Very good convergence

⇒ From  $N=13$  to  $N=11 \rightarrow 200 \text{ keV}$

$$E(N=13) = -1269.6 \text{ MeV}$$

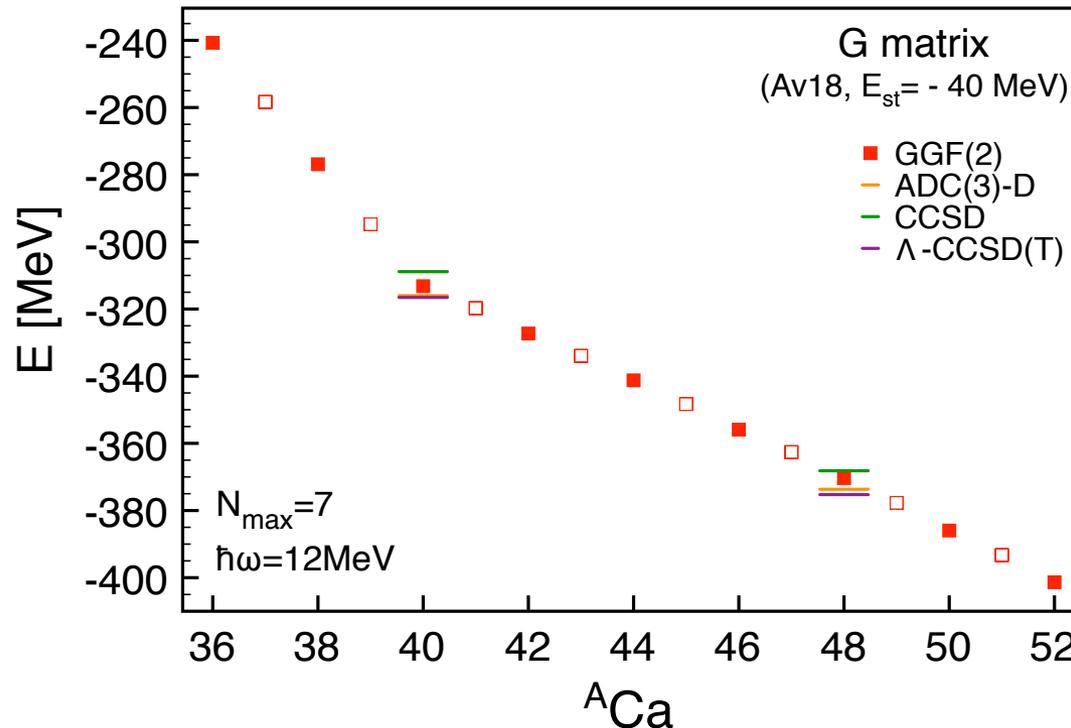
$$E(N=\infty) = -1269.7(2) \text{ MeV}$$

(Extrapolation to infinite model space from  
[Furnstahl, Hagen, Papenbrok 2012] and [Coon et al. 2012])

# Binding energies

Somà, CB, Duguet, Phys. Rev. C **87**, 011303 (2013)

\* Systematic along isotopic/isotonic chains has become available



- Accuracy is good (close to CCSD and FRPA) and improvable
- Systematic along isotopic/isotonic chains has become possible
- Of course, need proper interactions and (at least) NNN forces...

# Approaches in GF theory

Truncation  
scheme:

Dyson formulation  
(closed shells)

Gorkov formulation  
(semi-magic)

1<sup>st</sup> order:

Hartree-Fock

HF-Bogolioubov

2<sup>nd</sup> order:

2<sup>nd</sup> order

2<sup>nd</sup> order (w/ pairing)

...

...

3<sup>rd</sup> and all-orders  
sums,  
P-V coupling:

ADC(3)  
FRPA  
etc...

G-ADC(3)  
...work in progress



# Approaches in GF theory

Truncation scheme:

1<sup>st</sup> order:

2<sup>nd</sup> order:

...

3<sup>rd</sup> and all-order sums,  
P-V coupling

Dyson formulation  
(closed shells)

Hartree-Fock

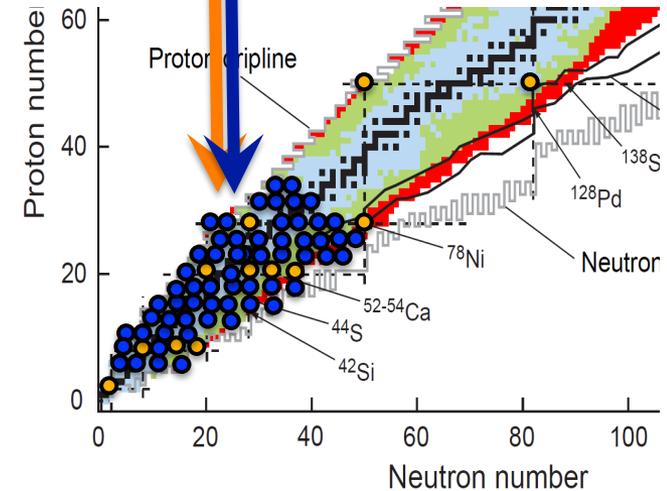
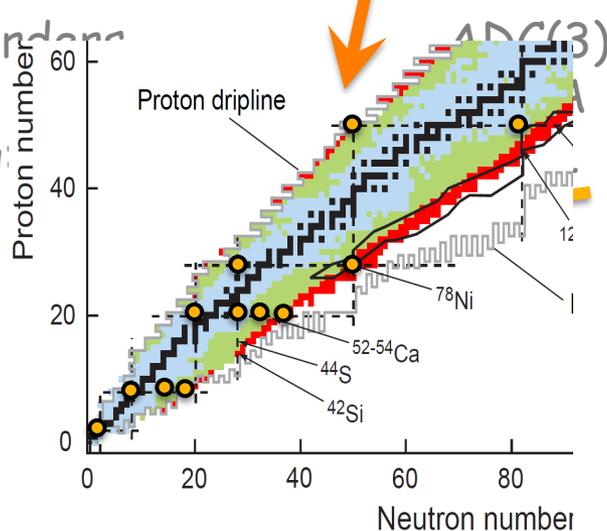
2<sup>nd</sup> order

...

Gorkov formulation  
(semi-magic)

HF-Bogoliubov

2<sup>nd</sup> order (w/ pairing)



# Ab-initio Nuclear Computation & BcDor code

BoccaDorata code:

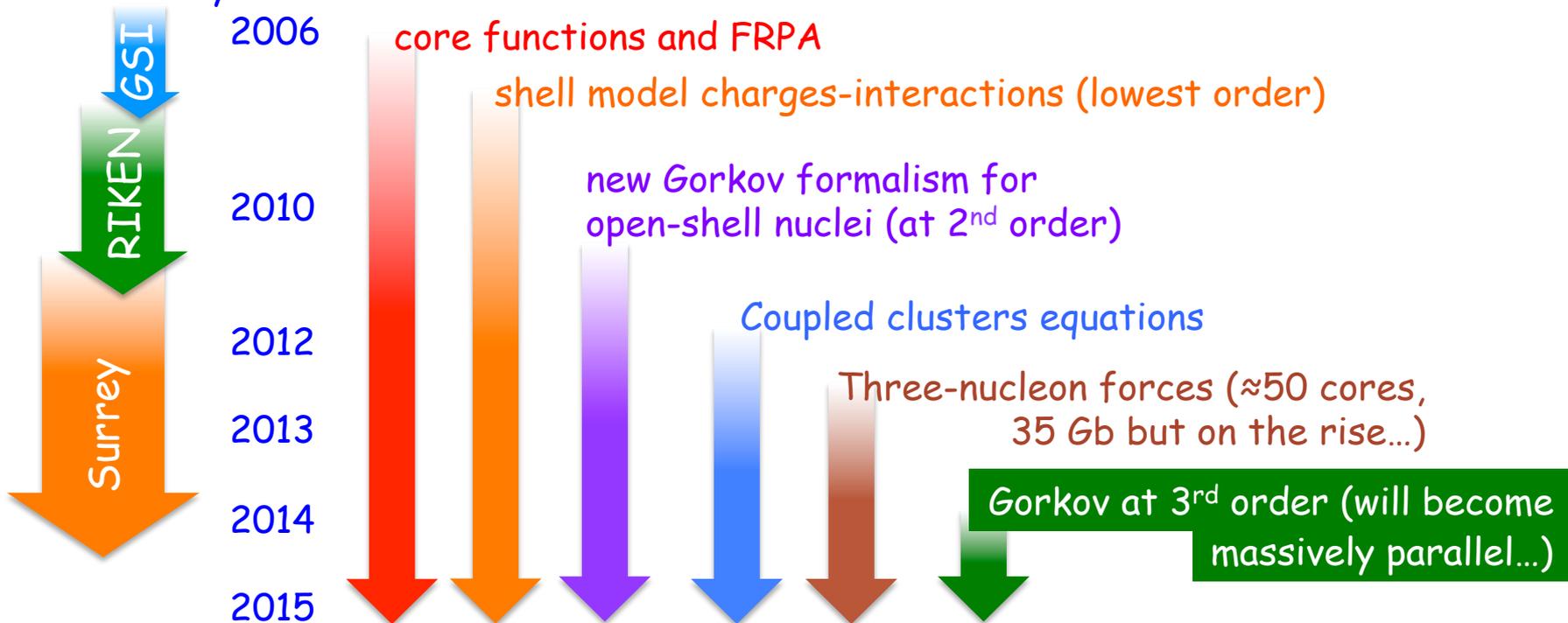
(C. Barbieri 2006-14

V. Somà 2011-14

A. Cipollone 2012-13)

- Provides a *C++ class library* for handling many-body propagators ( $\approx 40,000$  lines, OpenMPI based).
- Allows to solve for nuclear spectral functions, many-body propagators, RPA responses, coupled cluster equations and effective interaction/charges for the shell model.

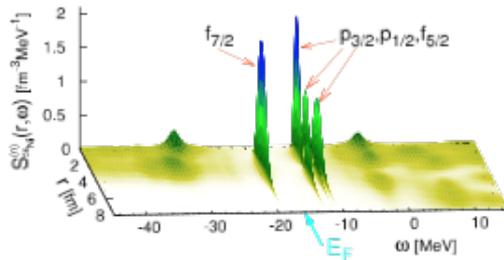
Code history:



# Ab-initio Nuclear Computation & BcDor code

<http://personal.ph.surrey.ac.uk/~cb0023/bcdor/>

## Computational Many-Body Physics



Download

Documentation

### Welcome

From here you can download a public version of my self-consistent Green's function (SCGF) code for nuclear physics. This is a code in J-coupled scheme that allows the calculation of the single particle propagators (a.k.a. one-body Green's functions) and other many-body properties of spherical nuclei.

This version allows to:

- Perform Hartree-Fock calculations.
- Calculate the correlation energy at second order in perturbation theory (MBPT2).
- Solve the Dyson equation for propagators (self consistently) up to second order in the self-energy.
- Solve coupled cluster CCD (doubles only!) equations.

When using this code you are kindly invited to follow the creative commons license agreement, as detailed at the weblinks below. In particular, we kindly ask you to refer to the publications that led the development of this software.

Relevant references (which can also help in using this code) are:

- Prog. Part. Nucl. Phys. 52, p. 377 (2004),
- Phys. Rev. A76, 052503 (2007),
- Phys. Rev. C79, 064313 (2009),
- Phys. Rev. C89, 024323 (2014)

# *Results*

# Spectroscopic Factors

# Quenching of absolute spectroscopic factors

[CB, Phys. Rev. Lett. **103**, 202520 (2009)]

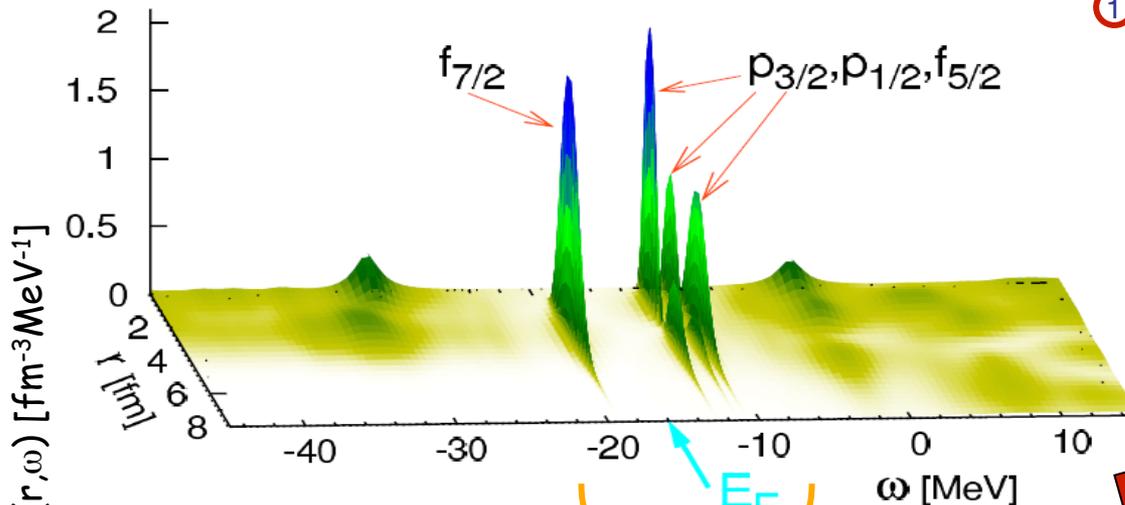
...with analogous conclusions for  $^{48}\text{Ca}$

Overall quenching of *spectroscopic factors* is driven by:

- SRC* → ~10%
- part-vibr. coupling* → dominant
- "shell-model"* → in open shell

	10 osc. shells		Exp. [30]	1p0f space		
	FRPA (SRC)	full FRPA		FRPA SM	$\Delta Z_\alpha$	

$^{57}\text{Ni}$	$\nu 1p_{1/2}$	0.96	0.63	0.61		0.79	0.77	-0.02
	$\nu 0f_{5/2}$	0.95	0.59	0.55		0.79	0.75	-0.04
	$\nu 1p_{3/2}$	0.95	0.65	0.62	0.58(11)	0.82	0.79	-0.03
$^{55}\text{Ni}$	$\nu 0f_{7/2}$	0.95	0.72	0.69		0.89	0.86	-0.03



$$Z_\alpha = \int d^3r |\psi_\alpha^{overlap}(\mathbf{r})|^2 = \frac{1}{1 - \left. \frac{\partial \Sigma_{\hat{\alpha}\hat{\alpha}}(\omega)}{\partial \omega} \right|_{\omega=\epsilon_\alpha}}$$

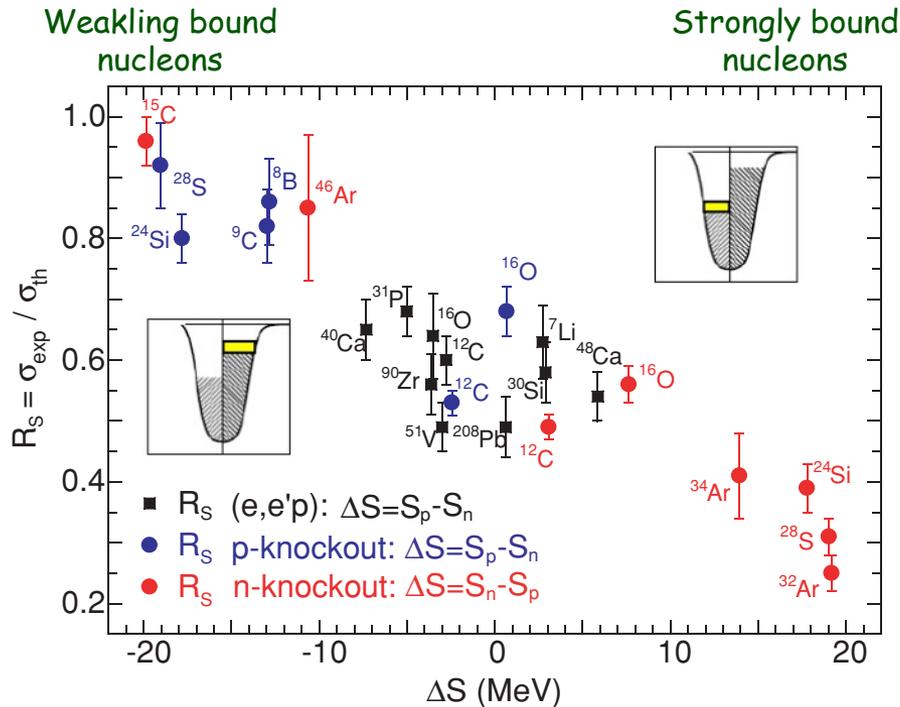
① SHORT RANGE CORRELATIONS

② PARTICLE-VIBRATION COUPLING

③ SHELL MODEL

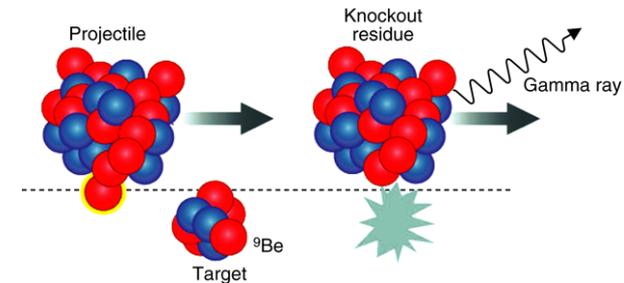
$^{56}\text{Ni}$   
NN-N3LO(500)

# Spectroscopic factors @ limits of stability



[Phys. Rev. C77, 044306 (2008)]

High energy knock-out in inverse kinematics



? **ORIGIN** ?  
**UNCLEAR**  
 ?

- Challenged by recent experiments

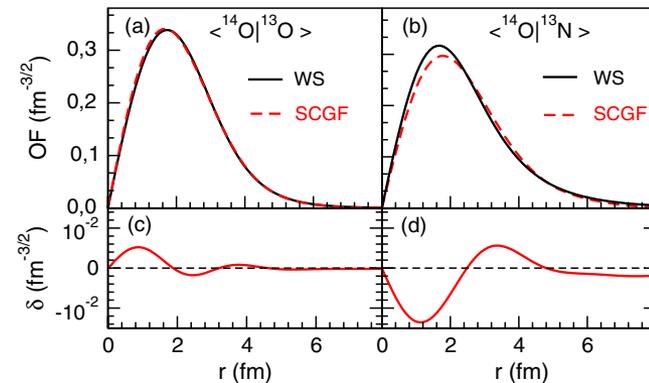
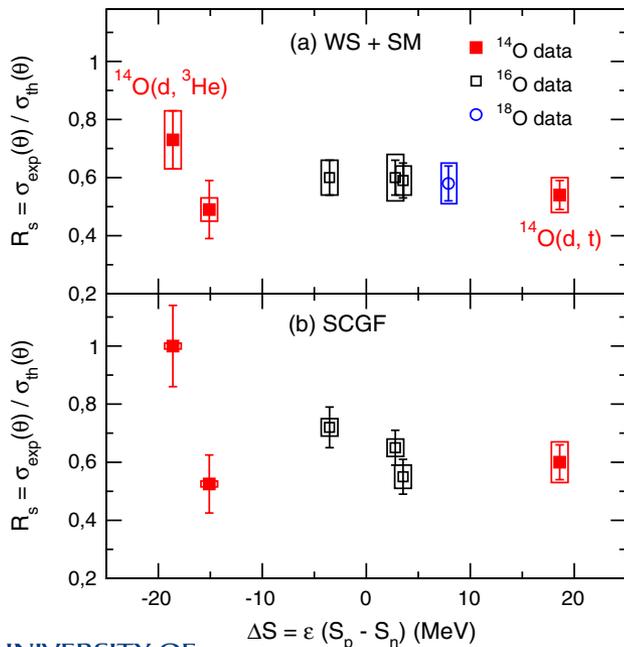
- May be correlations or scattering analysis

# Single nucleon transfer in the oxygen chain

[F. Flavigny et al, PRL110, 122503 (2013)]

→ Analysis of  $^{14}\text{O}(d,t)^{13}\text{O}$  and  $^{14}\text{O}(d,^3\text{He})^{13}\text{N}$  transfer reactions @ SPIRAL

Reaction	$E^*$ (MeV)	$J^\pi$	$R_{\text{rms}}^{\text{HFB}}$ (fm)	$r_0$ (fm)	$C^2S_{\text{exp}}$ (WS)	$C^2S_{\text{th}}$ $0p + 2\hbar\omega$	$R_s$ (WS)	$C^2S_{\text{exp}}$ (SCGF)	$C^2S_{\text{th}}$ (SCGF)	$R_s$ (SCGF)
$^{14}\text{O}(d,t)^{13}\text{O}$	0.00	$3/2^-$	2.69	1.40	1.69 (17)(20)	3.15	0.54(5)(6)	1.89(19)(22)	3.17	0.60(6)(7)
$^{14}\text{O}(d,^3\text{He})^{13}\text{N}$	0.00	$1/2^-$	3.03	1.23	1.14(16)(15)	1.55	0.73(10)(10)	1.58(22)(2)	1.58	1.00(14)(1)
	3.50	$3/2^-$	2.77	1.12	0.94(19)(7)	1.90	0.49(10)(4)	1.00(20)(1)	1.90	0.53(10)(1)
$^{16}\text{O}(d,t)^{15}\text{O}$	0.00	$1/2^-$	2.91	1.46	0.91(9)(8)	1.54	0.59(6)(5)	0.96(10)(7)	1.73	0.55(6)(4)
$^{16}\text{O}(d,^3\text{He})^{15}\text{N}$ [19,20]	0.00	$1/2^-$	2.95	1.46	0.93(9)(9)	1.54	0.60(6)(6)	1.25(12)(5)	1.74	0.72(7)(3)
	6.32	$3/2^-$	2.80	1.31	1.83(18)(24)	3.07	0.60(6)(8)	2.24(22)(10)	3.45	0.65(6)(3)
$^{18}\text{O}(d,^3\text{He})^{17}\text{N}$ [21]	0.00	$1/2^-$	2.91	1.46	0.92(9)(12)	1.58	0.58(6)(10)			

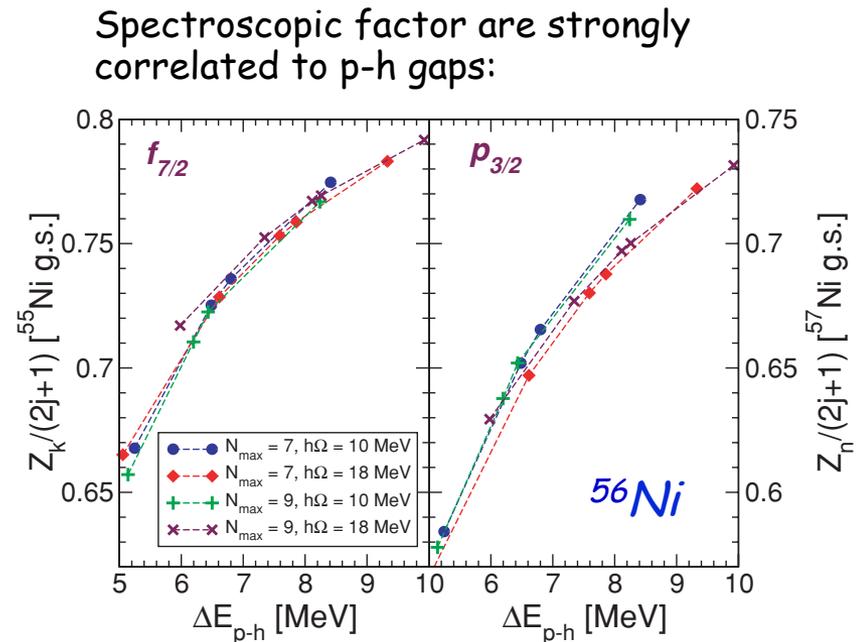
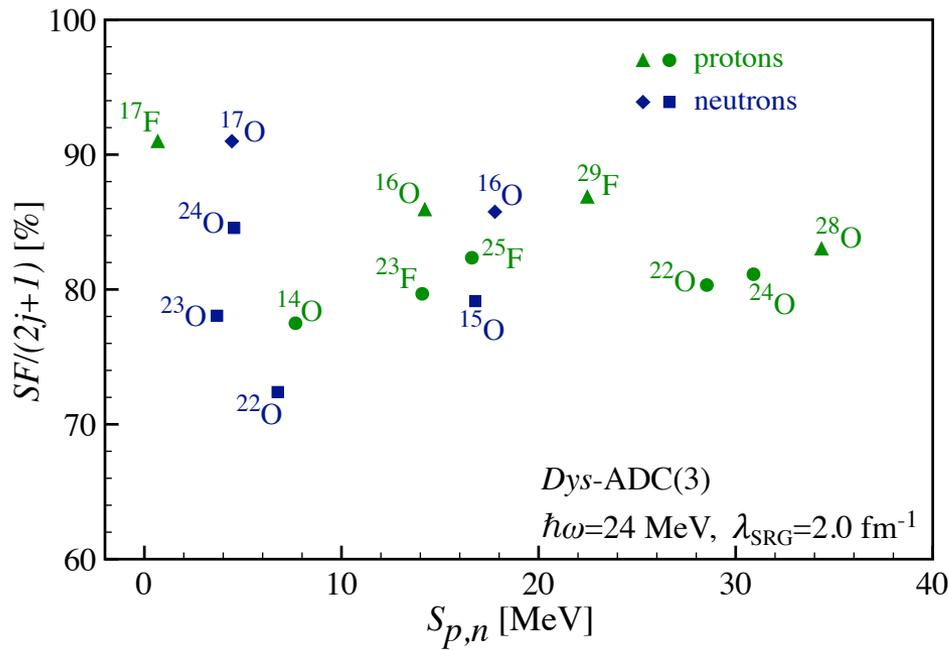


- Overlap functions and strengths from GF
- $R_s$  independent of asymmetry

# Z/N asymmetry dependence of SFs - Theory

Ab-initio calculations explain the Z/N dependence but the effect is much lower than suggested by direct knockout

Effects of continuum become important at the driplines



# Knockout & transfer experiments

✱ Neutron removal from proton- and neutron- Ar isotopes @ NSCL:

Isotopes	$lj^\pi$	Sn(MeV)	$\Delta S$ (MeV)	(theo.)	(expt.)		(expt.)	
				SF(LB-SM)	SF(JLM + HF)	$R_s$ (JLM + HF)	SF(CH89)	$R_s$ (CH89)
$^{34}\text{Ar}$	$s1/2^+$	17.07	12.41	1.31	$0.85 \pm 0.09$	$0.65 \pm 0.07$	$1.10 \pm 0.11$	$0.84 \pm 0.08$
$^{36}\text{Ar}$	$d3/2^+$	15.25	6.75	2.10	$1.60 \pm 0.16$	$0.76 \pm 0.08$	$2.29 \pm 0.23$	$1.09 \pm 0.11$
$^{46}\text{Ar}$	$f7/2^-$	8.07	-10.03	5.16	$3.93 \pm 0.39$	$0.76 \pm 0.08$	$5.29 \pm 0.53$	$1.02 \pm 0.10$

[Lee *et al.* 2010]

	Sn (MeV)	$\Delta S$ (MeV)	SF
$^{34}\text{Ar}$	33.0	18.6	1.46
$^{36}\text{Ar}$	27.7	7.5	1.46
$^{46}\text{Ar}$	16.0	-22.3	5.88

$$\Delta S = S_n - S_p$$

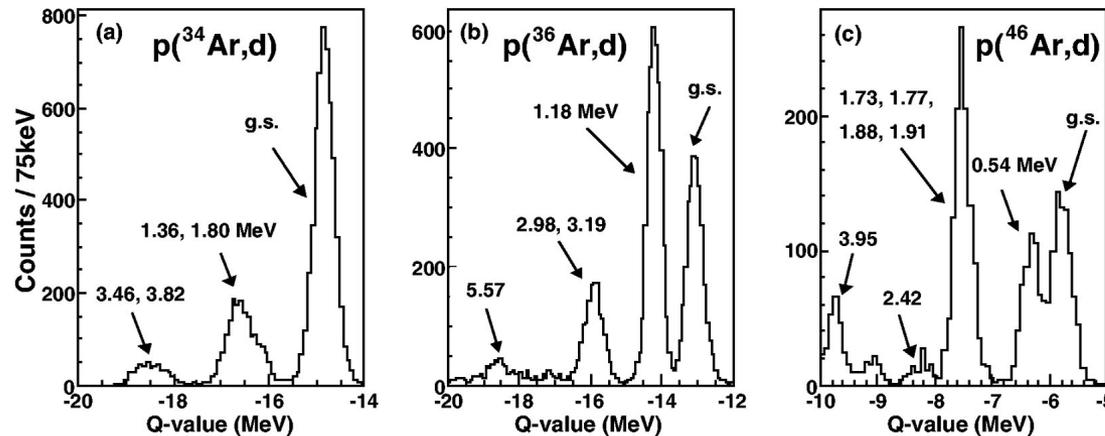
Gorkov GF NN

$^{34}\text{Ar}$	22.4	15.5	1.56
$^{36}\text{Ar}$	15.3	7.2	1.54
$^{46}\text{Ar}$	6.5	-15.7	6.64

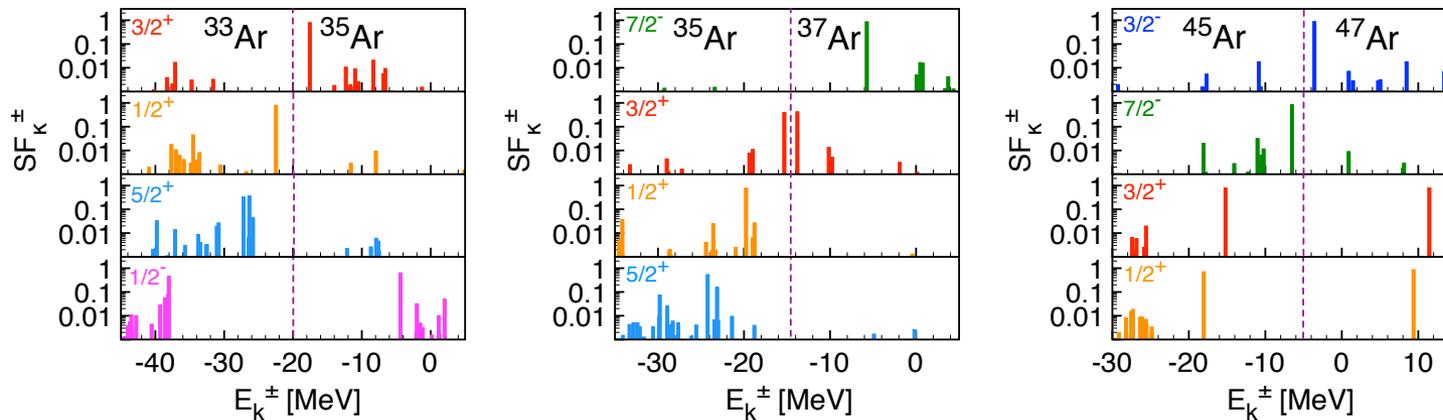
Gorkov GF NN + 3N

# Knockout & transfer experiments

✱ Neutron removal from proton- and neutron- Ar isotopes @ NSCL:

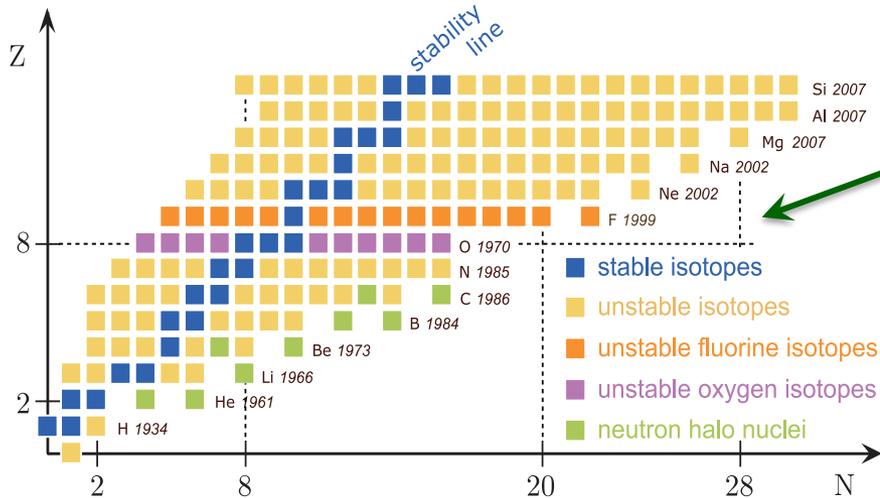


[Lee *et al.* 2010]



# Chiral Hamiltonian and 3NF

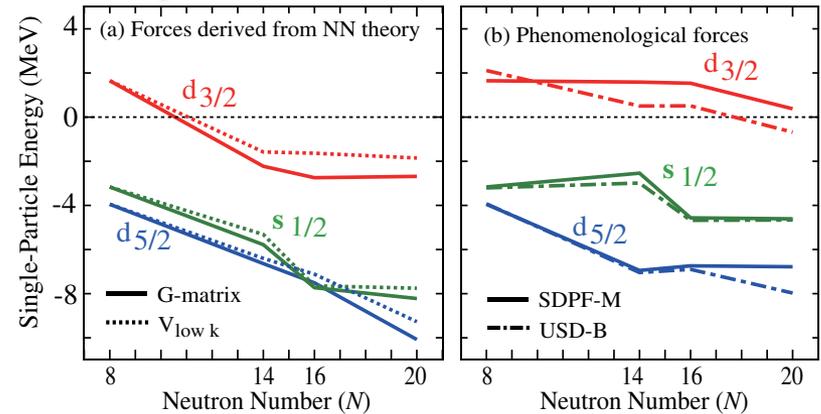
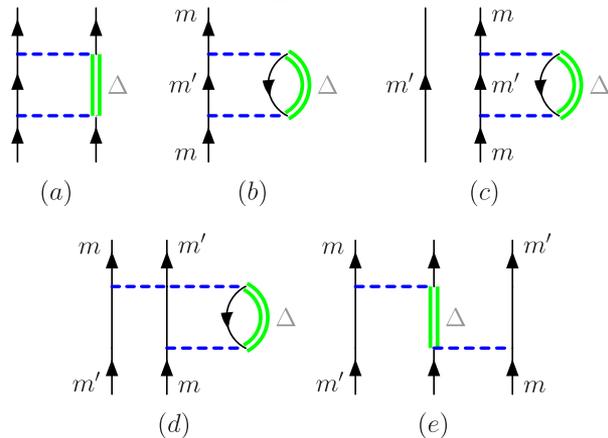
# Oxygen puzzle...



The oxygen dripline is at  $^{24}\text{O}$ , at odds with other neighbor isotope chains.

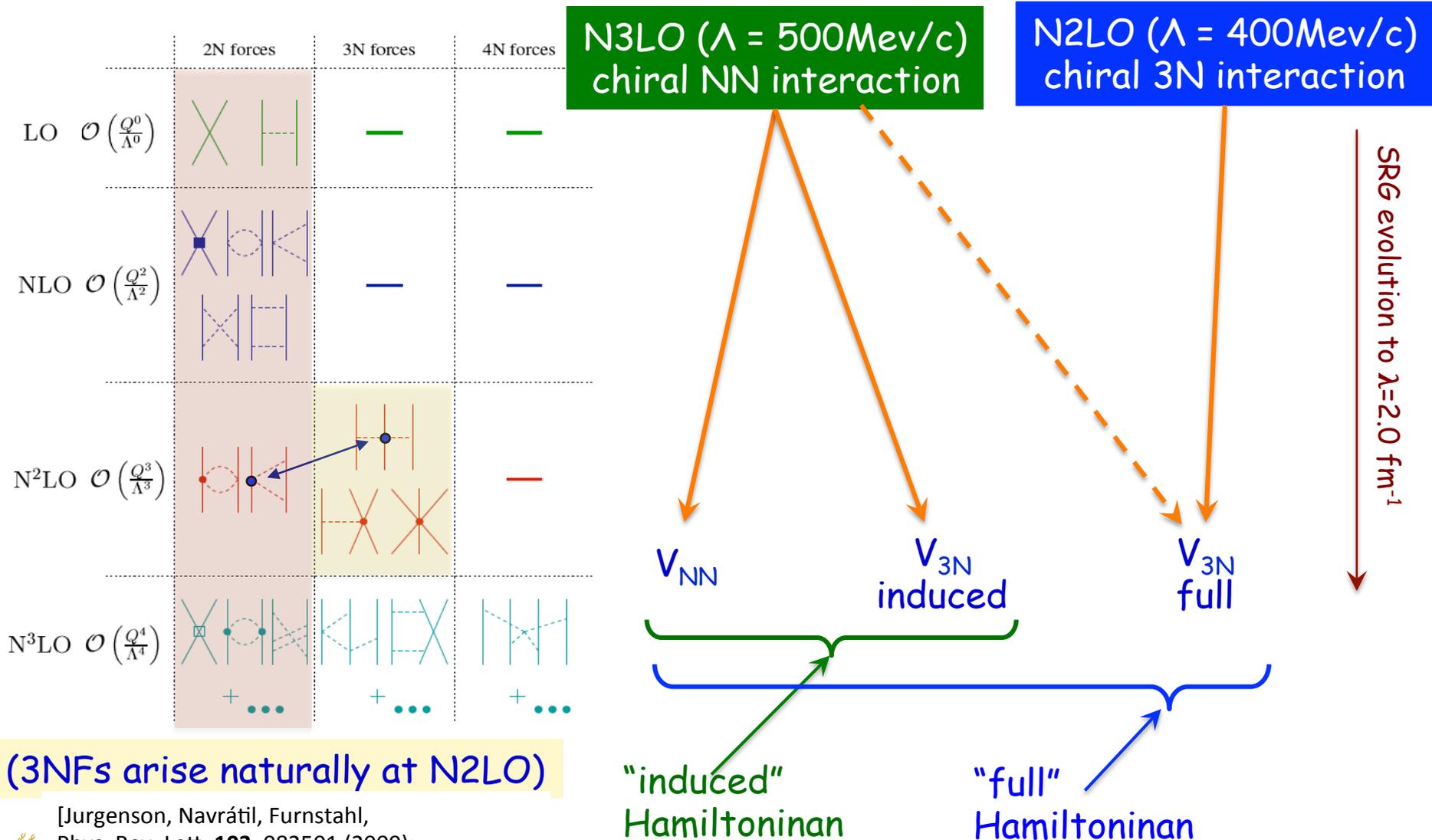
Phenomenological shell model interaction reflect this in the s.p. energies but no realistic NN interaction alone is capable of reproducing this...

The fujita-Miyazawa 3NF provides repulsion through Pauli screening of other 2NF terms:



[T. Otsuka et al., Phys Rev. Lett **105**, 32501 (2010)]

# Chiral Nuclear forces - SRG evolved

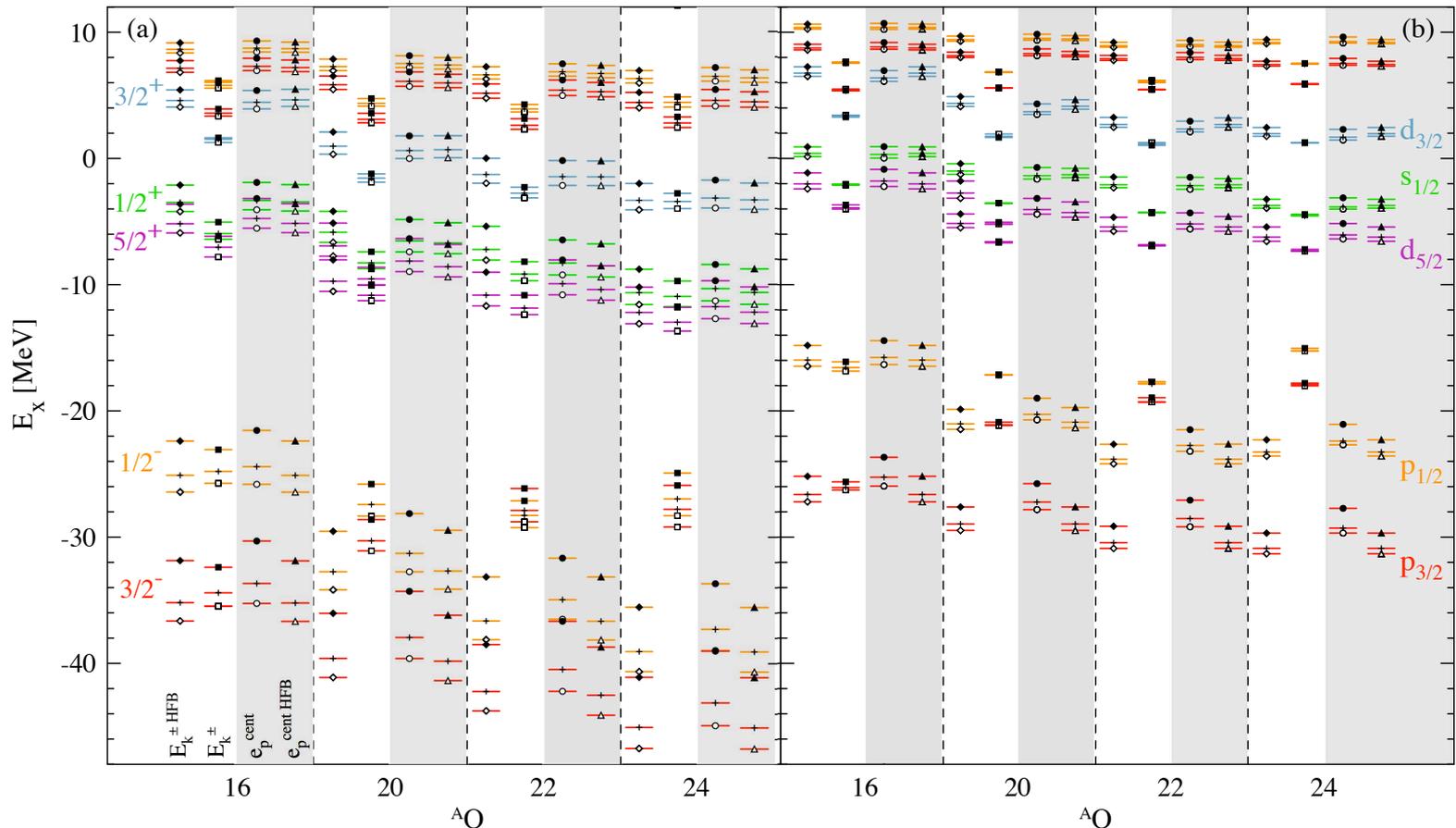


# Convergence of s.p. spectra w.r.t. SRG

Cutoff dependence is reduced, indicating good convergence of many-body truncation and many-body forces

arXiv:1411.1237 (2014)

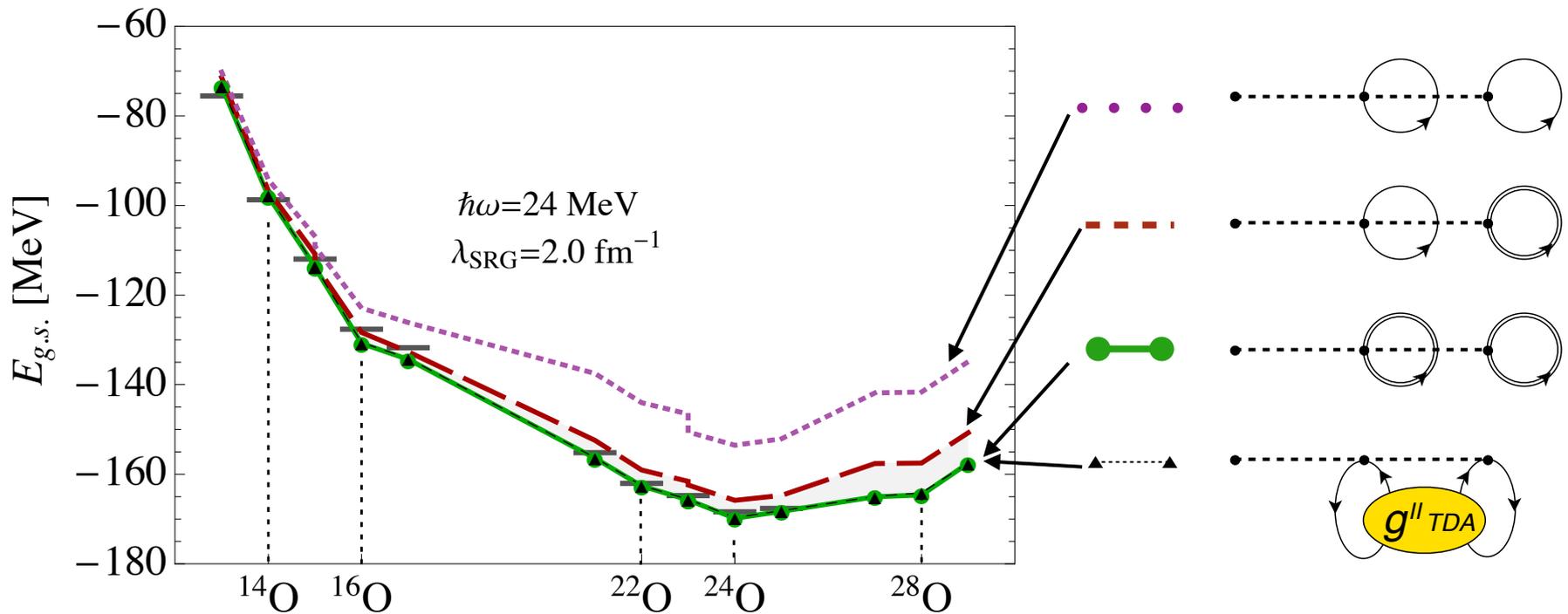
✓ only dominant s.p. states shown



NN terms (no induced 3NF)  $\leftrightarrow$  NN+3NF fully included

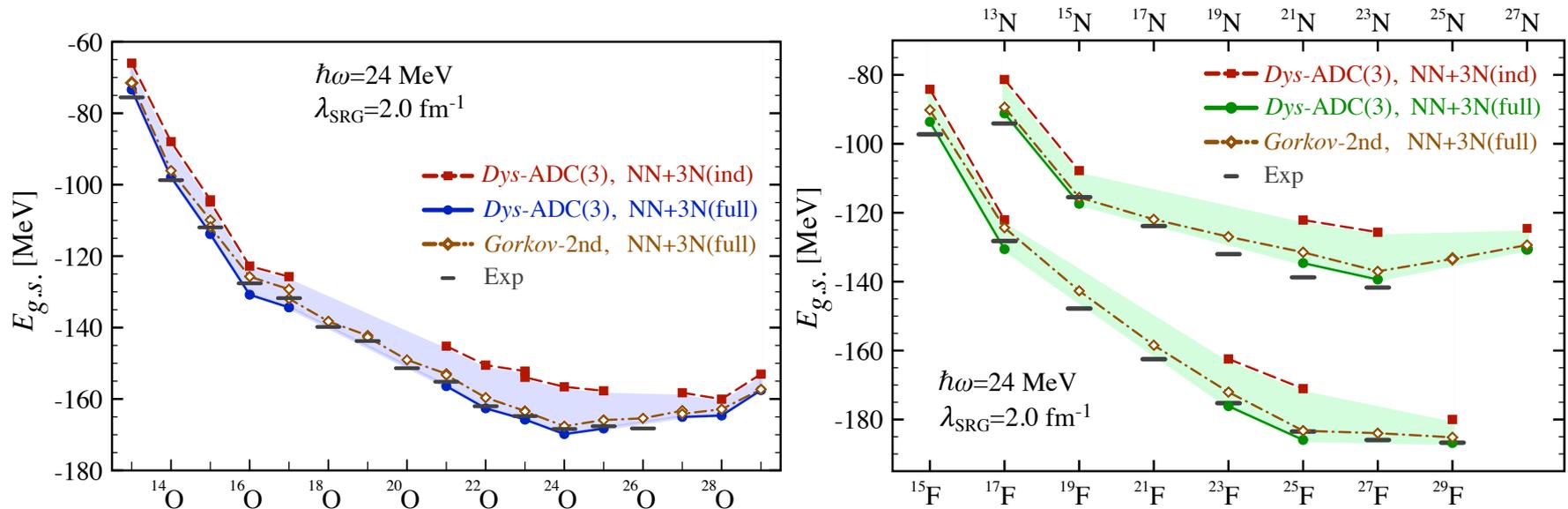
# 3N forces in FRPA/FTDA formalism

→ Ladder contributions to static self-energy are negligible (in oxygen)



# Results for the N-O-F chains

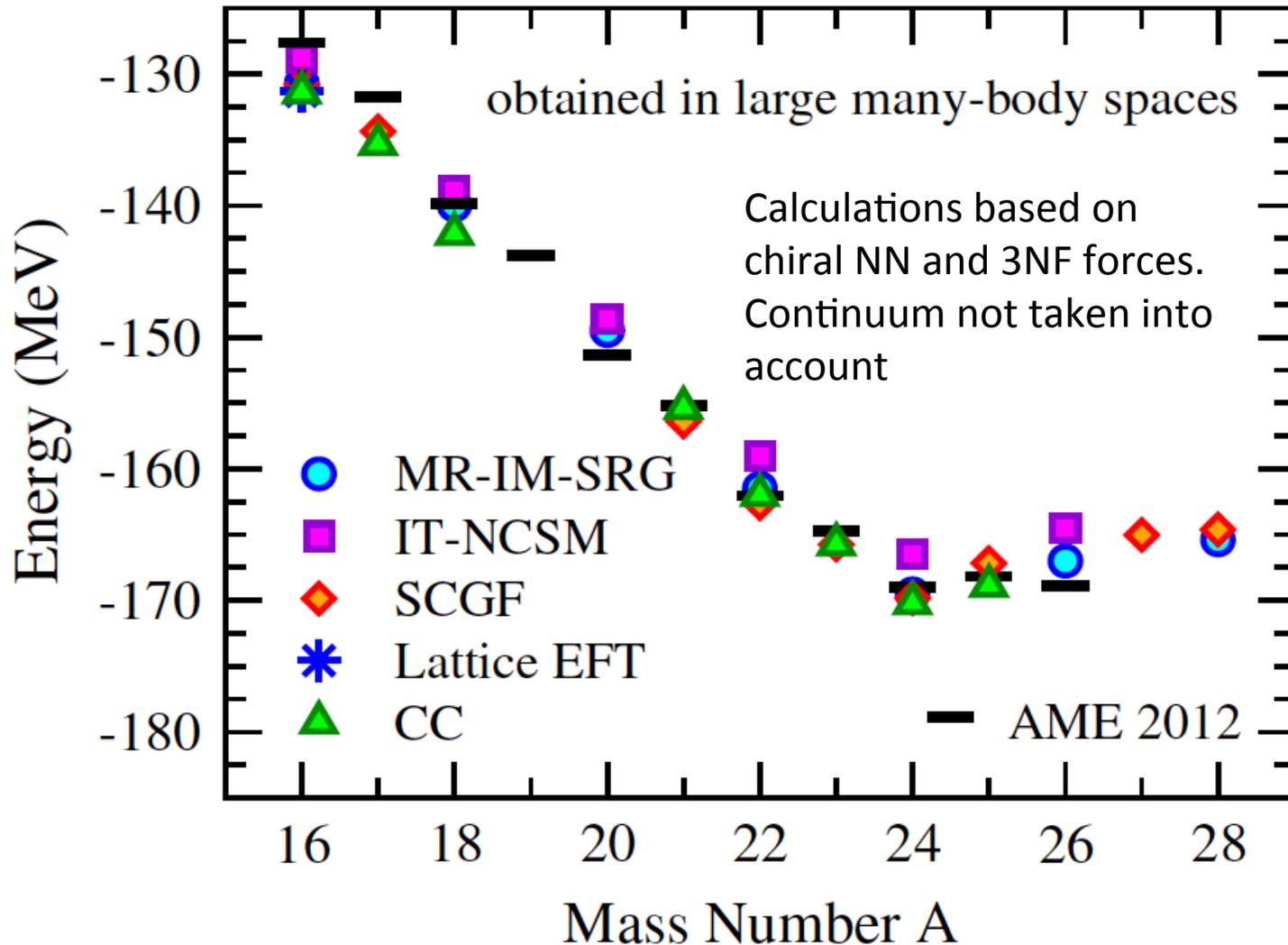
A. Cipollone, CB, P. Navrátil, Phys. Rev. Lett. **111**, 062501 (2013)  
and arXiv:1412.3002 [nucl-th] (2014)



→ 3NF crucial for reproducing binding energies and driplines around oxygen

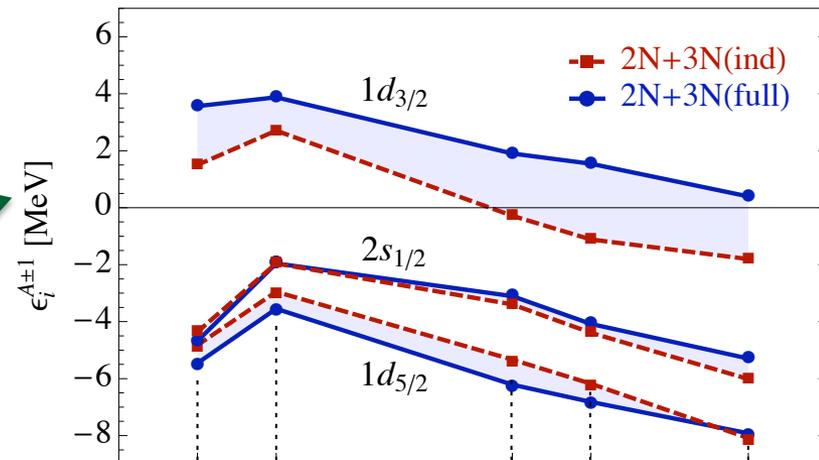
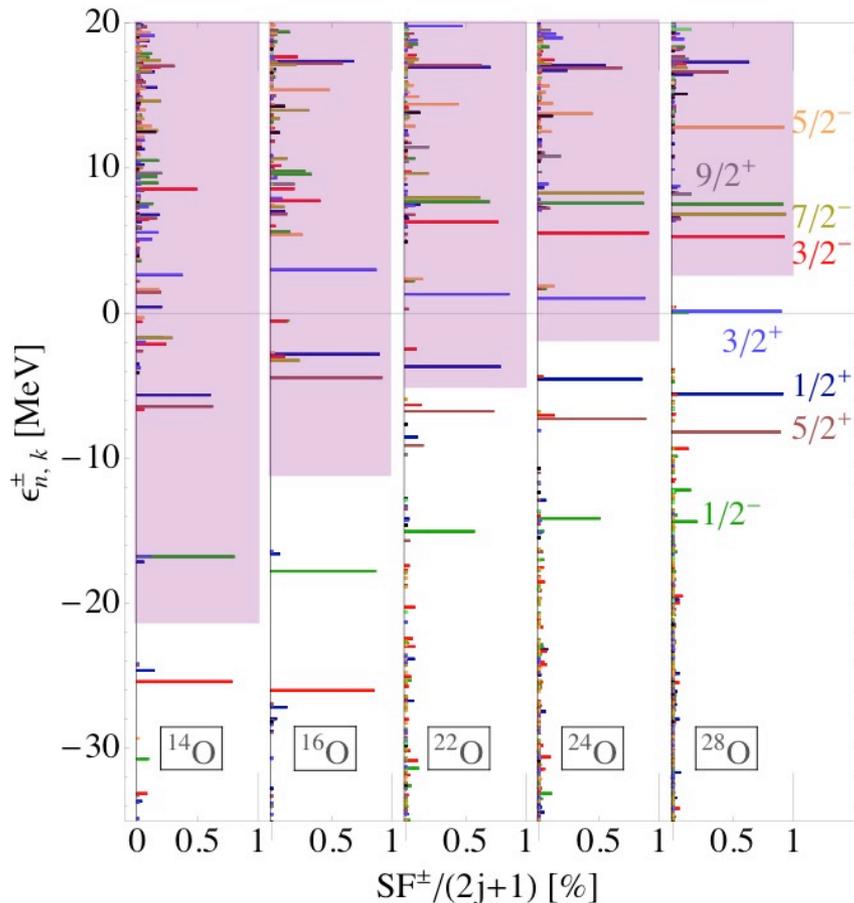
→ cf. microscopic shell model [Otsuka et al, PRL**105**, 032501 (2010).]

# Benchmark of *ab-initio* methods in the oxygen isotopic chain



# Results for the N-O-F chains

A. Cipollone, CB, P. Navrátil, Phys. Rev. Lett. **111**, 062501 (2013)  
and arXiv:1412.3002 [nucl-th] (2014)

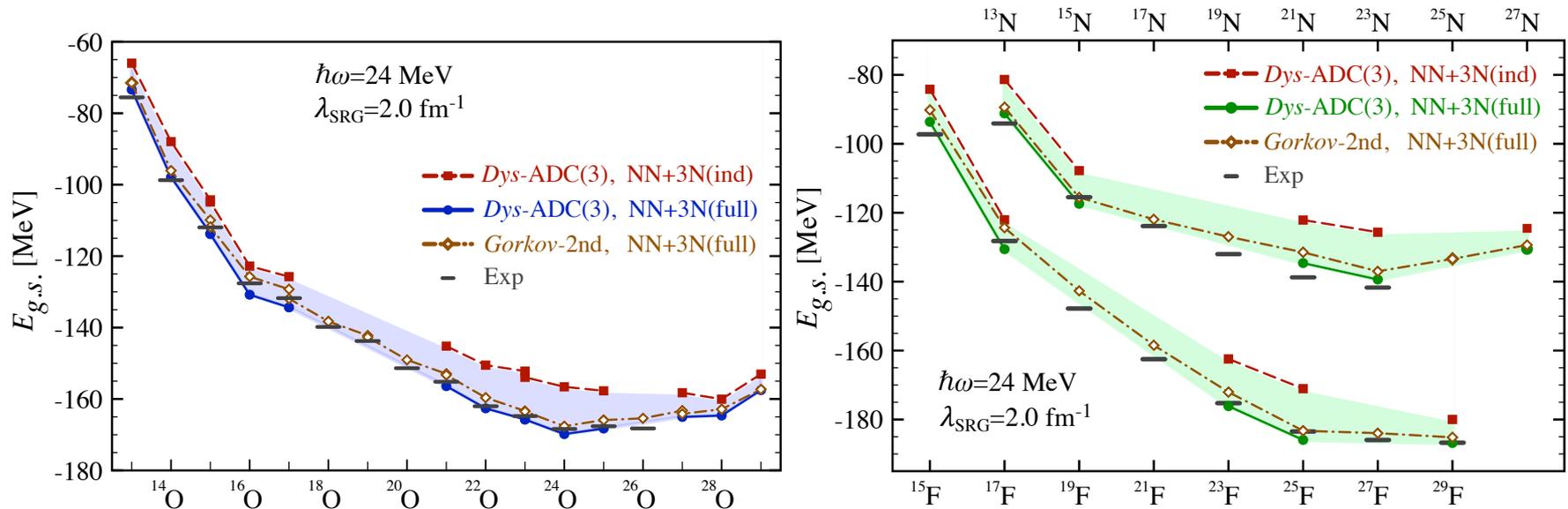


→  $d_{3/2}$  raised by genuine 3NF

→ cf. microscopic shell model [Otsuka et al, PRL**105**, 032501 (2010).]

# Results for the N-O-F chains

A. Cipollone, CB, P. Navrátil, Phys. Rev. Lett. **111**, 062501 (2013)  
and arXiv:1412.3002 [nucl-th] (2014)

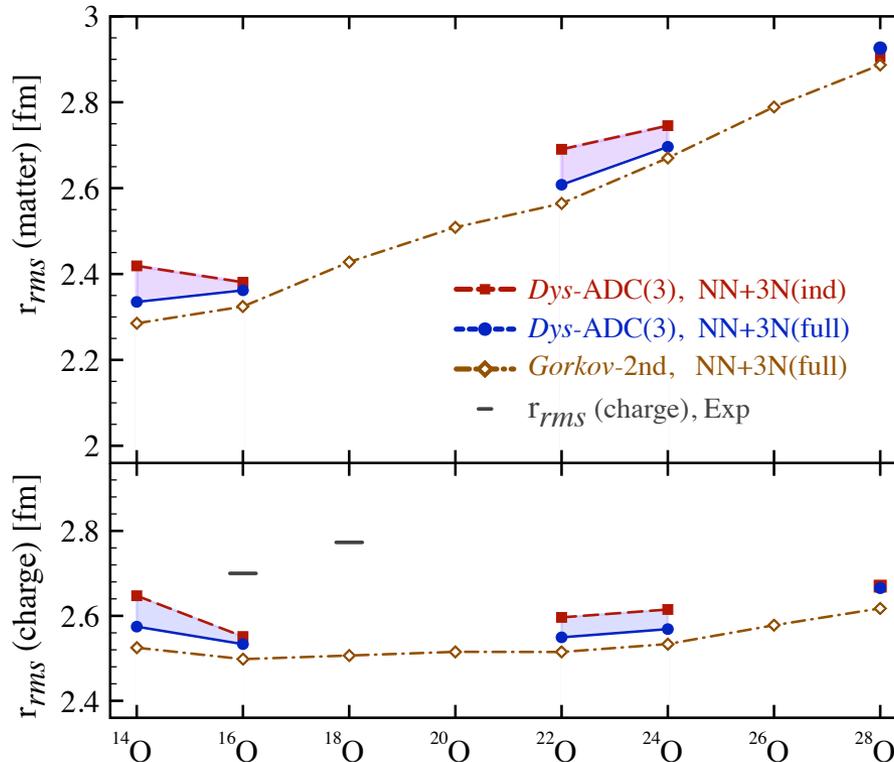


→ 3NF crucial for reproducing binding energies and driplines around oxygen

→ cf. microscopic shell model [Otsuka et al, PRL**105**, 032501 (2010).]

# Results for the oxygen chain

A. Cipollone, CB, P. Navrátil, arXiv:1412.3002 [nucl-th] (2014)

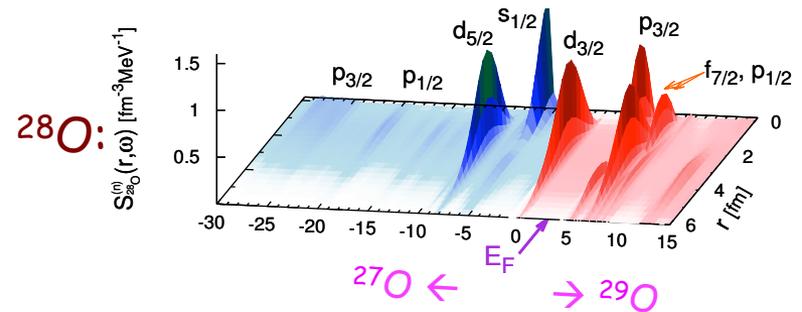
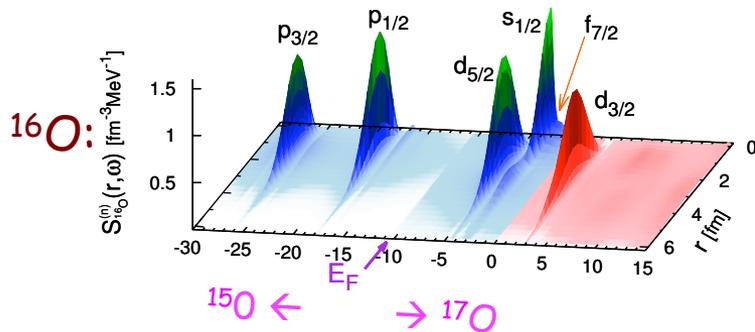
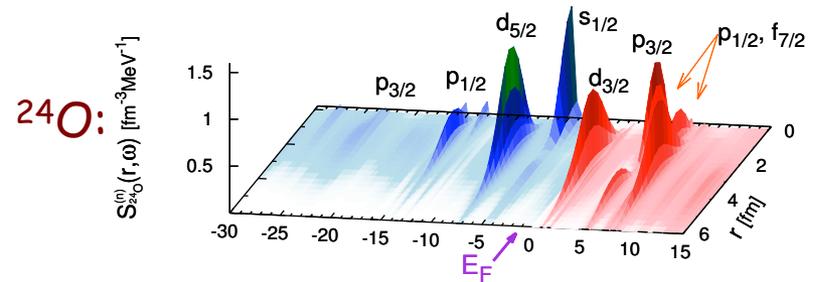
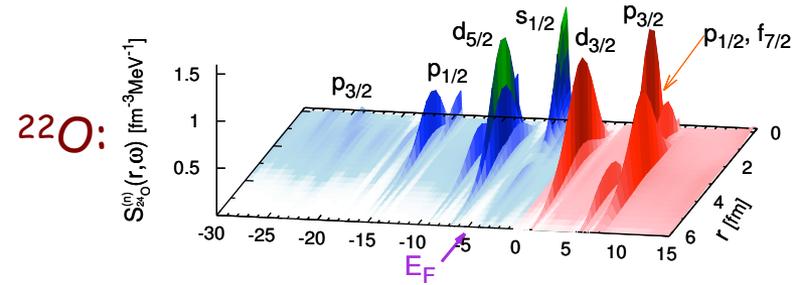
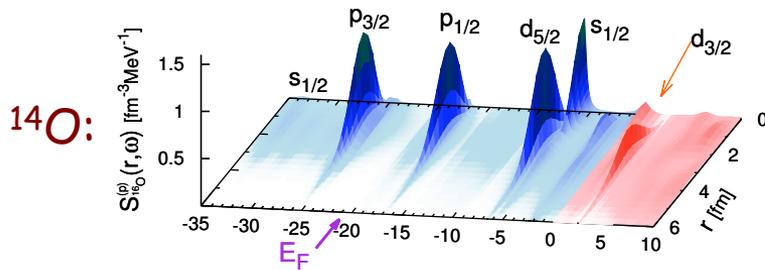
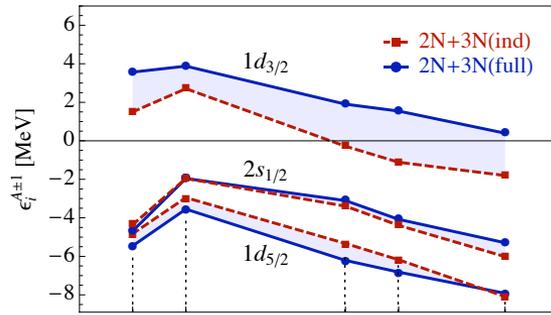
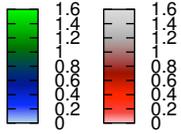


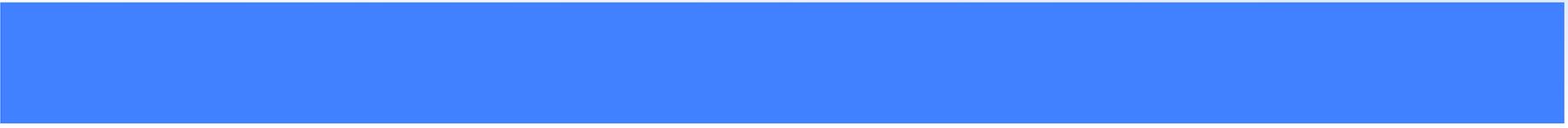
→ Single particle spectra slightly to spread and

→ systematic underestimation of radii

# Neutron spectral function of Oxygens

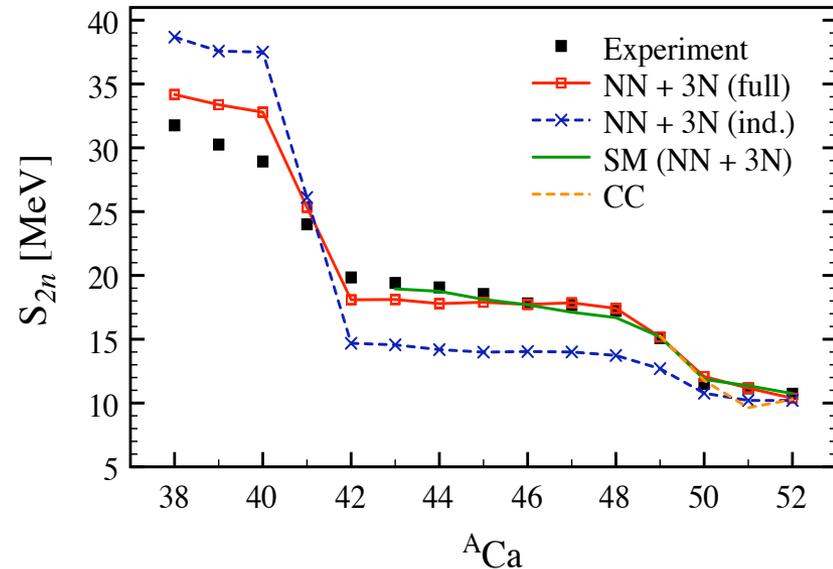
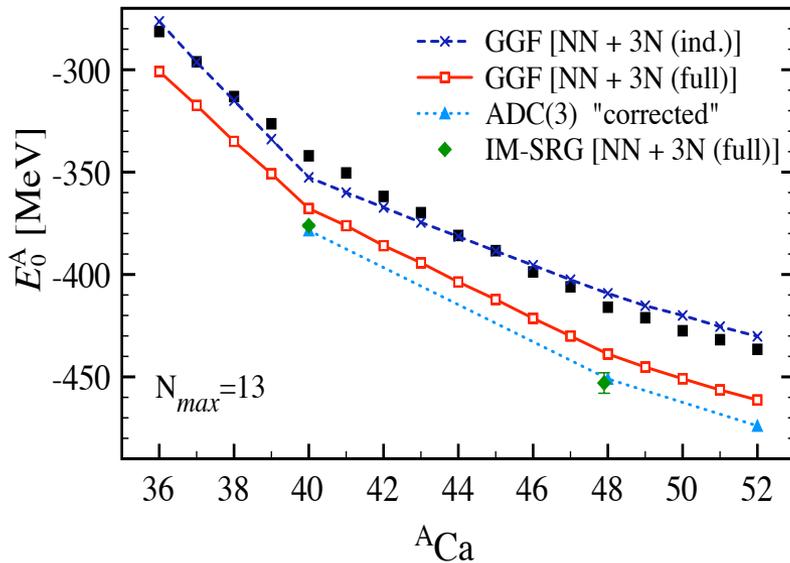
A. Cipollone, CB P. Navrátil, *PRC submitted* (2014)





# Calcium isotopic chain

Ab-initio calculation of the whole Ca: *induced* and *full* 3NF investigated



→ *induced* and *full* 3NF investigated

→ *genuine* (N2LO) 3NF needed to reproduce the energy curvature and  $S_{2n}$

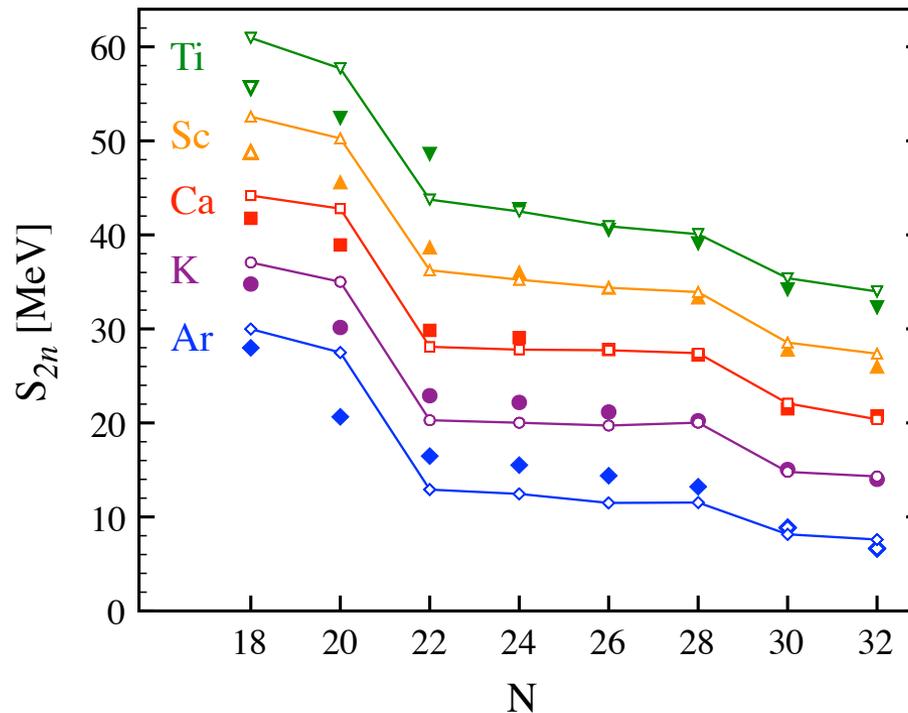
→ N=20 and Z=20 gaps *overestimated!*

→ Full 3NF give a *correct* trend but *over bind!*

# Neighbouring Ar, K, Ca, Sc, and Ti chains

V. Somà, CB *et al.* Phys. Rev. C89, 061301R (2014)

Two-neutron separation energies predicted by chiral NN+3NF forces:

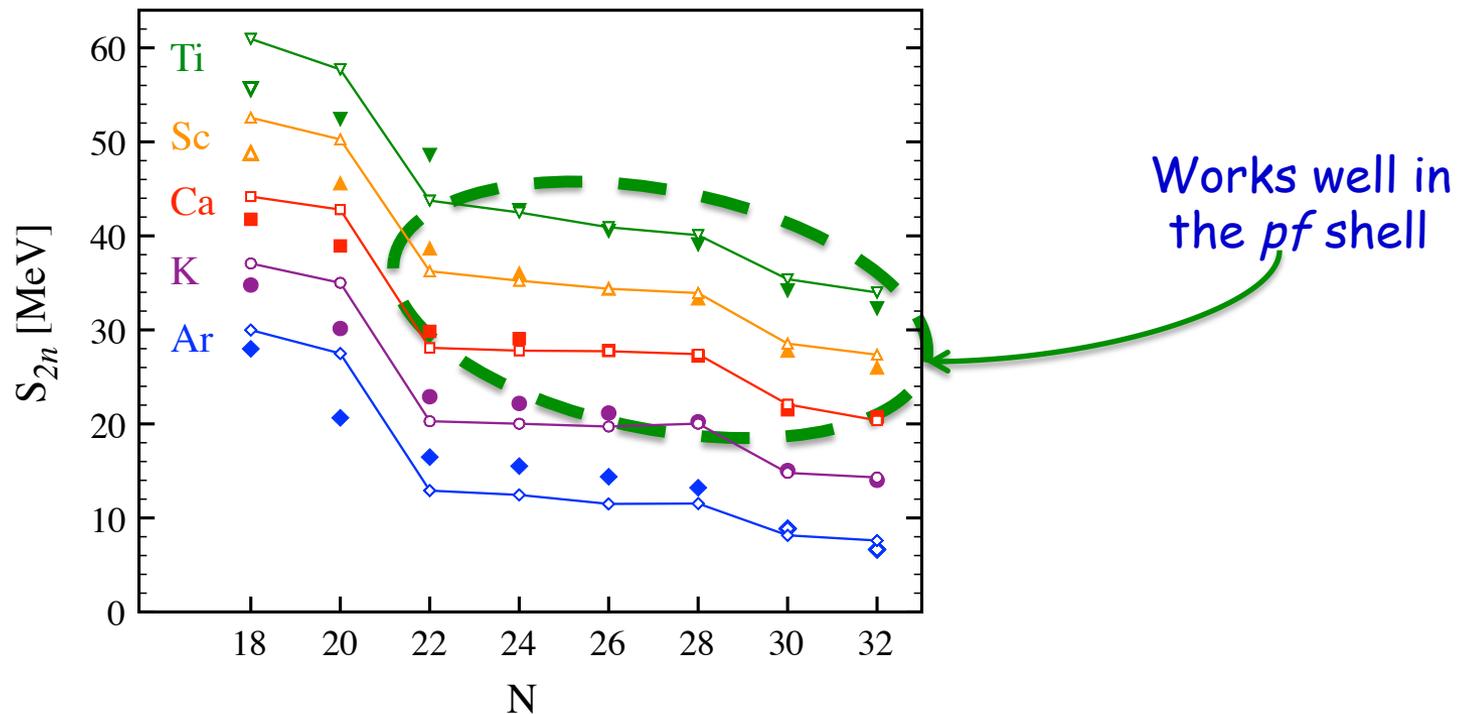


→ First *ab-initio* calculation over a contiguous portion of the nuclear chart—open shells are now possible through the Gorkov-GF formalism

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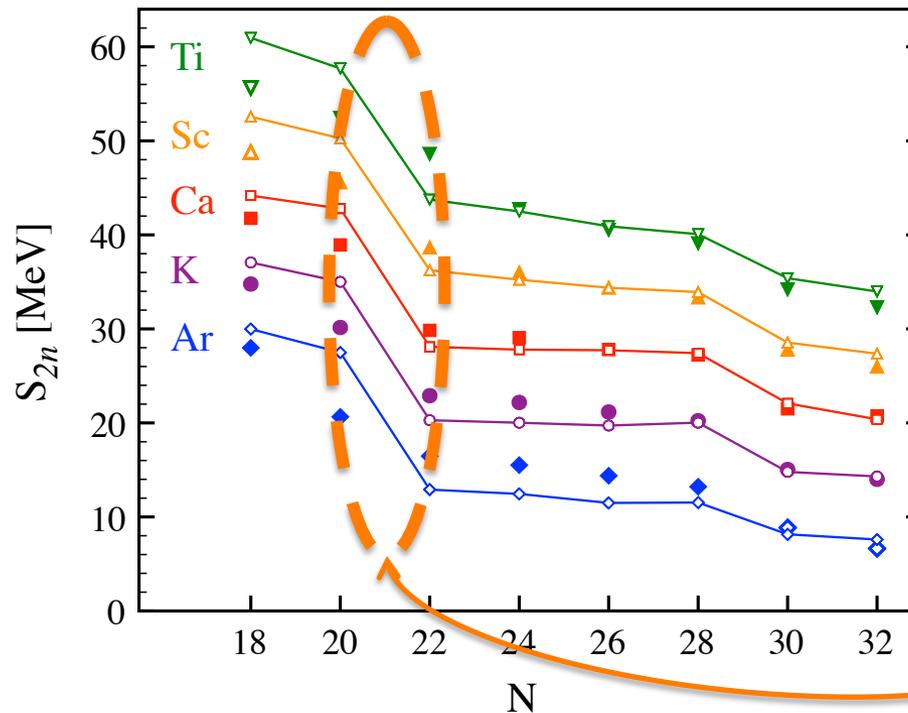


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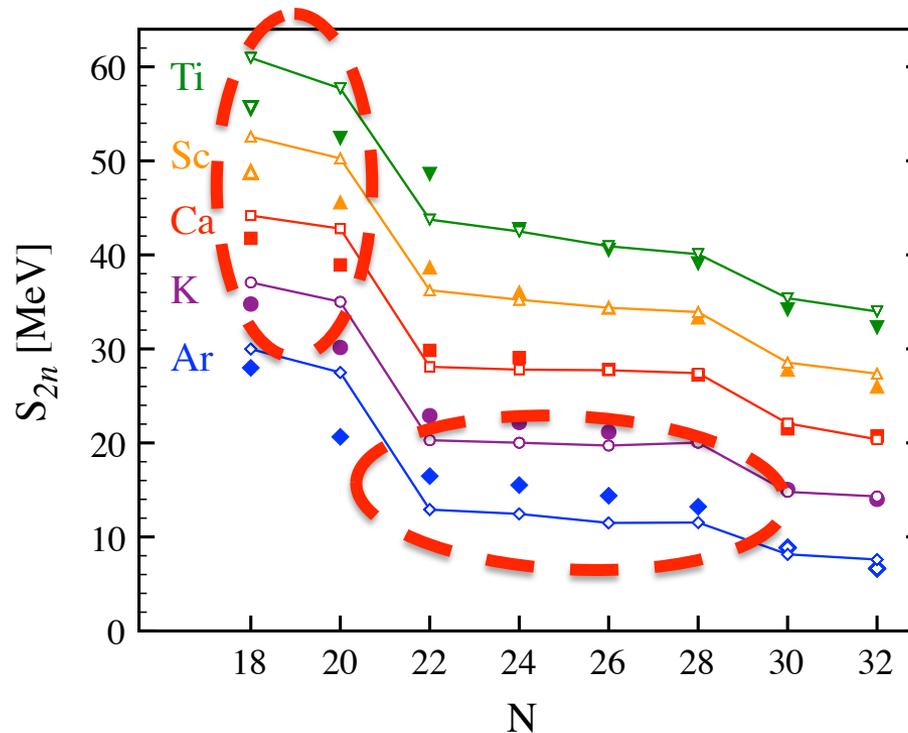
Over estimated  
N=20 and Z=20 gaps

→ First *ab-initio* calculation over a contiguous portion of the nuclear chart—open shells are now possible through the Gorkov-GF formalism

# Neighbouring Ar, K, Ca, Sc, and Ti chains

V. Somà, CB *et al.* Phys. Rev. C89, 061301R (2014)

Two-neutron separation energies predicted by chiral NN+3NF forces:



Lack of deformation due to quenched cross-shell quadrupole excitations

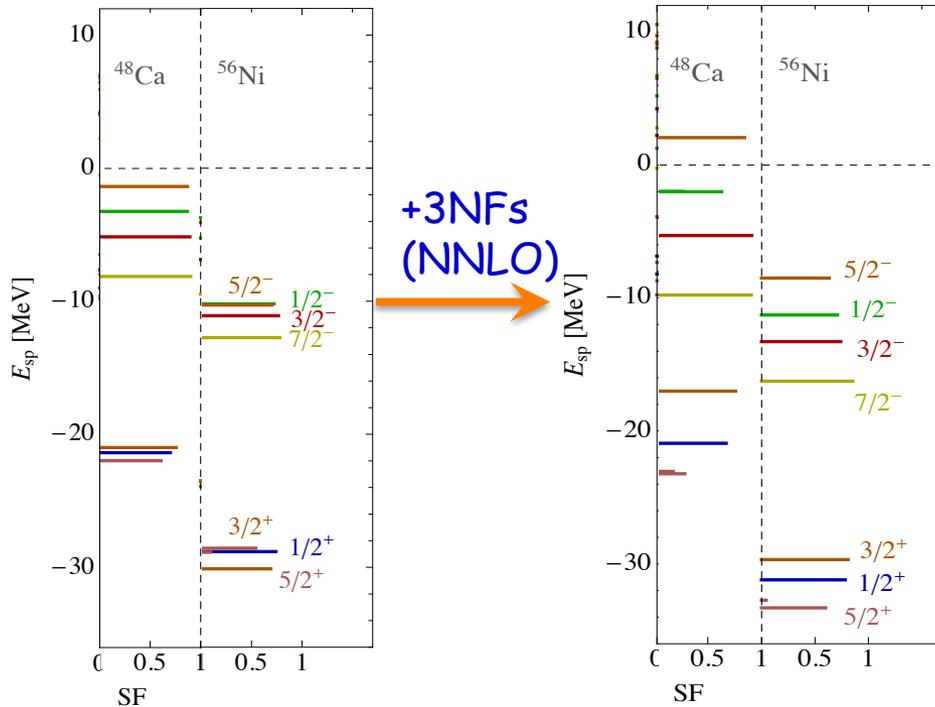
→ First *ab-initio* calculation over a contiguous portion of the nuclear chart—open shells are now possible through the Gorkov-GF formalism

# The *sd*-*pf* shell gap

Neutron spectral distributions for  $^{48}\text{Ca}$  and  $^{56}\text{Ni}$ :

2N + 3NF (induced)

2N + 3NF (FULL)

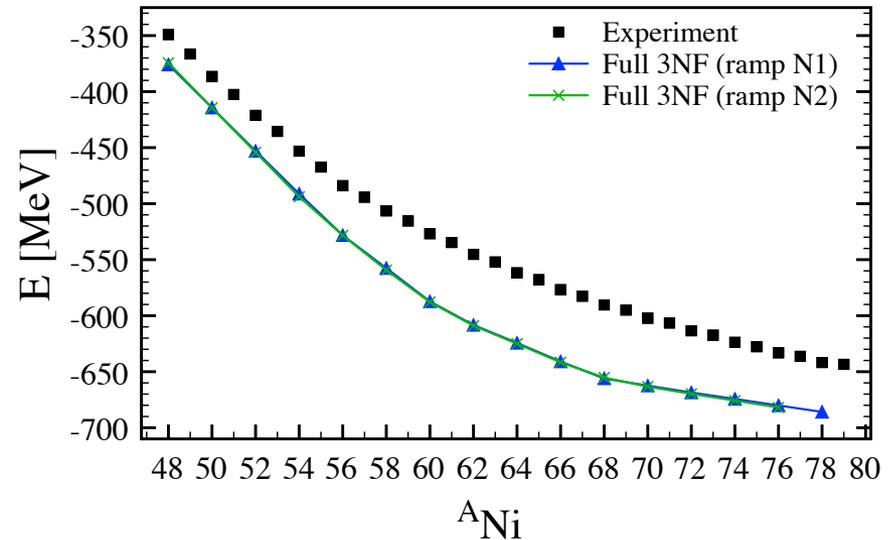
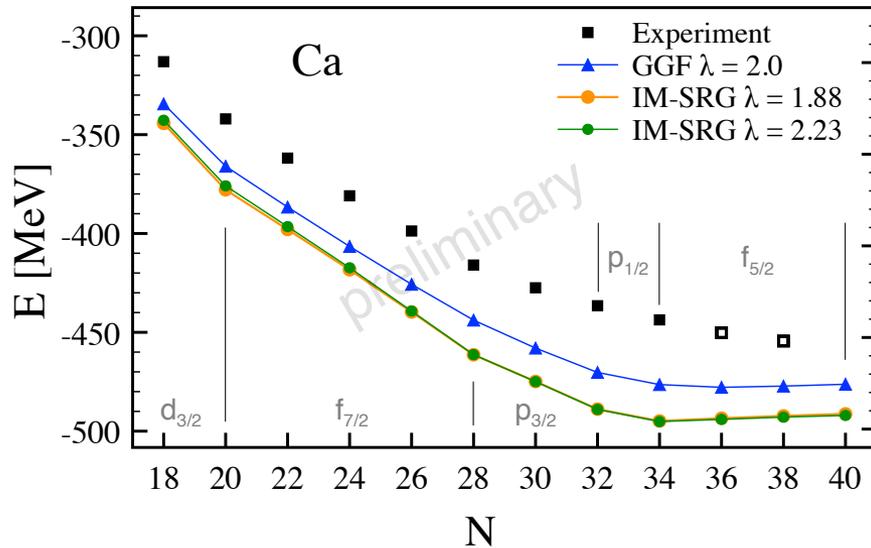


- *sd*-*pf* separation is *overestimated* even with leading order N2LO 3NF
- Correct increase of  $p_{3/2}$ - $f_{7/2}$  splitting (see Zuker 2003)

	2NF only	2+3NF(ind.)	2+3NF(full)	Experiment
$^{16}\text{O}$ :	2.10	2.41	2.38	$2.718 \pm 0.210$ [19]
$^{44}\text{Ca}$ :	2.48	2.93	2.94	$3.520 \pm 0.005$ [20]

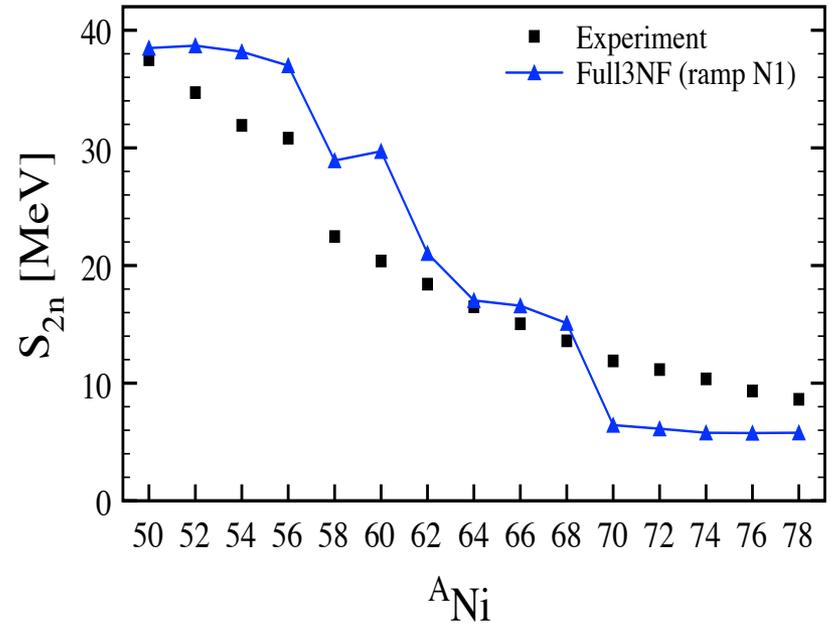
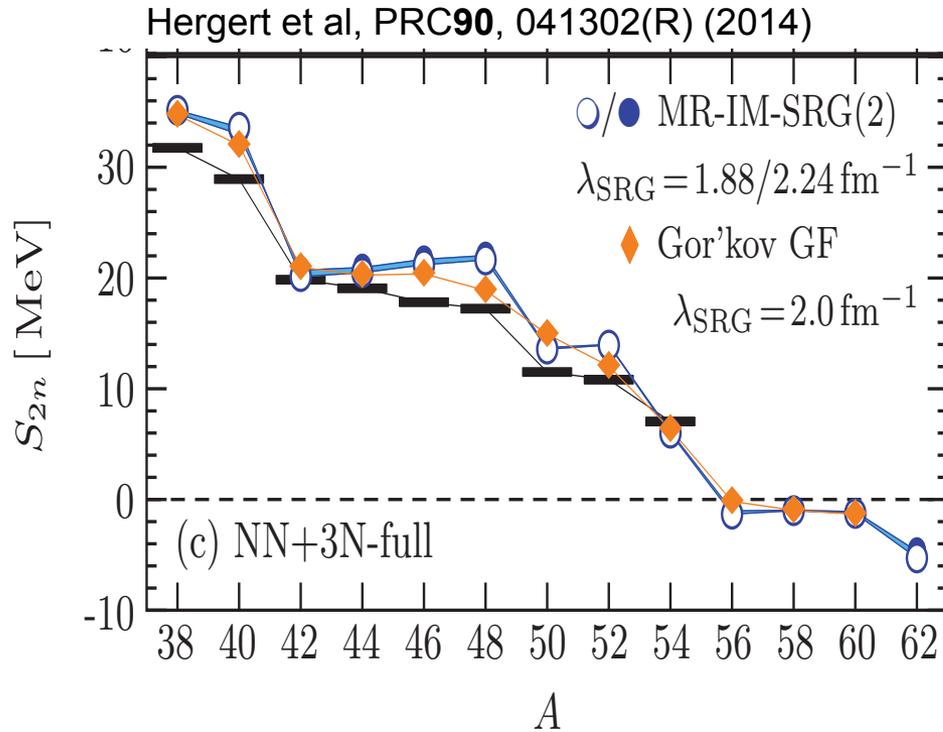
CB *et al.*, arXiv:1211.3315 [nucl-th]

# Ca and Ni isotopic chains



- Large  $J$  in free space SRG matter (must pay attention to its convergence)
- Overall conclusions regarding over binding and  $S_{2n}$  remain but details change

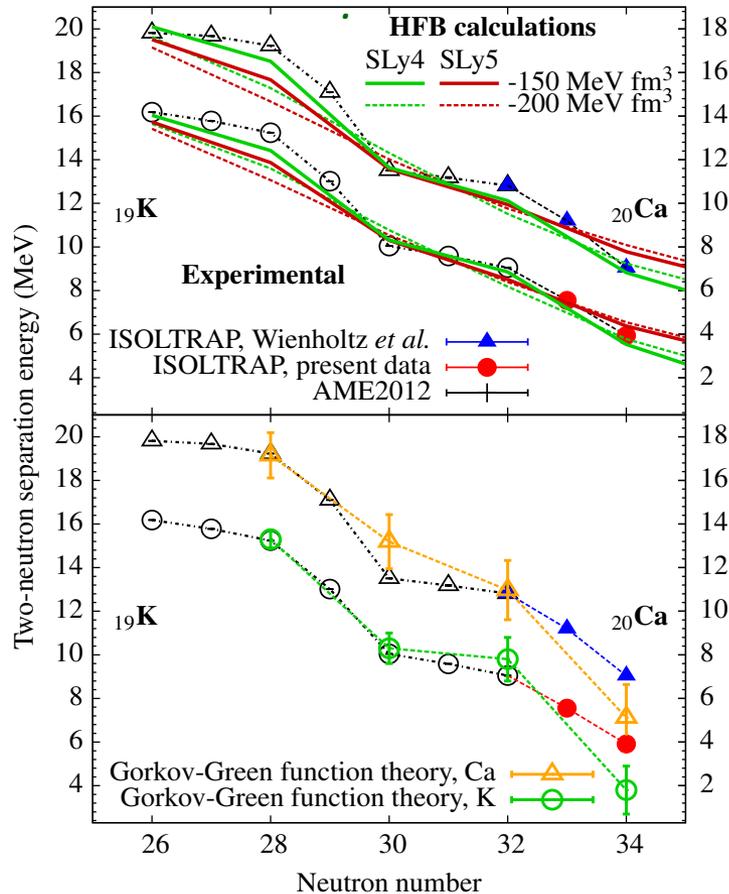
# Ca and Ni isotopic chains



- Large  $J$  in free space SRG matter (must pay attention to its convergence)
- Overall conclusions regarding over binding and  $S_{2n}$  remain but details change

# Two-neutron separation energies for neutron rich K isotopes

M. Rosenbusch, et al., PRL114, 202501 (2015)



Measurements  
@ ISOLTRAP

Theory tend to overestimate the gap at N=34, but overall good

→ Error bar in predictions are from extrapolating the many-body expansion to convergence of the model space.

# Inversion of $d_{3/2}-s_{1/2}$ at $N=28$

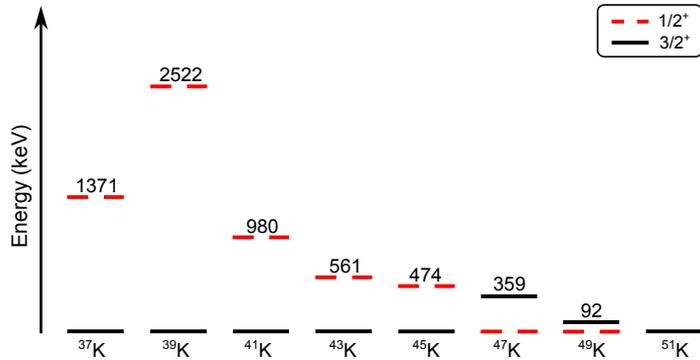


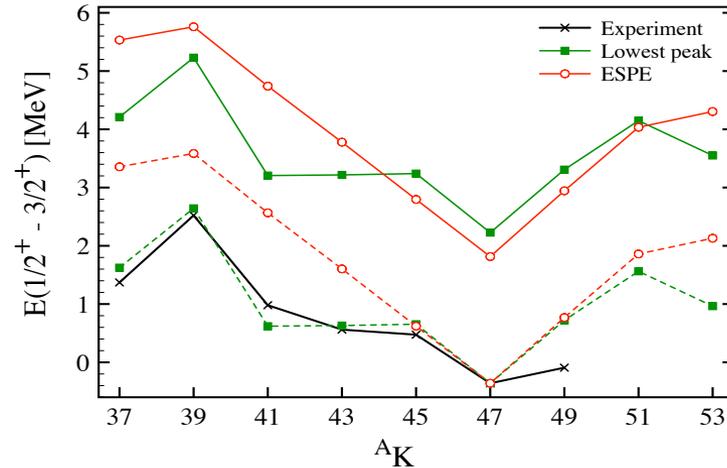
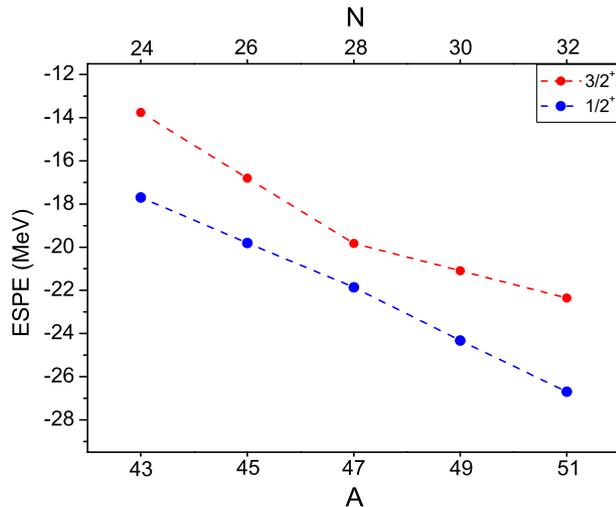
FIG. 1. (color online) Experimental energies for  $1/2^+$  and  $3/2^+$  states in odd- $A$  K isotopes. Inversion of the nuclear spin is obtained in  $^{47,49}\text{K}$  and reinversion back in  $^{51}\text{K}$ . Results are

J. Papuga, et al., Phys. Rev. Lett. **110**, 172503 (2013);  
Phys. Rev. C **90**, 034321 (2014)

$A$ K isotopes

Laser spectroscopy @ ISOLDE

Change in separation described by chiral NN+3NF:

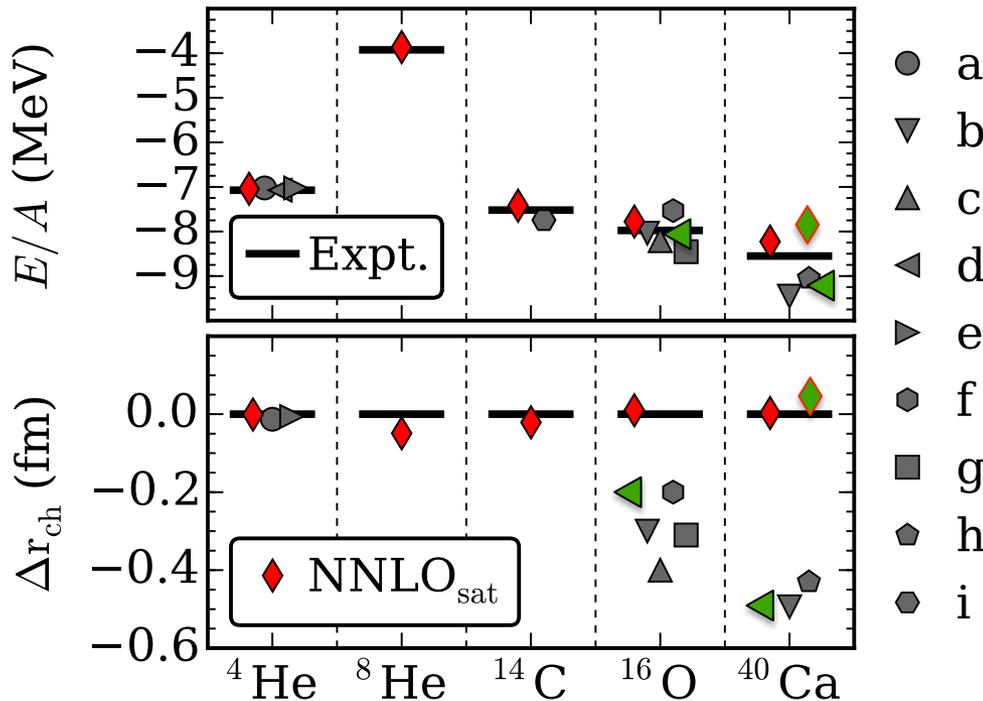


ESPE: "centroid" energies

(Gorkov calculations at 2<sup>nd</sup> order)

# NNLO-sat : a global fit up to $A \approx 24$

A. Ekström *et al.* Phys. Rev. C91, 051301(R) (2015)



- Constrain NN phase shifts

- Constrain radii and energies up to  $A \leq 24$

→ Provides saturation up to large masses!

◆ NNLOsat (V2 + W3) -- Grkv 2nd ord.

From SCGF:

◀ { V2-N3LO(500) + W3-NNLO(400MeV/c) w/ SRG at  $2.0 \text{ fm}^{-1}$   
 A. Cipollone, CB, P. Navrátil, Phys. Rev. Lett. **111**, 062501 (2013)  
 V. Somà, CB *et al.* Phys. Rev. C**89**, 061301R (2014)

# Collaborators



energies atomiques • énergies alternatives



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