

TALENT Course no. 2: Many-Body Methods for Nuclear Physics

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*

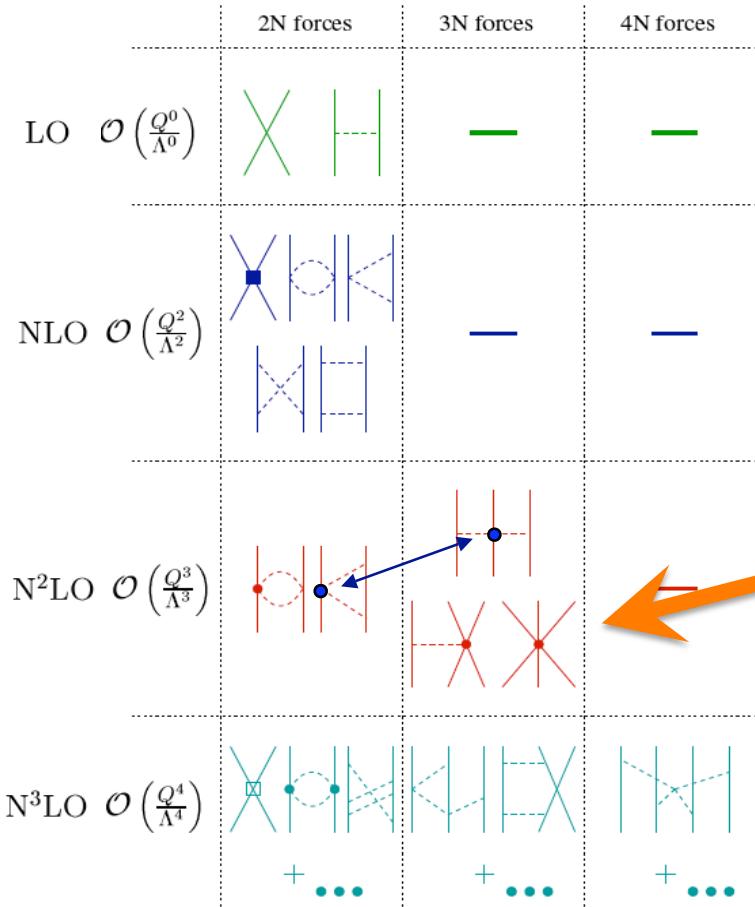


UNIVERSITY OF
SURREY

Adding 3-nucleon forces

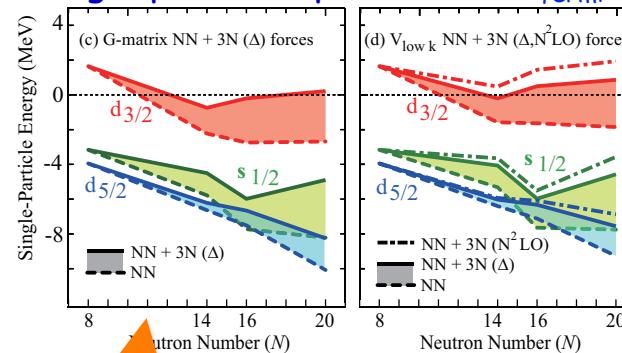
Modern realistic nuclear forces

Chiral EFT for nuclear forces:



(3NFs arise naturally at N²LO)

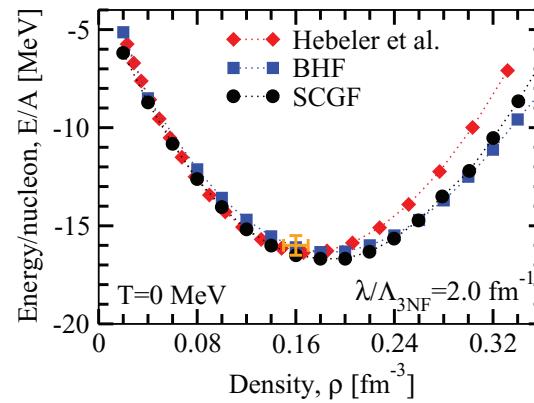
Single particle spectrum at E_{fermi} :



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

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

Saturation of nuclear matter:

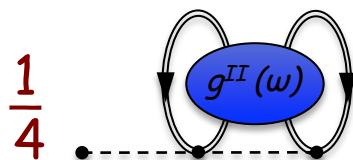


[A. Carbone et al.,
Phys Rev. C **88**, 044302 (2013)]

Inclusion of NNN forces

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

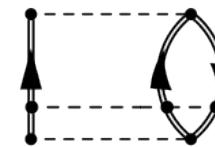
- ✿ NNN forces can enter diagrams in three different ways:



$\frac{1}{4}$.
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

$$\tilde{U} = \text{---} \times \equiv \text{---} \times + \text{---} \circlearrowleft + \frac{1}{4} \text{---} \circlearrowleft \text{---} \circlearrowright g^{II}(\omega)$$

$$\tilde{V} = \text{---} \bullet \equiv \text{---} \bullet + \text{---} \circlearrowleft$$

$$W = \text{---} \bullet \text{---} \bullet \equiv \text{---} \bullet \text{---} \bullet$$

- 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

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

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

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

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

Inclusion of NNN forces

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

- Second order PT
diagrams with 3BFs:

effectively:

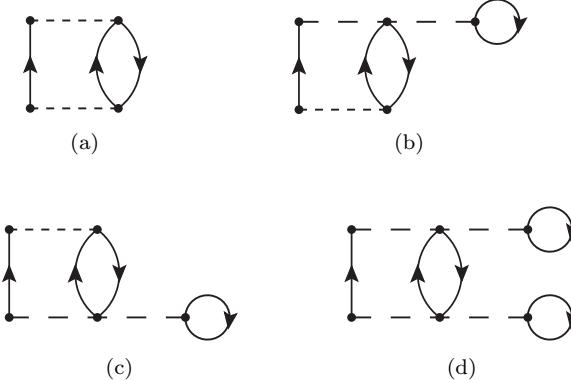
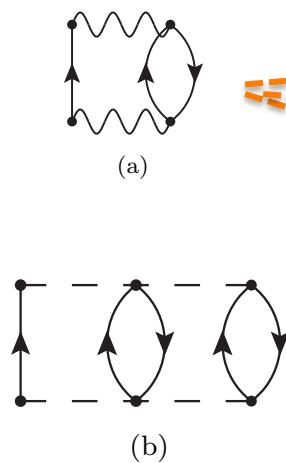
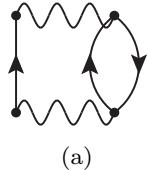


FIG. 4. The one *interaction irreducible* diagrams (a) and the three *interaction reducible* ones (b, c and d) that are contained in Fig. 3a.

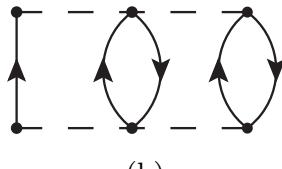
Inclusion of NNN forces

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

- Second order PT
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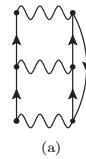


(a)

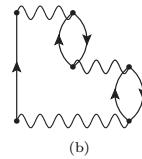


(b)

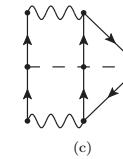
- Third order PT diagrams with 3BFs:



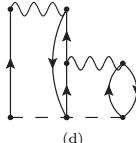
(a)



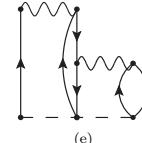
(b)



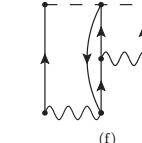
(c)



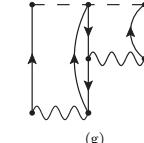
(d)



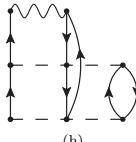
(e)



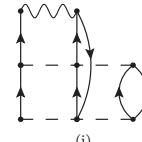
(f)



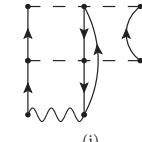
(g)



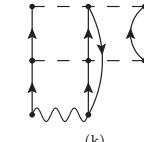
(h)



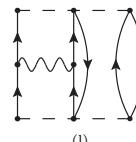
(i)



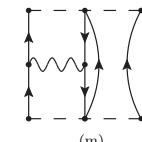
(j)



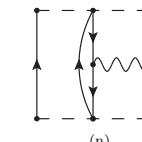
(k)



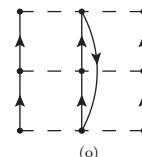
(l)



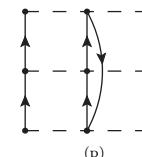
(m)



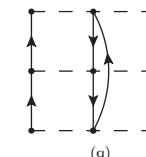
(n)



(o)



(p)



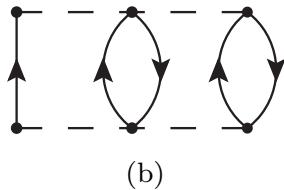
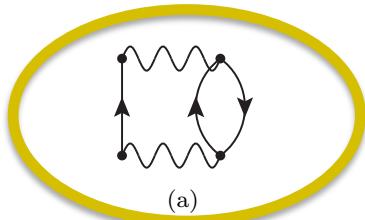
(q)

FIG. 5. 1PI, skeleton and interaction irreducible self-energy diagrams appearing at 3rd-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:

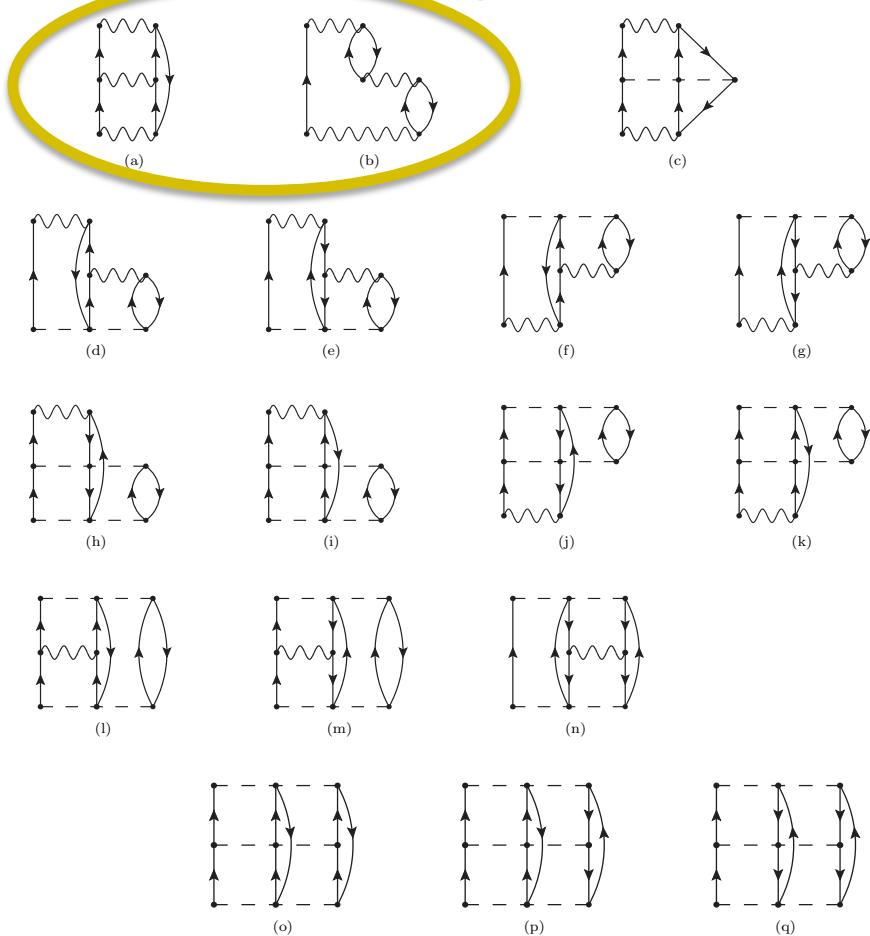


FIG. 5. 1PI, skeleton and interaction irreducible self-energy diagrams appearing at 3rd-order in perturbative expansion (7), making use of the effective hamiltonian of Eq. (9).

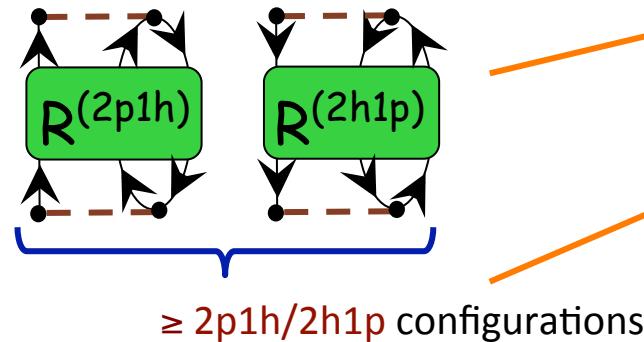
Gorkov method for the open-shells

Faddeev-RPA in two words...

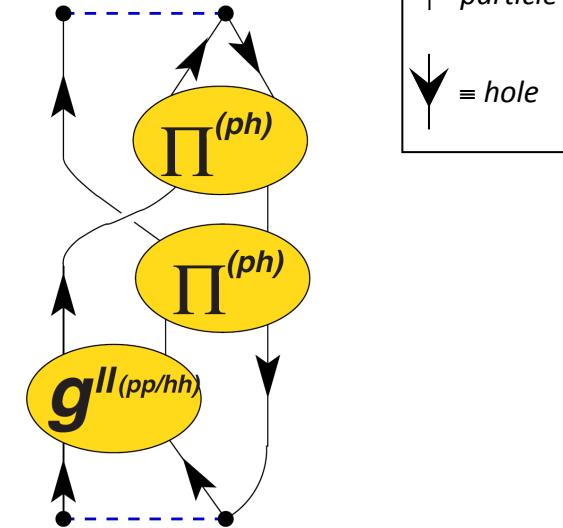
Self-energy
(optical potential):

$$\Sigma^*(\omega) = \text{---} \circlearrowleft$$

"Extended" Hartree Fock



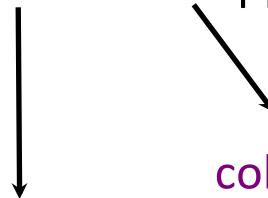
Faddeev-RPA:



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

Applications to doubly-magic nuclei

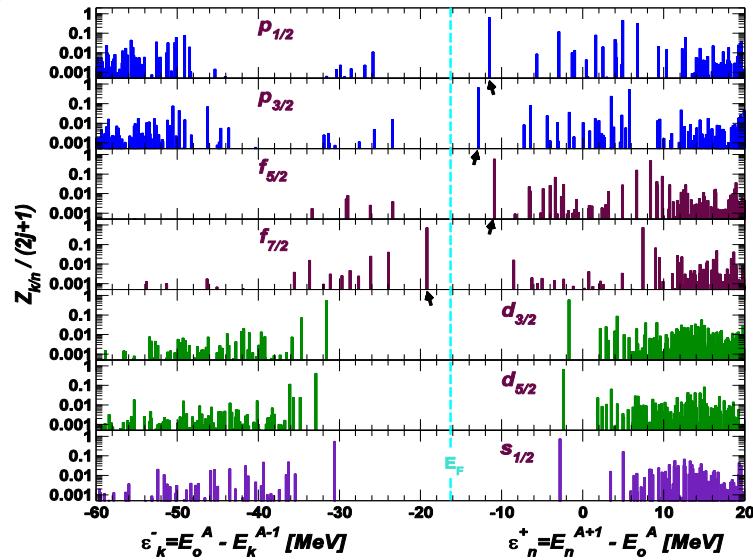
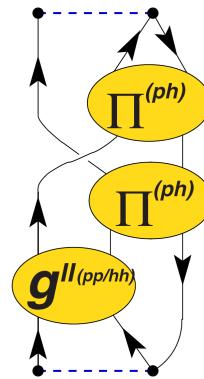
- ⌘ Faddeev-RPA approximation for the self-energy



collective vibrations

particle-vibration coupling

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



- ⌘ Successful in medium-mass doubly-magic systems

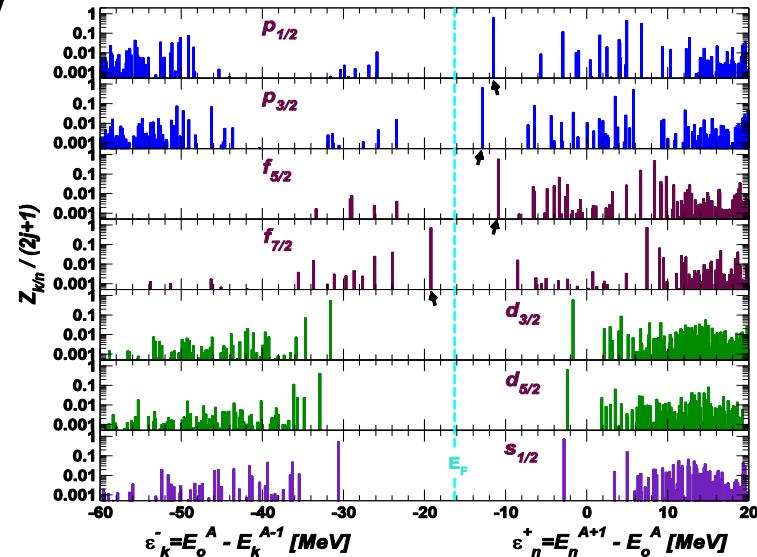
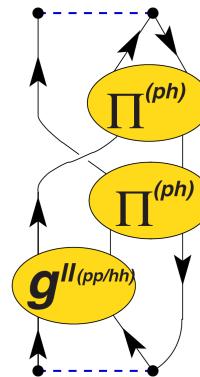
Applications to doubly-magic nuclei

- ⌘ 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]



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

Gorkov equations

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

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

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

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

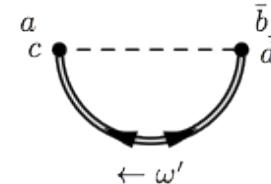
V. Somà, CB, T. Duguet, Phys. Rev. C **87**, 011303R (2013)

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

✳ 1st order → energy-independent self-energy

$$\Sigma_{ab}^{11(1)} = \begin{array}{c} a \\ \bullet \\ b \end{array} \cdots \begin{array}{c} c \\ d \end{array} \circlearrowleft \downarrow \omega'$$

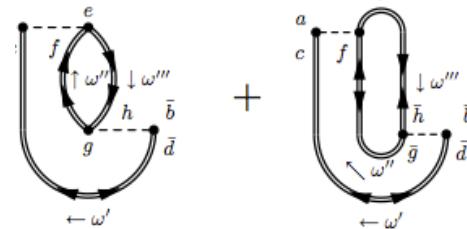
$$\Sigma_{ab}^{12(1)} =$$



✳ 2nd order → energy-dependent self-energy

$$\Sigma_{ab}^{11(2)}(\omega) = \begin{array}{c} a \\ \uparrow \omega' \\ c \\ \cdots \\ d \\ \downarrow \omega''' \\ b \end{array} + \begin{array}{c} e \\ \downarrow \omega''' \\ f \\ \cdots \\ g \\ h \end{array}$$

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



✳ Gorkov equations → eigenvalue problem

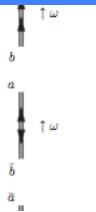
$$\sum_b \begin{pmatrix} t_{ab} - \mu_{ab} + \Sigma_{ab}^{11}(\omega) & \Sigma_{ab}^{12}(\omega) \\ \Sigma_{ab}^{21}(\omega) & -t_{ab} + \mu_{ab} + \Sigma_{ab}^{22}(\omega) \end{pmatrix} \Big|_{\omega_k} \begin{pmatrix} \mathcal{U}_b^k \\ \mathcal{V}_b^k \end{pmatrix} = \omega_k \begin{pmatrix} \mathcal{U}_a^k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

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

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

Expressions for 1st & 2nd order diagrams

$$G_{ab}^{11}(\omega) \equiv$$



(B5a)

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

V. SOMÀ, T. DUGUET, AND C. BARBIERI

$$G_{ab}^{12}(\omega) \equiv$$



(B5b)

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

$$\begin{aligned} \Sigma_{ab}^{21(1)} &= \frac{1}{2} \sum_{cd,k} \tilde{V}_{cdab} \tilde{U} \\ &= -\frac{1}{2} \sum_{n_i n_j n_k} \sum_{\gamma} f_{\alpha\gamma\beta\gamma}^{\alpha_i n_i n_j n_k} \frac{\sqrt{2J_c+1}}{\sqrt{2J_d+1}} (- \\ &= \delta_{ab} \delta_{m_a m_b} \frac{1}{2} \cdot \\ &\equiv \delta_{ab} \delta_{m_a m_b} \Sigma_{n_a}^{21} \\ &= \delta_{ab} \delta_{m_a m_b} \tilde{f}_{n_a}^{(a)} \end{aligned}$$

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-diagonality reflects in the various self-energy contributions, starting with the first one (C19) into Eq. (B7), and introducing the factor

$$f_{\alpha\beta\gamma\delta}^{n_i n_j n_k n_l} \equiv \sqrt{1 + \delta_{ab} \delta_{n_a}}$$

one obtains

$$\begin{aligned} \Sigma_{ab}^{11(1)} &= \sum_{cd,k} V_{abcd} \mathcal{V}_d^{k*} \mathcal{V}_c \\ &= \sum_{n_i n_j n_k} \sum_{\gamma} \sum_{M} f_{\alpha\gamma\beta\gamma}^{\alpha_i n_i n_j n_k} C_{j,M}^{J,M} \\ &= \delta_{ab} \delta_{m_a m_b} \sum_{n_i n_j} \sum_{\gamma} f_{\alpha\gamma\beta\gamma}^{\alpha_i n_i n_j n_k} \frac{2}{2} \\ &\equiv \delta_{ab} \delta_{m_a m_b} \Sigma_{n_a}^{11(1)} \\ &\equiv \delta_{ab} \delta_{m_a m_b} \Lambda_{n_a}^{(a)} \end{aligned}$$

where the block-diagonal normal density matrix is introduced through

$$\rho_{n_a n_b}^{(a)} = \sum_{n_i} \rho_{n_i}^{n_a}$$

and properties of Clebsch-Gordan coefficients has been used. The $\delta_{n_a n_b}$ and $\delta_{q_a q_b}$, leading to $\delta_{ab} = \delta_{j_a j_b} \delta_{n_a n_b} \delta_{q_a q_b}$. Similarly, for $\Sigma^{22(1)}$

$$\begin{aligned} \Sigma_{ab}^{22(1)} &= -\sum_{cd,k} V_{abcd} \tilde{V}_c^{k*} \tilde{V}_d \\ &= -\delta_{ab} \delta_{m_a m_b} \sum_{n_i n_j} \sum_{\gamma} f_{\alpha\gamma}^{n_i} \\ &\equiv \delta_{ab} \delta_{m_a m_b} \Sigma_{n_a}^{22(1)} \\ &= -\delta_{ab} \delta_{m_a m_b} \Lambda_{n_a}^{(a)} \\ &= -\delta_{ab} \delta_{m_a m_b} [\Lambda_{n_a}^{(a)}]^* . \end{aligned}$$

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

$$\begin{aligned} \Sigma_{ab}^{12(1)} &= \frac{1}{2} \sum_{cd,k} V_{abcd} \mathcal{V}_c^{k*} \tilde{U}_d^k \\ &= -\frac{1}{2} \sum_{n_i n_j n_k} \sum_{\gamma} \sum_{M} f_{\alpha\gamma\beta\gamma}^{\alpha_i n_i n_j n_k} \eta_{jk} \eta_{ci} C_{j,M}^{J,M} \\ &= -\frac{1}{2} \sum_{n_i n_j} \sum_{\gamma} \sum_{M} f_{\alpha\gamma\beta\gamma}^{\alpha_i n_i n_j n_k} \eta_{jk} \eta_{ci} C_{j,M}^{J,M} \\ &= -\frac{1}{2} \sum_{n_i n_j} \sum_{\gamma} f_{\alpha\gamma\beta\gamma}^{\alpha_i n_i n_j n_k} \eta_{jk} \pi_c (-1)^{2j} C_{j,M}^{J,M} \\ &= \delta_{ab} \delta_{m_a m_b} \frac{1}{2} \sum_{n_i n_j} \sum_{\gamma} f_{\alpha\gamma\beta\gamma}^{\alpha_i n_i n_j n_k} \pi_a \pi_c (-1)^{2j} C_{j,M}^{J,M} \\ &\equiv \delta_{ab} \delta_{m_a m_b} \Sigma_{n_a}^{12(1)} \\ &\equiv \delta_{ab} \delta_{m_a m_b} \tilde{f}_{n_a}^{(a)} . \end{aligned}$$

where the block-diagonal anomalous density matrix is introduced through

$$\tilde{\rho}_{n_a n_b}^{(a)} = \sum_{n_i} \tilde{\rho}_{n_i}^{n_a} V_{n_i}^{n_b} .$$

$$\begin{aligned} &= \sum_{n_i n_j n_k} \sum_{\gamma} \sum_{M} \eta_{jk} \eta_{ki} f_{\alpha\gamma\beta\gamma}^{\alpha_i n_i n_j n_k} C_{j,M}^{J,M} \\ &= \sum_{n_i n_j n_k} \sum_{\gamma} \eta_{jk} \pi_k f_{\alpha\gamma\beta\gamma}^{\alpha_i n_i n_j n_k} \frac{\sqrt{2J_c+1}}{\sqrt{2J_d+1}} (- \\ &= \delta_{j_a j_b} \delta_{M_{ab} - m_a} \sum_{n_i n_j n_k} \eta_{jk} \pi_k f_{\alpha\gamma\beta\gamma}^{\alpha_i n_i n_j n_k} \frac{\sqrt{2J_c+1}}{\sqrt{2J_d+1}} \\ &= -\delta_{j_a j_b} \delta_{M_{ab} - m_a} \eta_{jk} \mathcal{N}_{n_a [n_b n_c n_k]} J_c \end{aligned}$$

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

$$= \sum_{n_i n_j n_k} \sum_{\gamma} \eta_{jk} \pi_k f_{\alpha\gamma\beta\gamma}^{\alpha_i n_i n_j n_k} \frac{\sqrt{2J_c+1}}{\sqrt{2J_d+1}} (-$$

$$= \delta_{j_a j_b} \delta_{M_{ab} - m_a} \sum_{n_i n_j n_k} \eta_{jk} \pi_k f_{\alpha\gamma\beta\gamma}^{\alpha_i n_i n_j n_k} \frac{\sqrt{2J_c+1}}{\sqrt{2J_d+1}}$$

$$= -\delta_{j_a j_b} \delta_{M_{ab} - m_a} \eta_{jk} \mathcal{N}_{n_a [n_b n_c n_k]} J_c ,$$

which recovers relation (72a). The remaining quantities $\langle k_1, k_2, k_3 \rangle$ indices and can be obtained from Eqs. (C44a)-(C44d).

j_{k_1} to J_{k_1} and J_c as follows:

$$\mathcal{P}_{a(J, J_{k_1})}^{k_1 k_2 k_3} = \sum_{J_c} (-1)^{J_c + j_{k_2} + j_{k_3}} \sqrt{2J_c}$$

$$= -\delta_{j_a j_b} \delta_{M_{ab} - m_a} \sum_{n_i n_j n_k} \pi_k$$

$$\times \tilde{V}_{n_a [n_b n_c n_k]}^J U_{n_i [n_c]}^{n_k} U_{n_j [n_k]}^{n_i}$$

$$\equiv \delta_{j_a j_b} \delta_{M_{ab} - m_a} \mathcal{P}_{n_a [n_b n_c n_k]}^{k_1 k_2 k_3} J_c$$

$$\mathcal{Q}_{a(J, J_{k_1})}^{k_1 k_2 k_3} = \sum_{J_c} (-1)^{J_c + j_{k_2} + j_{k_3}} \sqrt{2J_c + 1}$$

$$= \delta_{j_a j_b} \delta_{M_{ab} - m_a} \sum_{n_i n_j n_k} \pi_k .$$

$$\times \tilde{V}_{n_a [n_b n_c n_k]}^J Y_{n_i [n_c]}^{n_k} Y_{n_j [n_k]}^{n_i}$$

$$\equiv \delta_{j_a j_b} \delta_{M_{ab} - m_a} \mathcal{Q}_{n_a [n_b n_c n_k]}^{k_1 k_2 k_3} J_c$$

$$\mathcal{R}_{a(J, J_{k_1})}^{k_1 k_2 k_3} = \sum_{J_c} (-1)^{2j_{k_1} + 2j_{k_2}} \sqrt{2J_c + 1}$$

$$= -\delta_{j_a j_b} \delta_{M_{ab} - m_a} \sum_{n_i n_j n_k} \pi_k$$

$$\times \tilde{V}_{n_a [n_b n_c n_k]}^J U_{n_i [n_c]}^{n_k} U_{n_j [n_k]}^{n_i}$$

$$\equiv \delta_{j_a j_b} \delta_{M_{ab} - m_a} \mathcal{R}_{n_a [n_b n_c n_k]}^{k_1 k_2 k_3} J_c$$

$$\mathcal{S}_{a(J, J_{k_1})}^{k_1 k_2 k_3} = \sum_{J_c} (-1)^{2j_{k_1} + 2j_{k_2}} \sqrt{2J_c + 1}$$

$$= \delta_{j_a j_b} \delta_{M_{ab} - m_a} \sum_{n_i n_j n_k} \pi_k$$

$$\times \tilde{V}_{n_a [n_b n_c n_k]}^J Y_{n_i [n_c]}^{n_k} Y_{n_j [n_k]}^{n_i}$$

$$\equiv \delta_{j_a j_b} \delta_{M_{ab} - m_a} \mathcal{S}_{n_a [n_b n_c n_k]}^{k_1 k_2 k_3} J_c .$$

where general properties of Clebsch-Gord

$$\begin{aligned} \mathcal{N}_{a(J, J_{k_1})}^{k_1 k_2 k_3} &= \delta_{j_a j_b} \delta_{M_{ab} - m_a} \sum_{n_i n_j n_k} \\ &\equiv \delta_{j_a j_b} \delta_{M_{ab} - m_a} \mathcal{N}_a^{k_1 k_2 k_3} \end{aligned}$$

One can show that the same result is obtained

$$\begin{aligned} \mathcal{N}_{a(J, J_{k_1})}^{k_1 k_2 k_3} &= \sum_{m_1 m_2 m_3 M_c} C_{j_1 m_1 j_2 m_2}^{J,M} C_{j_3 M_c M_c}^{J,M} \\ &= \sum_{m_1 m_2 m_3} \sum_{M_c} \sum_{J_c} C_{j_1 m_1 j_2 m_2}^{J,M} C_{j_3 M_c}^{J_c} \\ &= \sum_{m_1 m_2 m_3} \sum_{M_c} \sum_{J_c} \delta_{j_1, 0} \delta_{m_2 - m_1} \delta_{j_2, 0} \delta_{m_3 - m_2} \delta_{j_3, 0} \eta_{jk} \eta_{ci} f_{\alpha\beta\gamma\gamma}^{\alpha_i n_i n_j n_k} \\ &\quad \times C_{j_1 m_1 j_2 m_2}^{J,M} C_{j_3 M_c M_c}^{J,M} C_{j_3 m_1 j_2 m_2 - m_1}^{J,M} \tilde{V}_{n_a [n_b n_c n_k]}^J \mathcal{V}_{n_i [n_c]}^{n_k} \mathcal{U}_{n_j [n_k]}^{n_i} \end{aligned}$$

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$$\mathcal{C}_{n_a [n_b n_c n_k]}^{k_1 k_2 k_3} J_c \equiv \frac{1}{\sqrt{6}} [\mathcal{M}_{n_a [n_b n_c n_k]}^{k_1 k_2 k_3} J_c - \mathcal{P}_{n_a [n_b n_c n_k]}^{k_1 k_2 k_3} J_c - \mathcal{R}_{n_a [n_b n_c n_k]}^{k_1 k_2 k_3} J_c] .$$

(C43a)

$$= \frac{1}{\sqrt{6}} [\mathcal{N}_{n_a [n_b n_c n_k]}^{k_1 k_2 k_3} J_c - \mathcal{E}_{n_a [n_b n_c n_k]}^{k_1 k_2 k_3} J_c - \mathcal{Z}_{n_a [n_b n_c n_k]}^{k_1 k_2 k_3} J_c] .$$

(C43b)

$$\Sigma_{n_a n_b}^{11(a)}(2) = \sum_{n_1 n_2 n_3} \sum_{J_c} \sum_{k_1 k_2 k_3} \left\{ \frac{\mathcal{C}_{n_a [n_b n_c n_k]}^{k_1 k_2 k_3} J_c}{\omega - (\omega_k + \omega_{k_2} + \omega_{k_3}) + i\eta} + \frac{(\mathcal{D}_{n_a [n_b n_c n_k]}^{k_1 k_2 k_3} J_c)^*}{\omega + (\omega_k + \omega_{k_2} + \omega_{k_3}) - i\eta} \right\} .$$

(C44a)

$$\Sigma_{n_a n_b}^{12(a)}(2) = \sum_{n_1 n_2 n_3} \sum_{J_c} \sum_{k_1 k_2 k_3} \left\{ \frac{\mathcal{C}_{n_a [n_b n_c n_k]}^{k_1 k_2 k_3} J_c}{\omega - (\omega_k + \omega_{k_2} + \omega_{k_3}) + i\eta} + \frac{(\mathcal{D}_{n_a [n_b n_c n_k]}^{k_1 k_2 k_3} J_c)^*}{\omega + (\omega_k + \omega_{k_2} + \omega_{k_3}) - i\eta} \right\} .$$

(C44b)

$$\Sigma_{n_a n_b}^{21(a)}(2) = \sum_{n_1 n_2 n_3} \sum_{J_c} \sum_{k_1 k_2 k_3} \left\{ \frac{\mathcal{D}_{n_a [n_b n_c n_k]}^{k_1 k_2 k_3} J_c}{\omega - (\omega_k + \omega_{k_2} + \omega_{k_3}) + i\eta} + \frac{(\mathcal{C}_{n_a [n_b n_c n_k]}^{k_1 k_2 k_3} J_c)^*}{\omega + (\omega_k + \omega_{k_2} + \omega_{k_3}) - i\eta} \right\} .$$

(C44c)

$$\Sigma_{n_a n_b}^{22(a)}(2) = \sum_{n_1 n_2 n_3} \sum_{J_c} \sum_{k_1 k_2 k_3} \left\{ \frac{\mathcal{D}_{n_a [n_b n_c n_k]}^{k_1 k_2 k_3} J_c}{\omega - (\omega_k + \omega_{k_2} + \omega_{k_3}) + i\eta} + \frac{(\mathcal{C}_{n_a [n_b n_c n_k]}^{k_1 k_2 k_3} J_c)^*}{\omega + (\omega_k + \omega_{k_2} + \omega_{k_3}) - i\eta} \right\} .$$

(C44d)

6. Block-diagonal structure of Gorkov's equations

(101)

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

$$T_{ab} - \mu_{ab} \equiv \delta_{ab} \delta_{m_a m_b} [T_{n_a n_b}^{(a)} - \mu_{n_a}^{(a)} \delta_{n_a n_b}] ,$$

(C45)

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

$$\mathcal{W}_{k(J, J_{k_1})}^{k_1 k_2 k_3} \equiv \delta_{j_a j_b} \delta_{M_{ab} - m_a} \mathcal{W}_{n_a [n_b n_c n_k]}^{k_1 k_2 k_3} J_c ,$$

(C46a)

$$\mathcal{Z}_{k(J, J_{k_1})}^{k_1 k_2 k_3} \equiv -\delta_{j_a j_b} \delta_{M_{ab} - m_a} \eta_{jk} \mathcal{Z}_{n_a [n_b n_c n_k]}^{k_1 k_2 k_3} J_c ,$$

(C46b)

with

$$(\omega_k - E_{k_1 k_2 k_3}) \mathcal{W}_{n_a [n_b n_c n_k]}^{k_1 k_2 k_3} J_c \equiv \sum_{n_i} [(C_{n_a [n_b n_c n_k]}^{k_1 k_2 k_3})^* \mathcal{U}_{n_i [a]}^{n_k} + (\mathcal{D}_{n_a [n_b n_c n_k]}^{k_1 k_2 k_3})^* \mathcal{V}_{n_i [a]}^{n_k}] ,$$

(C47a)

$$(\omega_k + E_{k_1 k_2 k_3}) \mathcal{Z}_{n_a [n_b n_c n_k]}^{k_1 k_2 k_3} J_c \equiv \sum_{n_i} [\mathcal{D}_{n_a [n_b n_c n_k]}^{k_1 k_2 k_3} \mathcal{U}_{n_i [a]}^{n_k} + \mathcal{C}_{n_a [n_b n_c n_k]}^{k_1 k_2 k_3} \mathcal{V}_{n_i [a]}^{n_k}] ,$$

(C47b)

$$\begin{aligned} \omega_k \mathcal{U}_{n_a [a]}^{n_k} &= \sum_{n_b} [(T_{n_a n_b}^{(a)} - \mu_{n_a}^{(a)} \delta_{n_a n_b} + \Lambda_{n_a}^{(a)}) \mathcal{U}_{n_b [a]}^{n_k} + \tilde{U}_{n_a [a]}^{n_k} \mathcal{V}_{n_b [a]}^{n_k}] \\ &\quad + \sum_{n_1 n_2 n_3} \sum_{J_c} \sum_{k_1 k_2 k_3} [\mathcal{C}_{n_a [n_b n_c n_k]}^{k_1 k_2 k_3} J_c \mathcal{W}_{n_b [n_c n_k]}^{k_1 k_2 k_3} + (\mathcal{D}_{n_a [n_b n_c n_k]}^{k_1 k_2 k_3} J_c)^* \mathcal{Z}_{n_b [n_c n_k]}^{k_1 k_2 k_3}] , \end{aligned}$$

(C48a)

$$\omega_k \mathcal{V}_{n_a [a]}^{n_k} = \sum_{n_b} [(-T_{n_a n_b}^{(a)} - \mu_{n_a}^{(a)} \delta_{n_a n_b} + \Lambda_{n_a}^{(a)}) \mathcal{V}_{n_b [a]}^{n_k} + \tilde{U}_{n_a [a]}^{n_k} \mathcal{U}_{n_b [a]}^{n_k}]$$

(C48b)

$$+ \sum_{n_1 n_2 n_3} \sum_{J_c} \sum_{k_1 k_2 k_3} [\mathcal{D}_{n_a [n_b n_c n_k]}^{k_1 k_2 k_3} J_c \mathcal{W}_{n_b [n_c n_k]}^{k_1 k_2 k_3} + (\mathcal{C}_{n_a [n_b n_c n_k]}^{k_1 k_2 k_3} J_c)^* \mathcal{Z}_{n_b [n_c n_k]}^{k_1 k_2 k_3}] .$$

(C48c)

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$$\begin{aligned} &e \quad \uparrow \omega'' \\ &h \quad \uparrow \omega''' \\ &g \quad \uparrow \omega''' \end{aligned}$$

(B31)

$$\frac{1}{\omega} \mathcal{U}_{\alpha}^{(a)} G_{\alpha b}^{12}(\omega'') G_{\beta b}^{21}(\omega' + \omega' - \omega)$$

(B32)

$$- \frac{1}{\omega} \sum_{cdefgh, k_1 k_2 k_3} \mathcal{V}_{cdefgh} \mathcal{V}_{k_1 k_2 k_3} \left[\frac{\mathcal{U}_c^{k_1} \mathcal{U}_d^{k_2} * \mathcal{U}_e^{k_3} \mathcal{U}_f^{k_4} \mathcal{U}_g^{k_5} \mathcal{V}_h^{k_6}}{\omega - (\omega_k + \omega_{k_2} + \omega_{k_3}) + i\eta} + \frac{\mathcal{U}_c^{k_1} * \mathcal{U}_d^{k_2} \mathcal{U}_e^{k_3} \mathcal{U}_f^{k_4} \mathcal{U}_g^{k_5} \mathcal{U}_h^{k_6}}{\omega + (\omega_k + \omega_{k_2} + \omega_{k_3}) - i\eta} \right] .$$

(B32)

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Gorkov equations

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

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



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

Energy independent eigenvalue problem

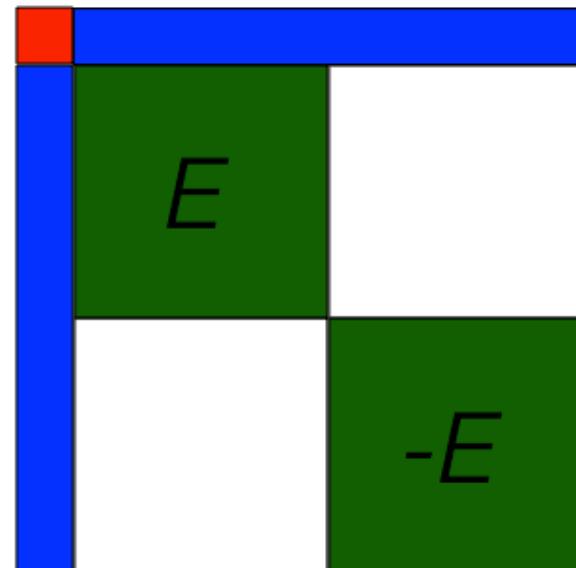
with the normalization condition $\sum_a \left[|\mathcal{U}_a^k|^2 + |\mathcal{V}_a^k|^2 \right] + \sum_{k_1 k_2 k_3} \left[|\mathcal{W}_k^{k_1 k_2 k_3}|^2 + |\mathcal{Z}_k^{k_1 k_2 k_3}|^2 \right] = 1$

Lanczos reduction of self-energy

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

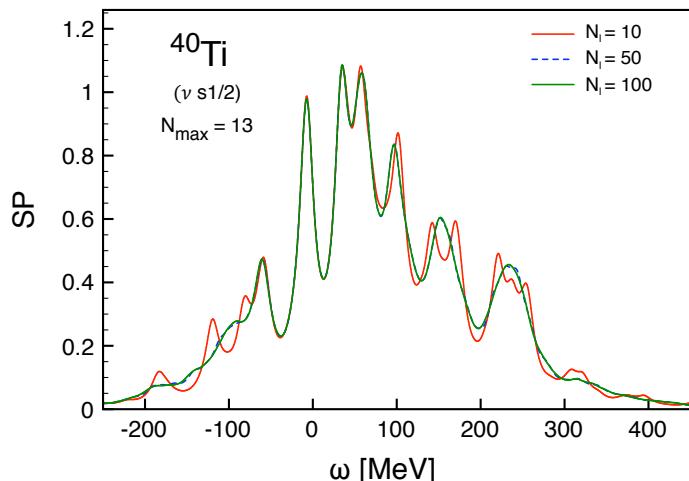
$$\begin{pmatrix} T - \mu + \Lambda & \tilde{h} & \mathcal{C} & -\mathcal{D}^\dagger \\ \tilde{h}^\dagger & -T + \mu - \Lambda & -\mathcal{D}^\dagger & \mathcal{C} \\ \mathcal{C}^\dagger & -\mathcal{D} & E & 0 \\ -\mathcal{D} & \mathcal{C}^\dagger & 0 & -E \end{pmatrix} \begin{pmatrix} \mathcal{U}^k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

HFB

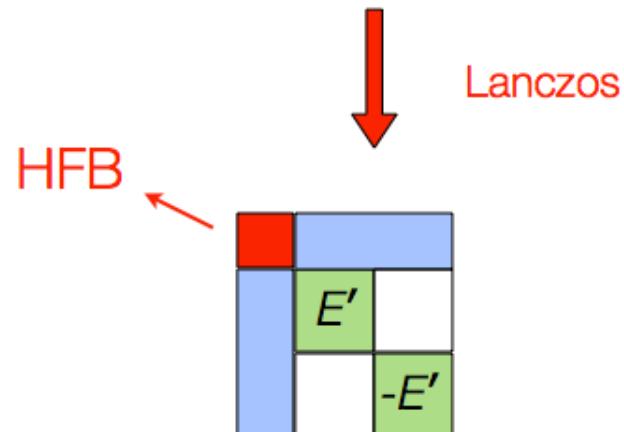


- Conserves moments of spectral functions
- Equivalent to exact diagonalization
for $N_L \rightarrow \dim(E)$

Spectral strength



HFB



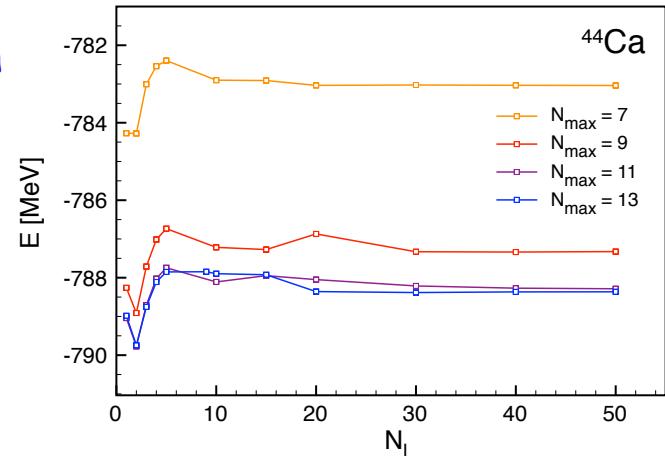
Testing Krylov projection

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

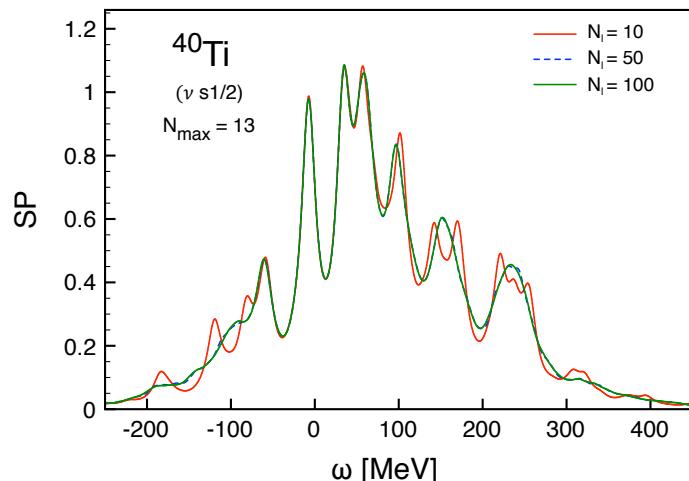
- Energy and spectra independent of the projection
- Same behavior for all model spaces



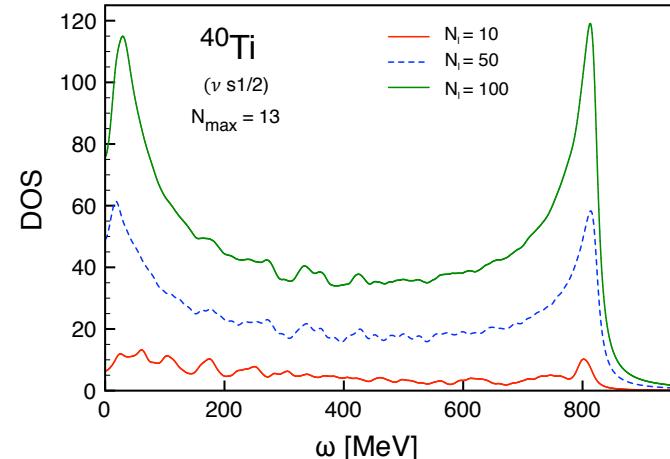
Favourable scaling



Spectral strength

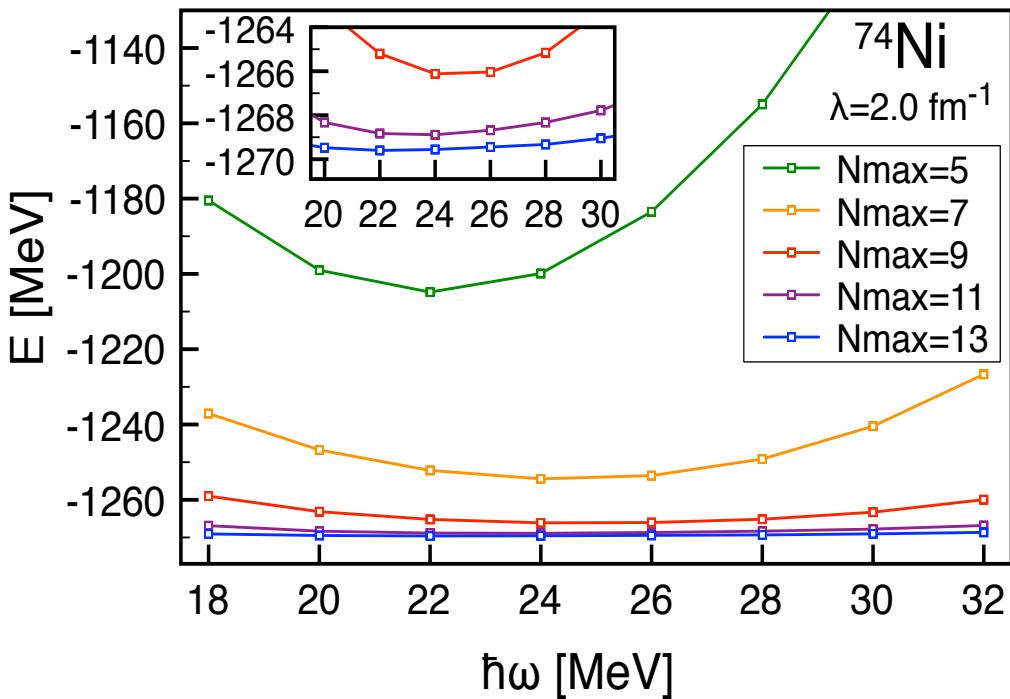


Deinsity of states



Binding energies

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



→ NN interaction:
chiral N³LO SRG-evolved to 2.0 fm⁻¹

[Entem and Machleidt 2003]

- Very good convergence
- From N=13 to N=11 → 200 keV

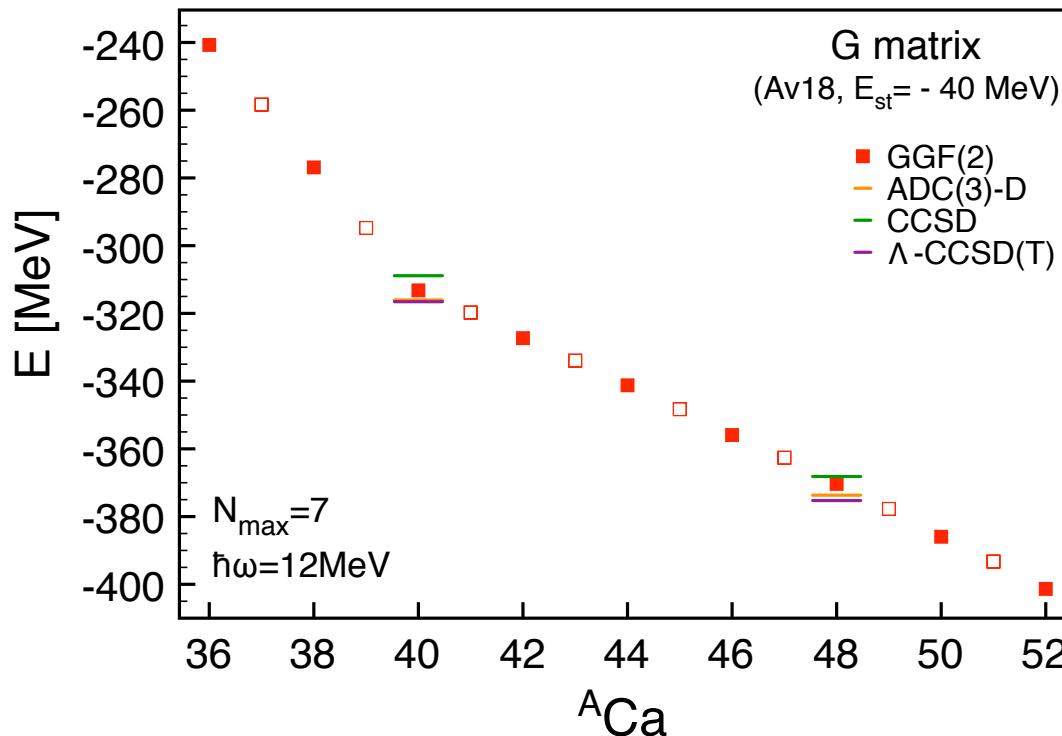
$E(N=13) = -1269.6 \text{ MeV}$
 $E(N=\infty) = -1269.7(2) \text{ MeV}$

(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:

1st order:

2nd order:

...

3rd and all-orders
sums,
P-V coupling:

Dyson formulation
(closed shells)

Hartree-Fock

2nd order

ADC(3)
FRPA
etc...

Gorkov formulation
(semi-magic)

HF-Bogoliubov

2nd order (w/ pairing)

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



Approaches in GF theory

Truncation scheme:

1st order:

2nd order:

...

3rd and all-orders sums,
P-V coupling

Dyson formulation
(closed shells)

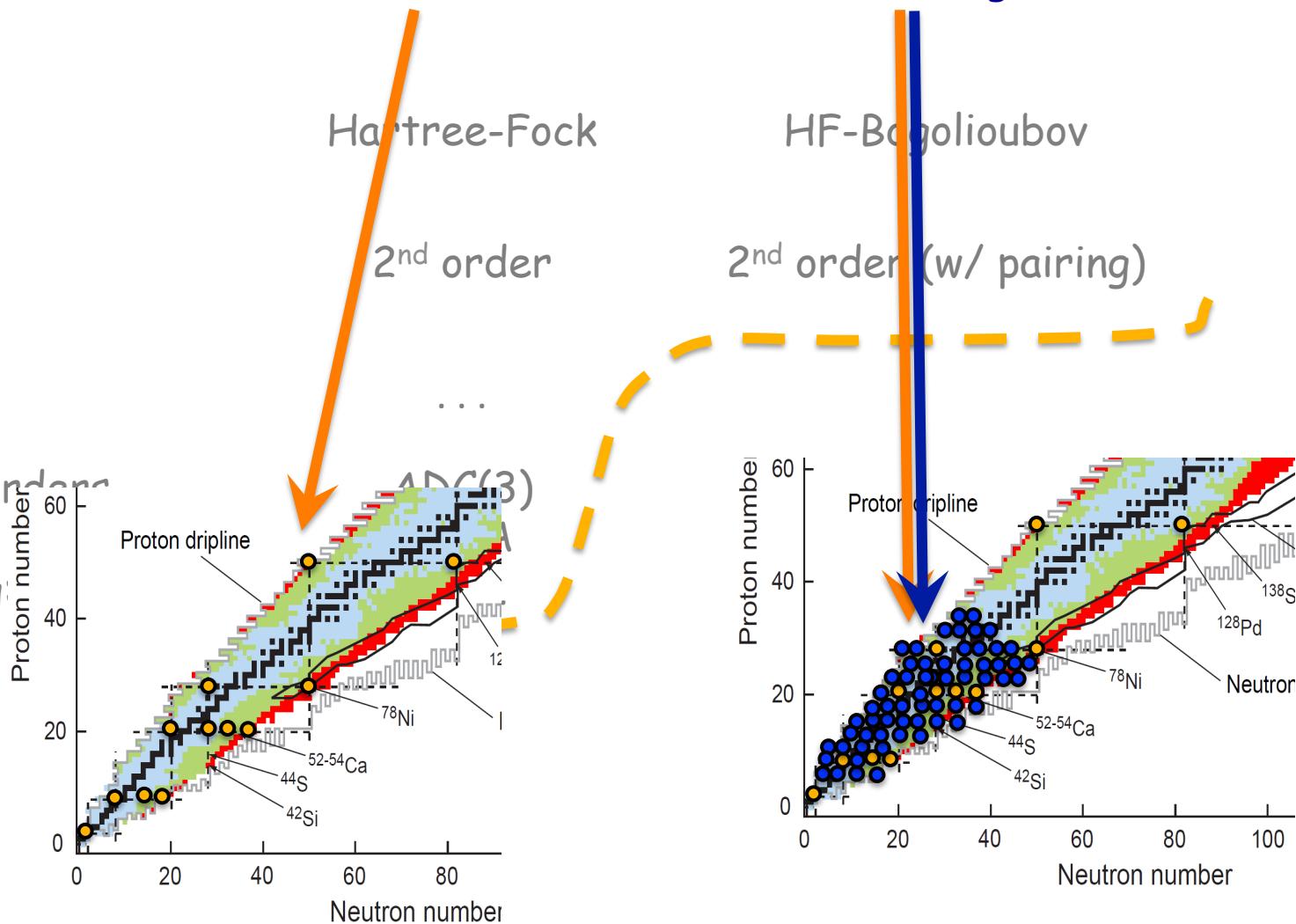
Hartree-Fock

2nd order

Gorkov formulation
(semi-magic)

HF-Bogoliubov

2nd order (w/ pairing)



Ab-initio Nuclear Computation & BcDor code

BoccaDorata code:

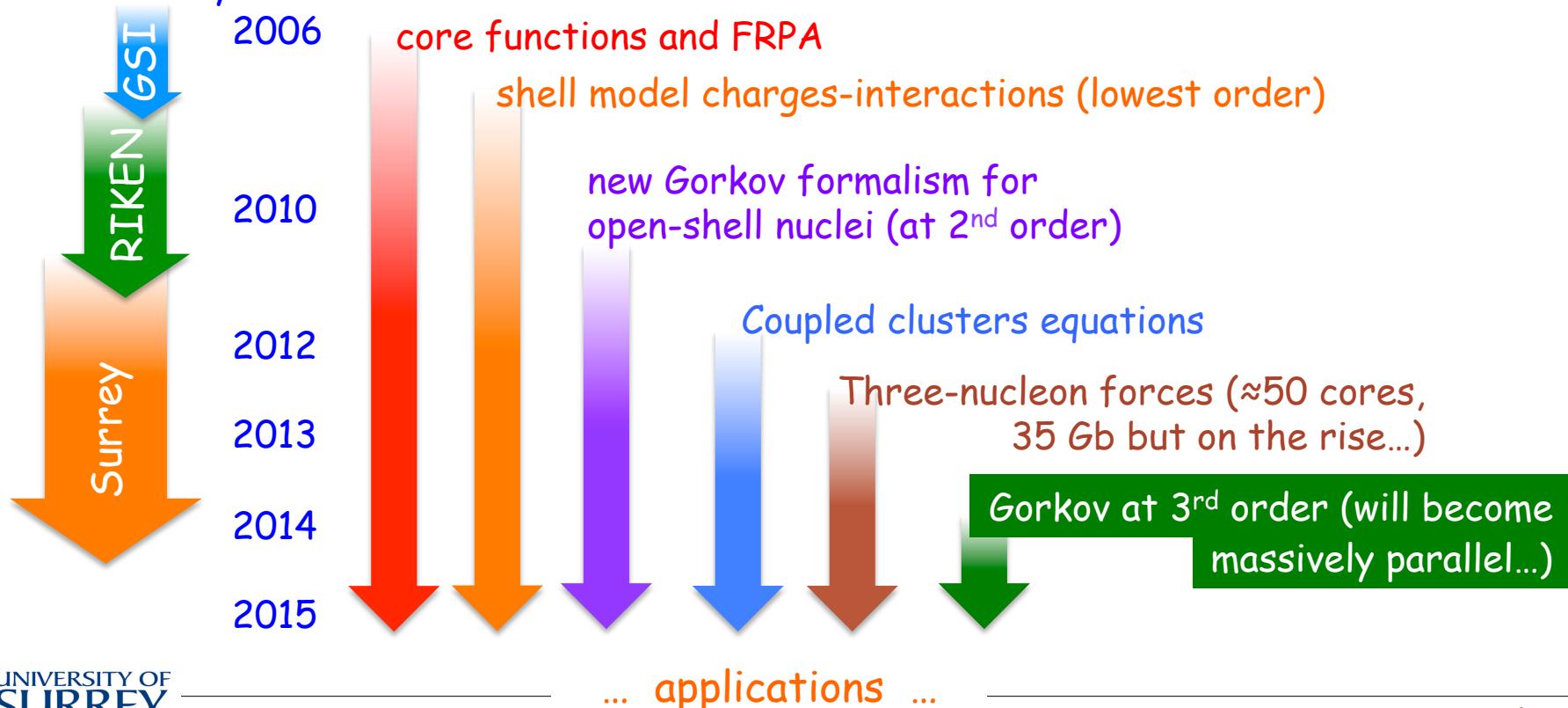
(C. Barbieri 2006-14)

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.

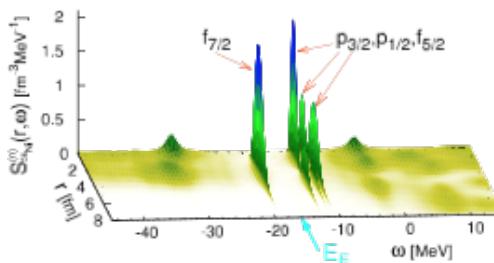
Code history:



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)]

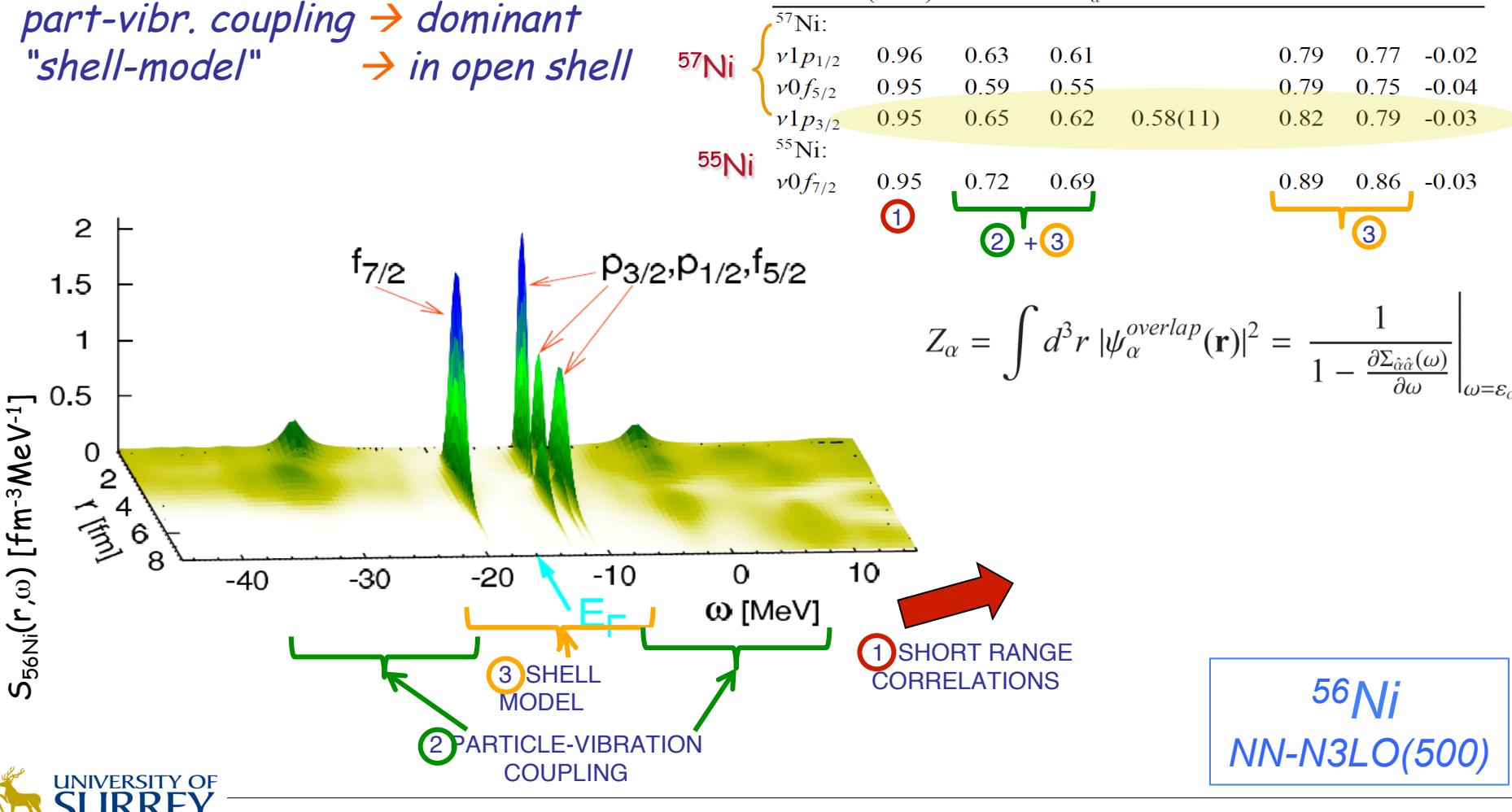
...with analogous conclusions for ^{48}Ca

Overall quenching of *spectroscopic factors* is driven by:

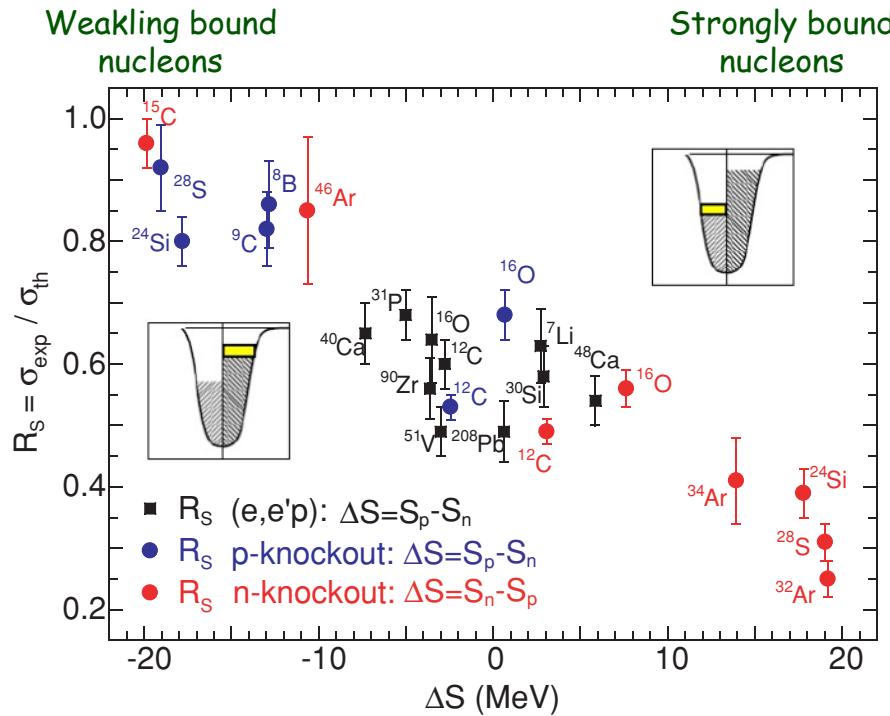
SRC $\rightarrow \sim 10\%$

part-vibr. coupling \rightarrow dominant

"shell-model" \rightarrow in open shell

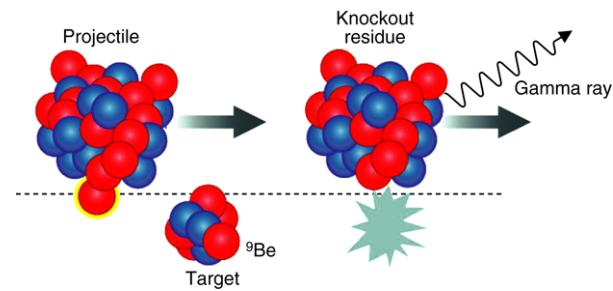


Spectroscopic factors @ limits of stability



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

High energy knock-out in inverse kinematics



? ORIGIN ?
UNCLEAR

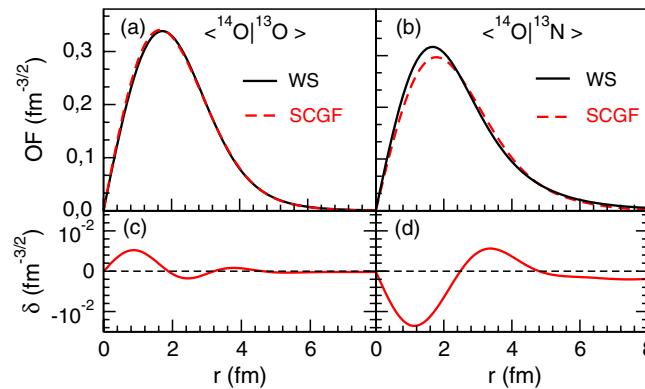
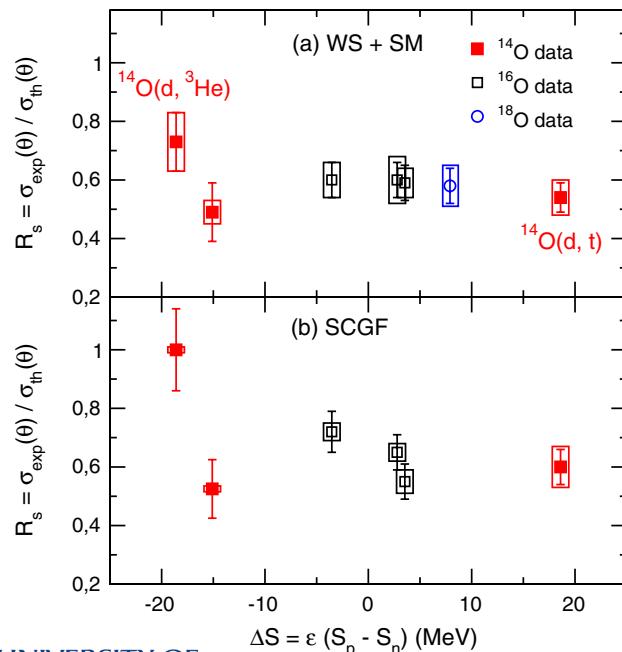
- Challenged by recent experiments
- May be correlations or scattering analysis

Single nucleon transfer in the oxygen chain

[F. Flavigny et al, PRL **110**, 122503 (2013)]

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

Reaction	E^* (MeV)	J^π	$R_{\text{rms}}^{\text{HFB}}$ (fm)	r_0 (fm)	$C^2 S_{\text{exp}}$ (WS)	$C^2 S_{\text{th}}$ $0p + 2\hbar\omega$	R_s (WS)	$C^2 S_{\text{exp}}$ (SCGF)	$C^2 S_{\text{th}}$ (SCGF)	R_s (SCGF)
$^{14}\text{O}(\text{d}, \text{t})^{13}\text{O}$	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)
$^{14}\text{O}(\text{d}, ^3\text{He})^{13}\text{N}$	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)
$^{16}\text{O}(\text{d}, \text{t})^{15}\text{O}$	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)
$^{16}\text{O}(\text{d}, ^3\text{He})^{15}\text{N}$ [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)
$^{18}\text{O}(\text{d}, ^3\text{He})^{17}\text{N}$ [21]	0.00	$1/2^-$	2.91	1.46	0.92(9)(12)	1.58	0.58(6)(10)			

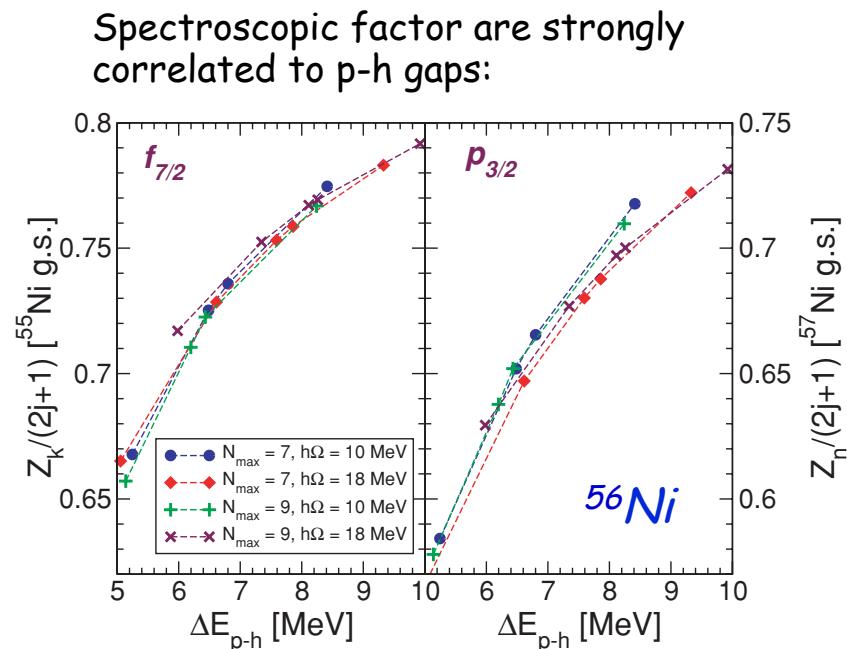
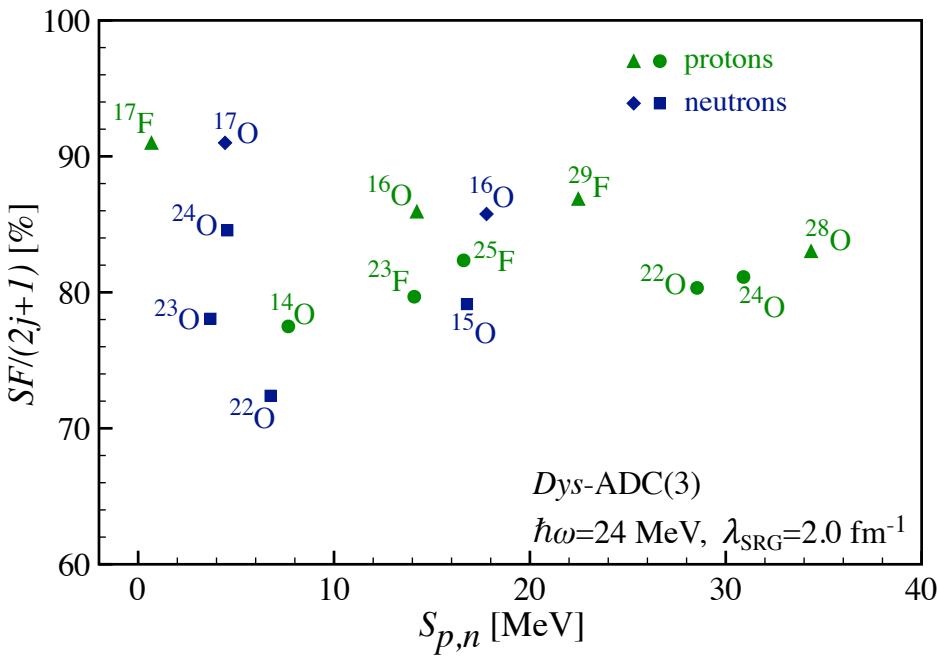


- Overlap functions and strengths from GF
- R_s independent of asymmetry

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

[Lee *et al.* 2010]

	Sn (MeV)	ΔS (MeV)	SF
^{34}Ar	33.0	18.6	1.46
^{36}Ar	27.7	7.5	1.46
^{46}Ar	16.0	-22.3	5.88

$$\Delta S = Sn - Sp$$

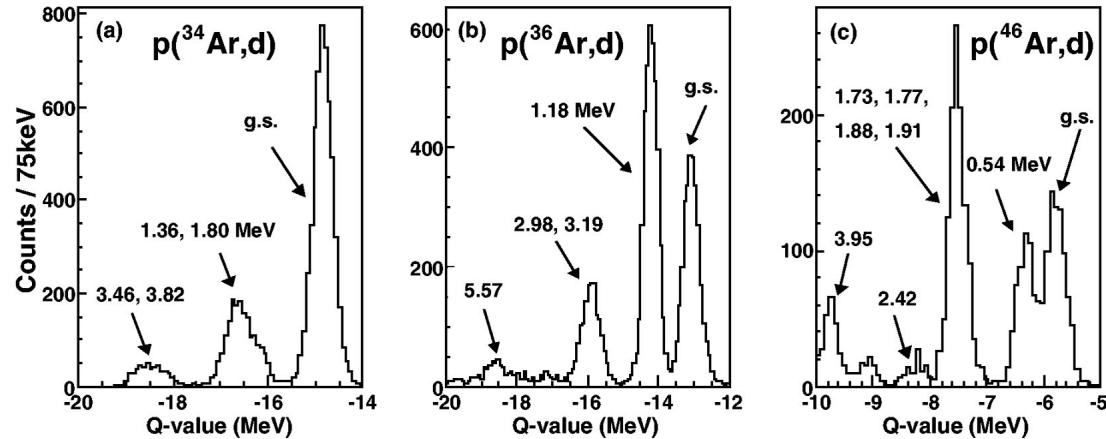
Gorkov GF NN

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

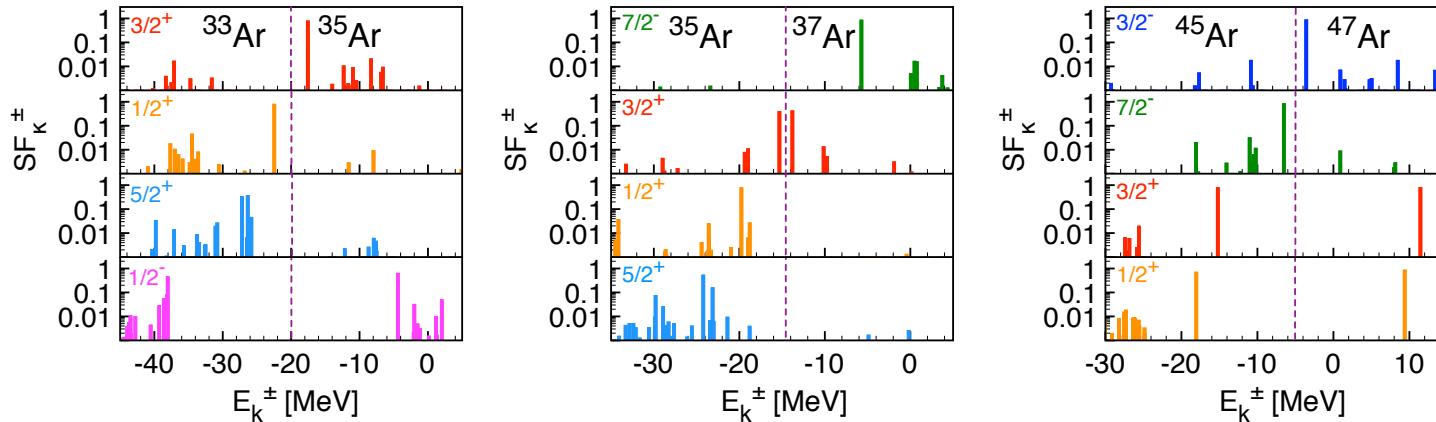
Gorkov GF NN + 3N

Knockout & transfer experiments

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

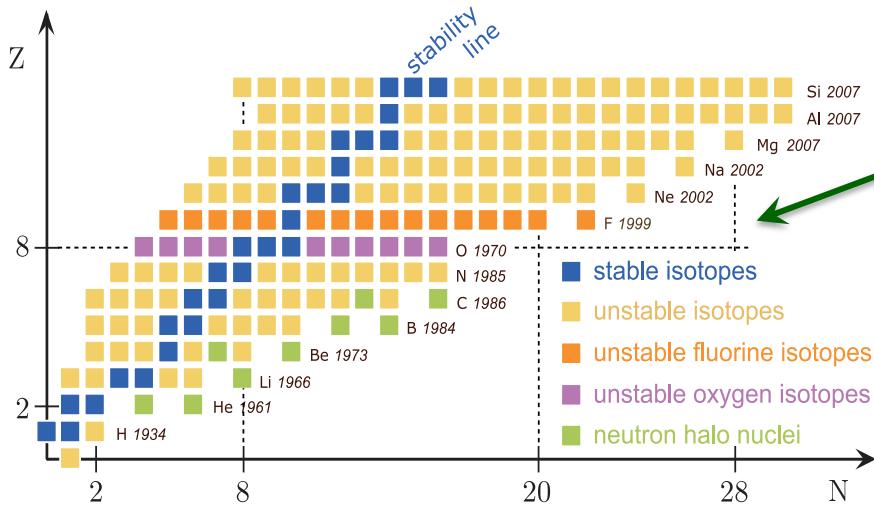


[Lee *et al.* 2010]



Chiral Hamiltonian and 3NF

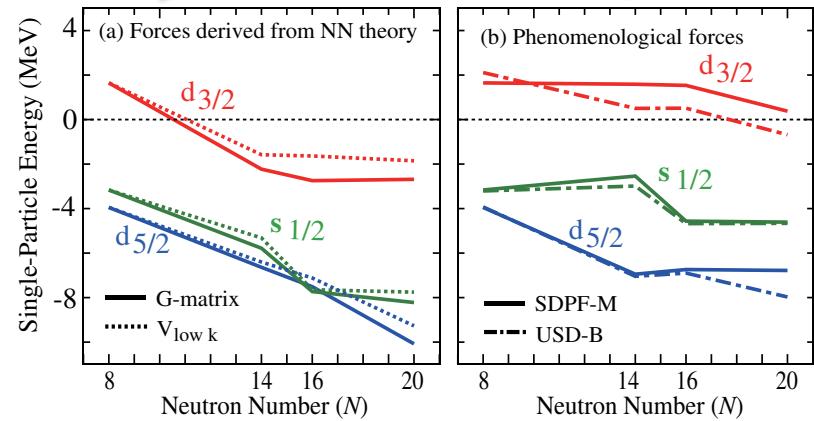
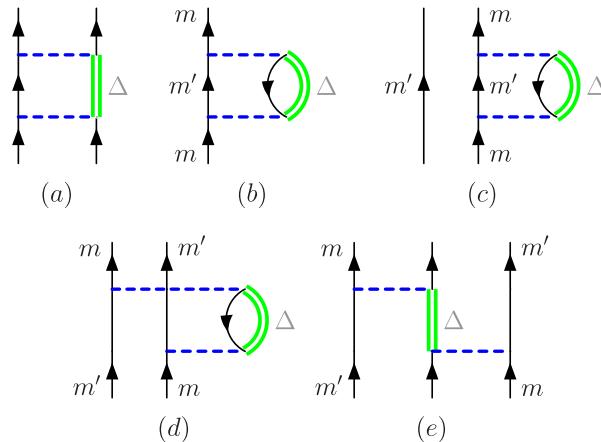
Oxygen puzzle...



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

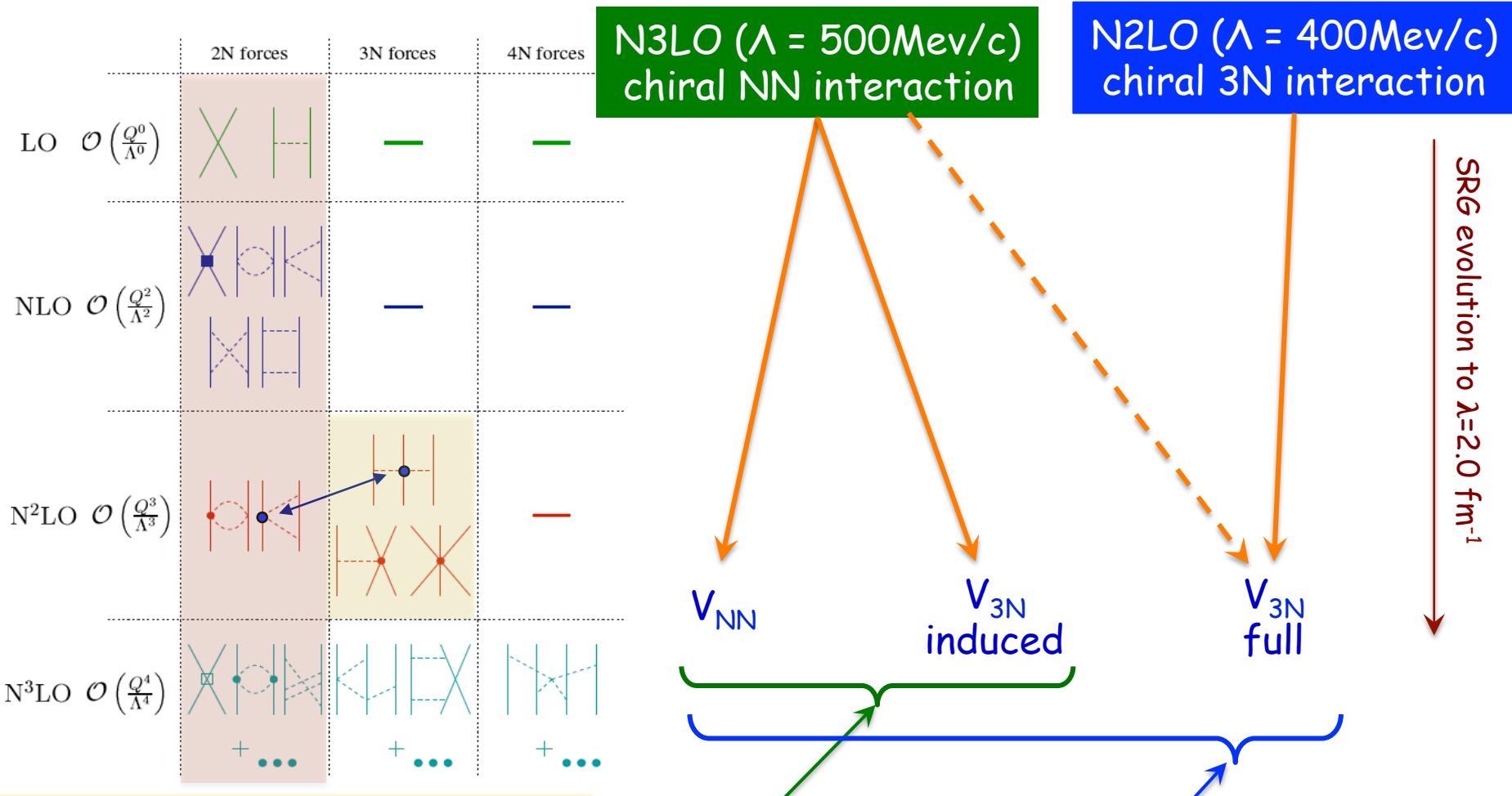
Phenomenological shell model interaction reflect this in the s.p. energies but no realistic NN interaction alone is capable of reproducing this...

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



[Jurgenson, Navrátil, Furnstahl,
Phys. Rev. Lett. **103**, 082501 (2009);
Hebeler, Phys. Rev. C **85**, 021002 (2012)]

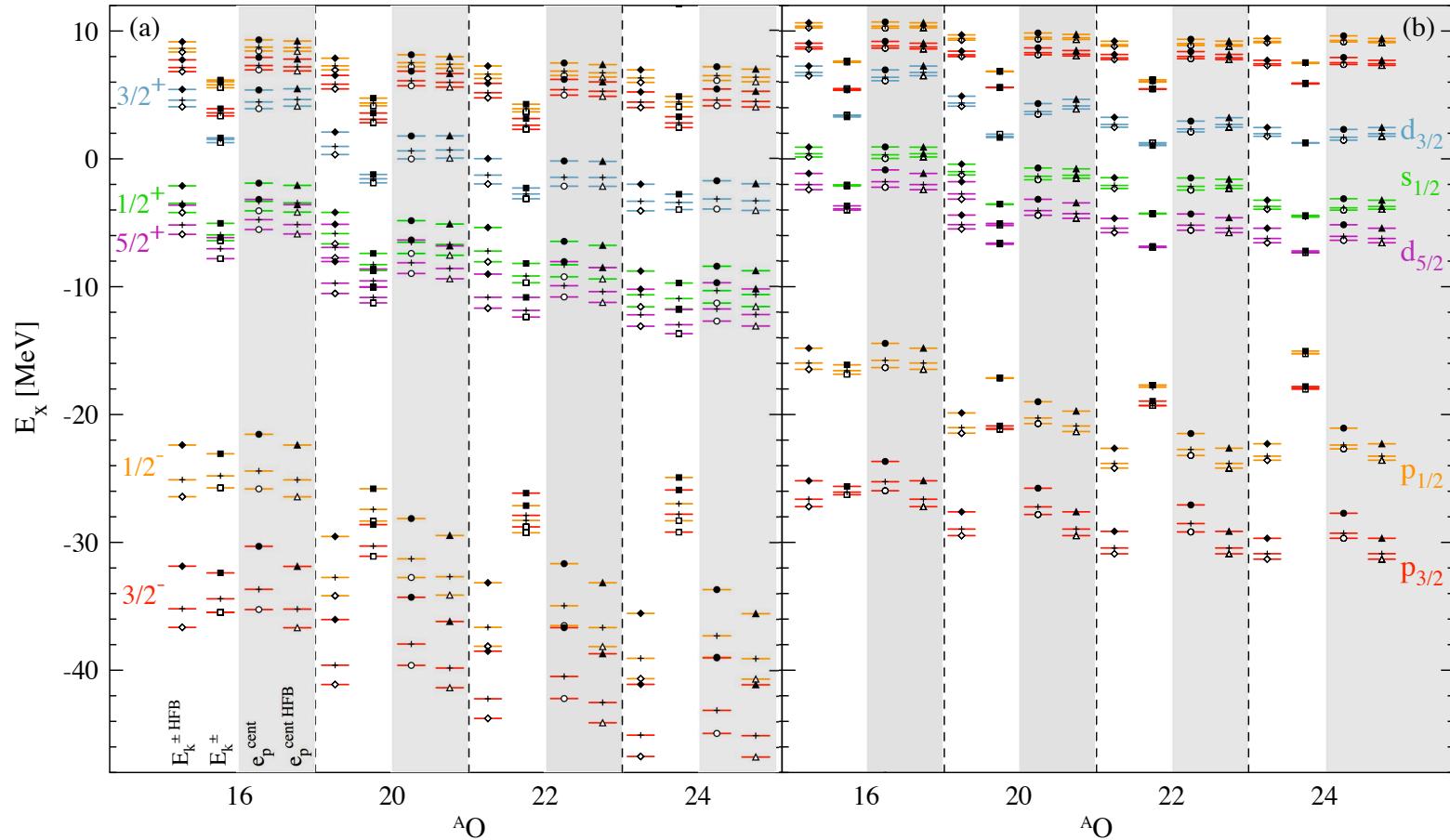


Convergence of s.p. spectra w.r.t. SRG

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

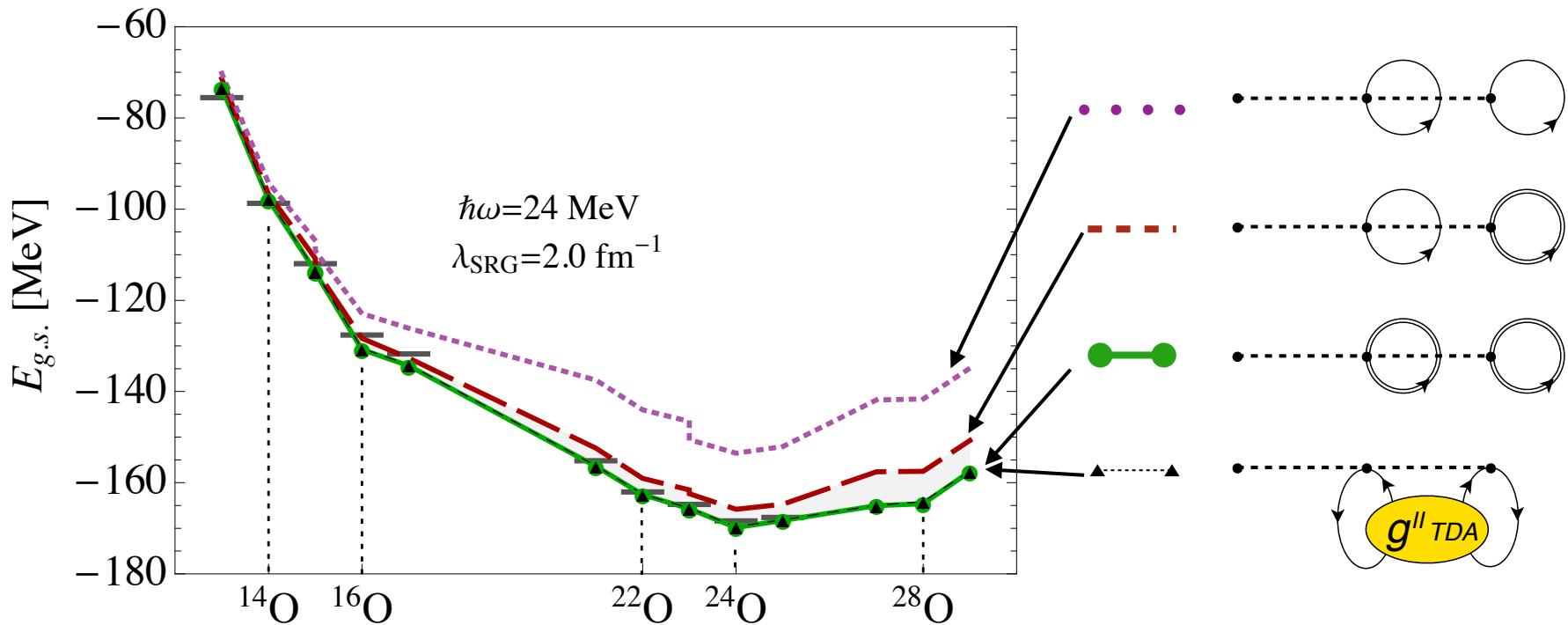
arXiv:1411.1237 (2014)

✓ only dominant s.p. states shown



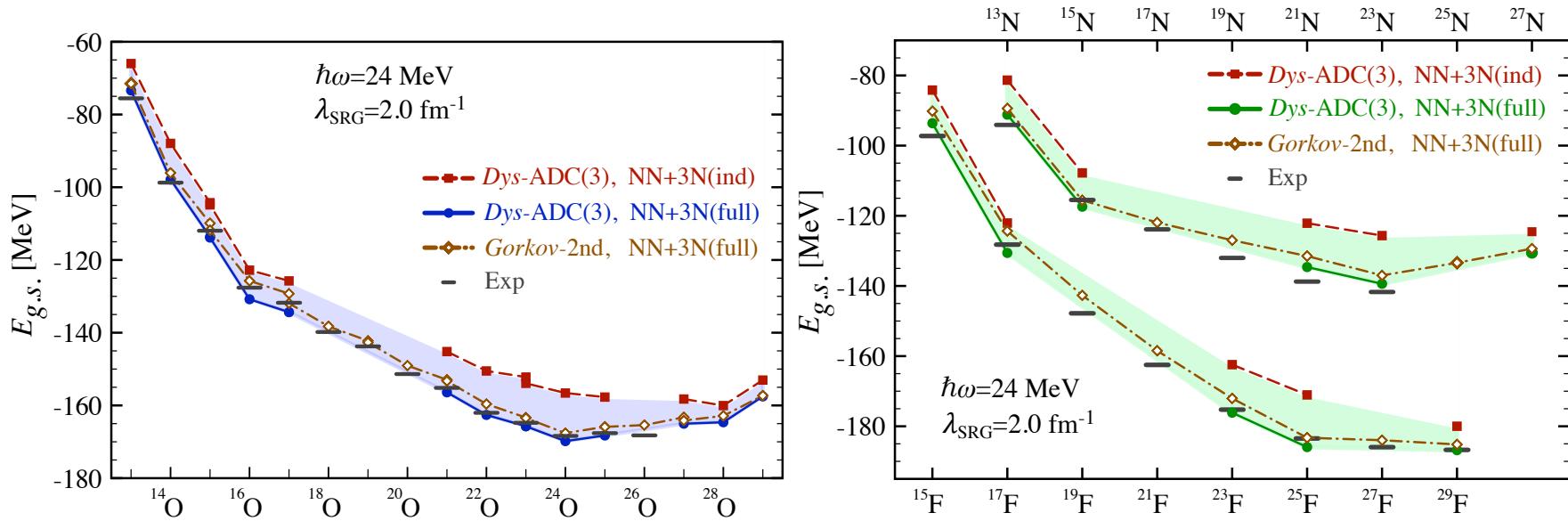
3N forces in FRPA/FTDA formalism

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



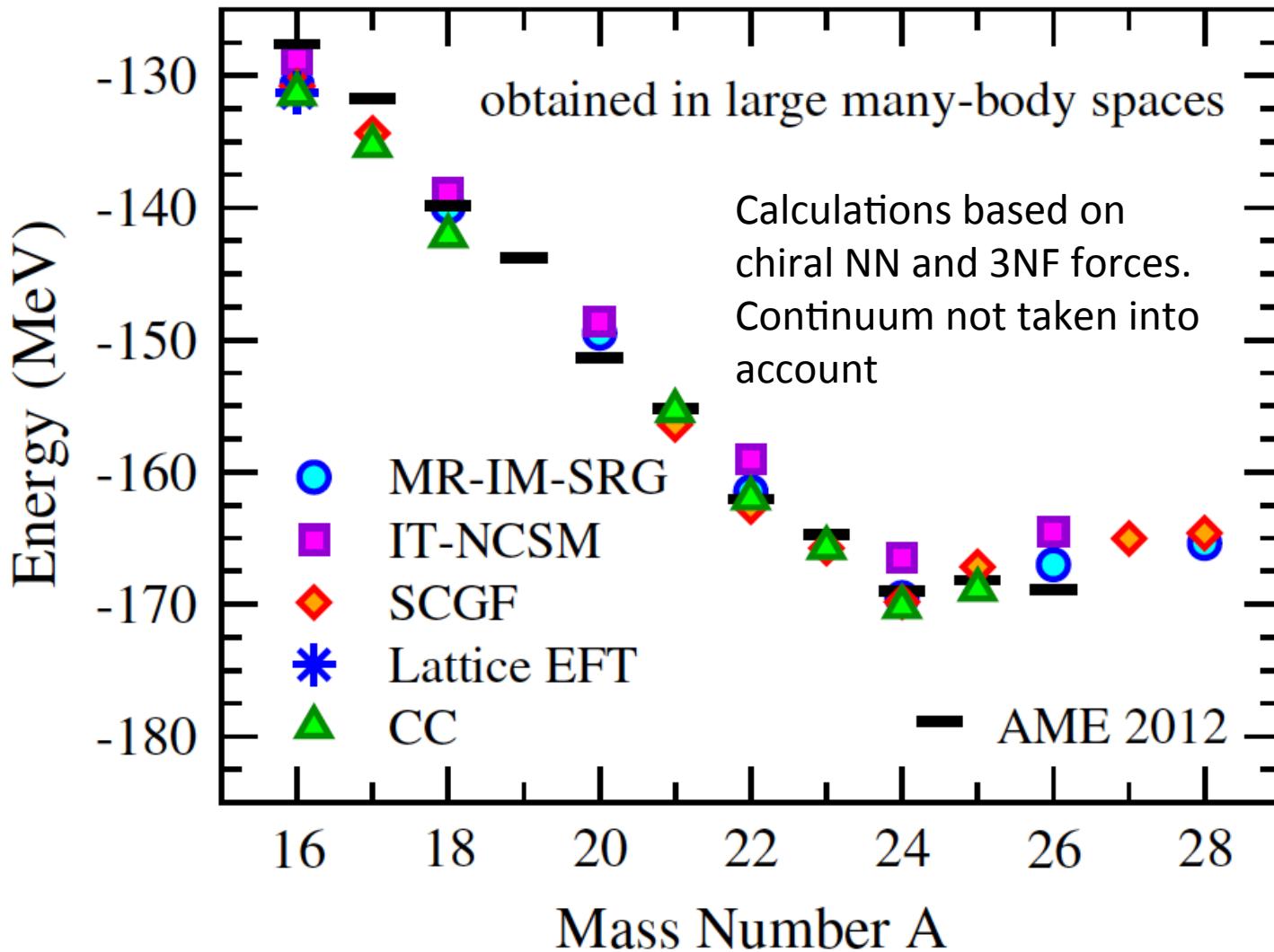
Results for the N-O-F chains

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



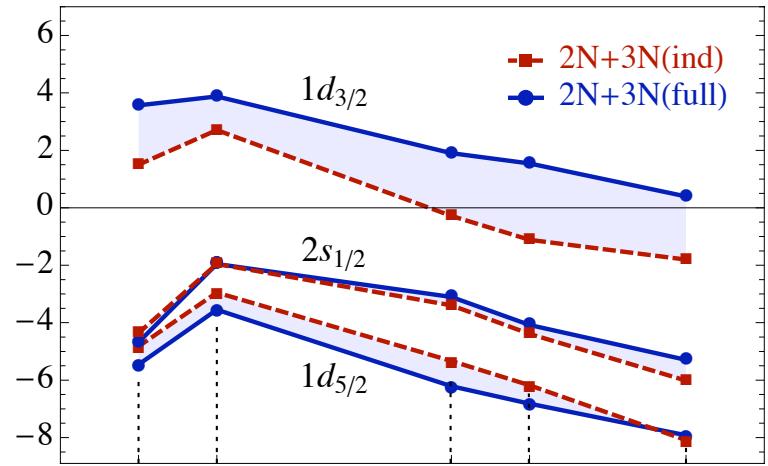
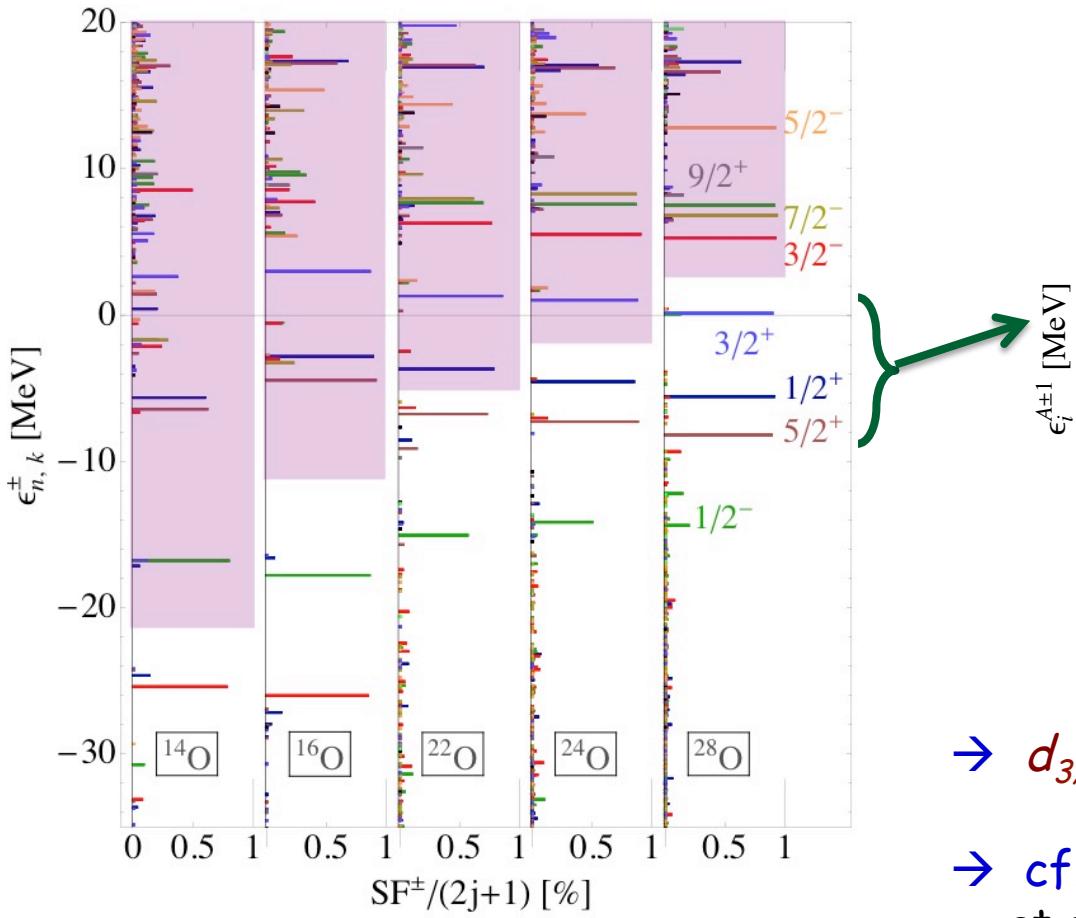
- 3NF crucial for reproducing binding energies and driplines around oxygen
- cf. microscopic shell model [Otsuka et al, PRL **105**, 032501 (2010).]

Benchmark of ab-initio methods in the oxygen isotopic chain



Results for the N-O-F chains

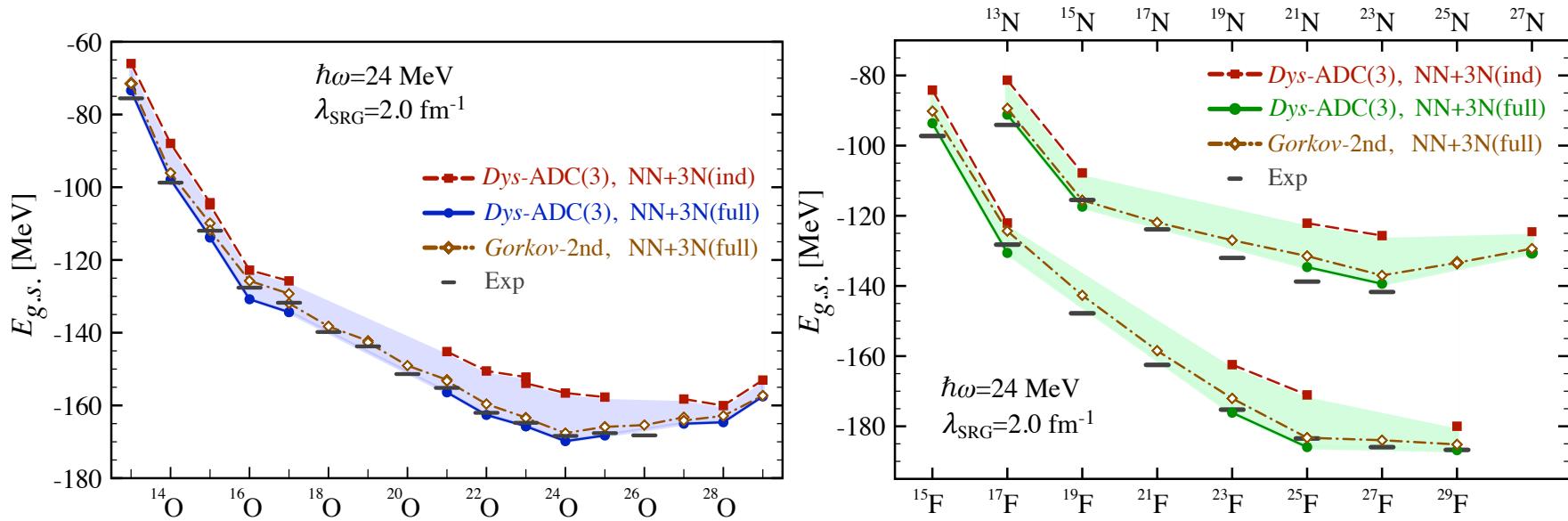
A. Cipollone, CB, P. Navrátil, Phys. Rev. Lett. **111**, 062501 (2013)
and arXiv:1412.3002 [nucl-th] (2014)



- $d_{3/2}$ raised by genuine 3NF
- cf. microscopic shell model [Otsuka et al, PRL **105**, 032501 (2010).]

Results for the N-O-F chains

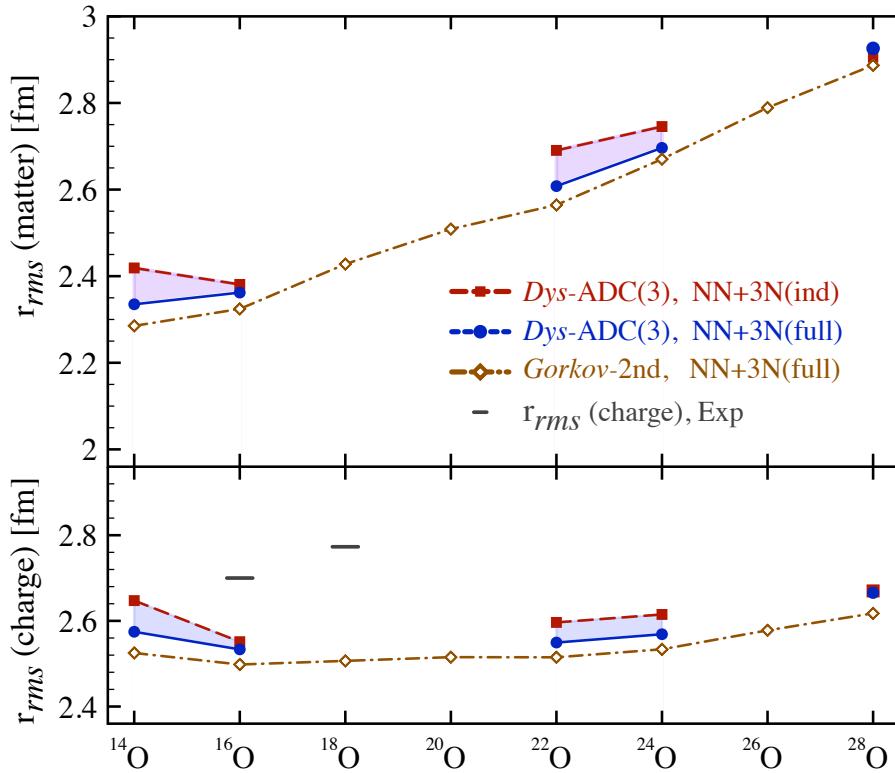
A. Cipollone, CB, P. Navrátil, Phys. Rev. Lett. **111**, 062501 (2013)
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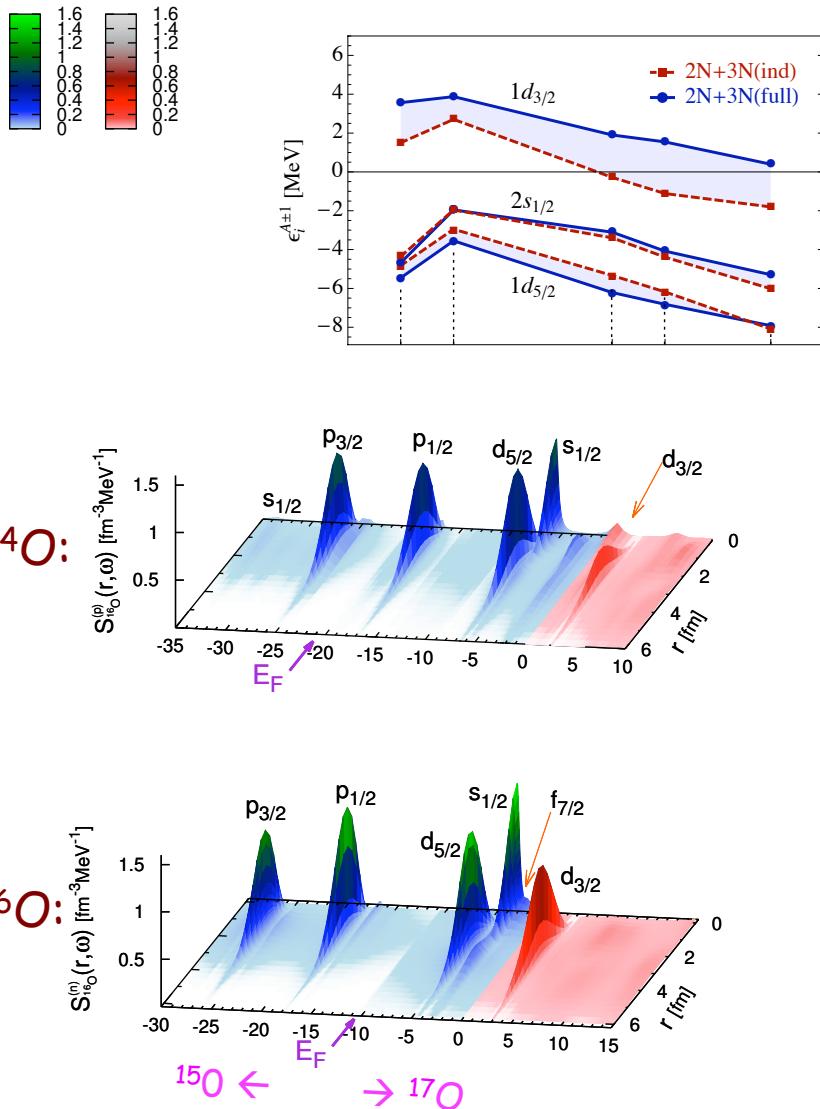
Results for the oxygen chain

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

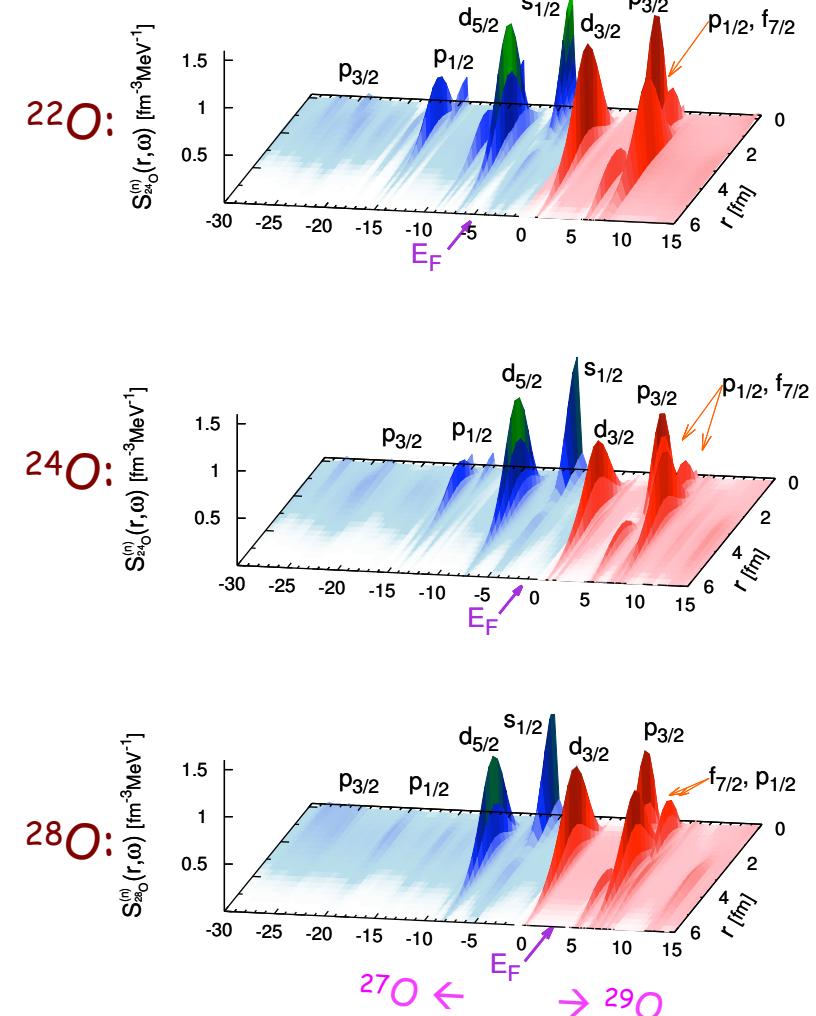


- Single particle spectra slightly to spread and
- systematic underestimation of radii

Neutron spectral function of Oxygens

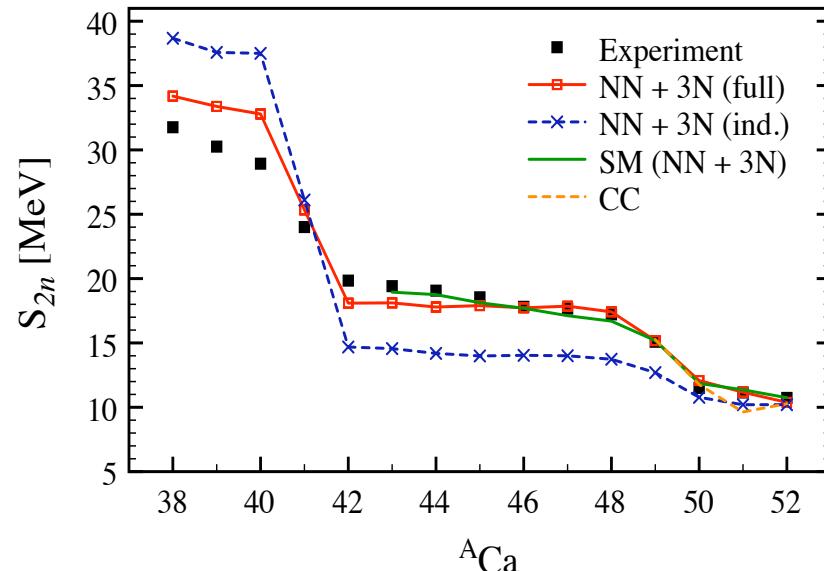
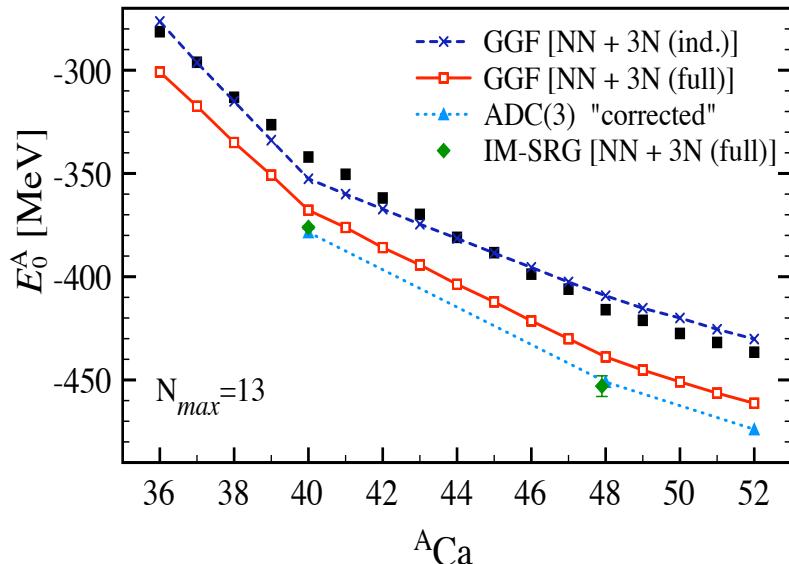


A. Cipollone, CB P. Navrátil, *PRC submitted* (2014)



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}

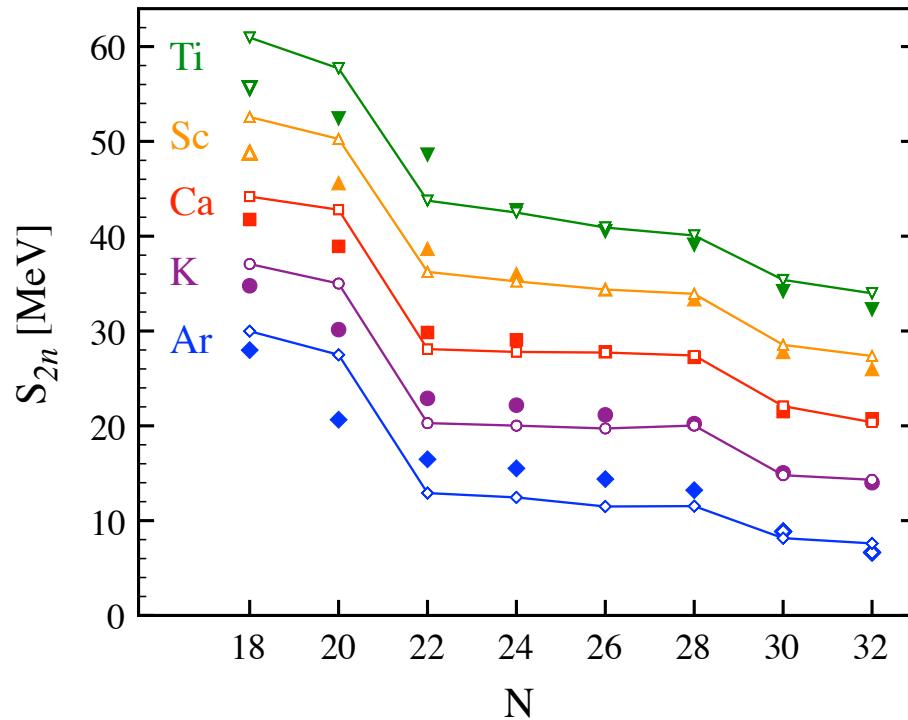
→ N=20 and Z=20 gaps overestimated!

→ 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:

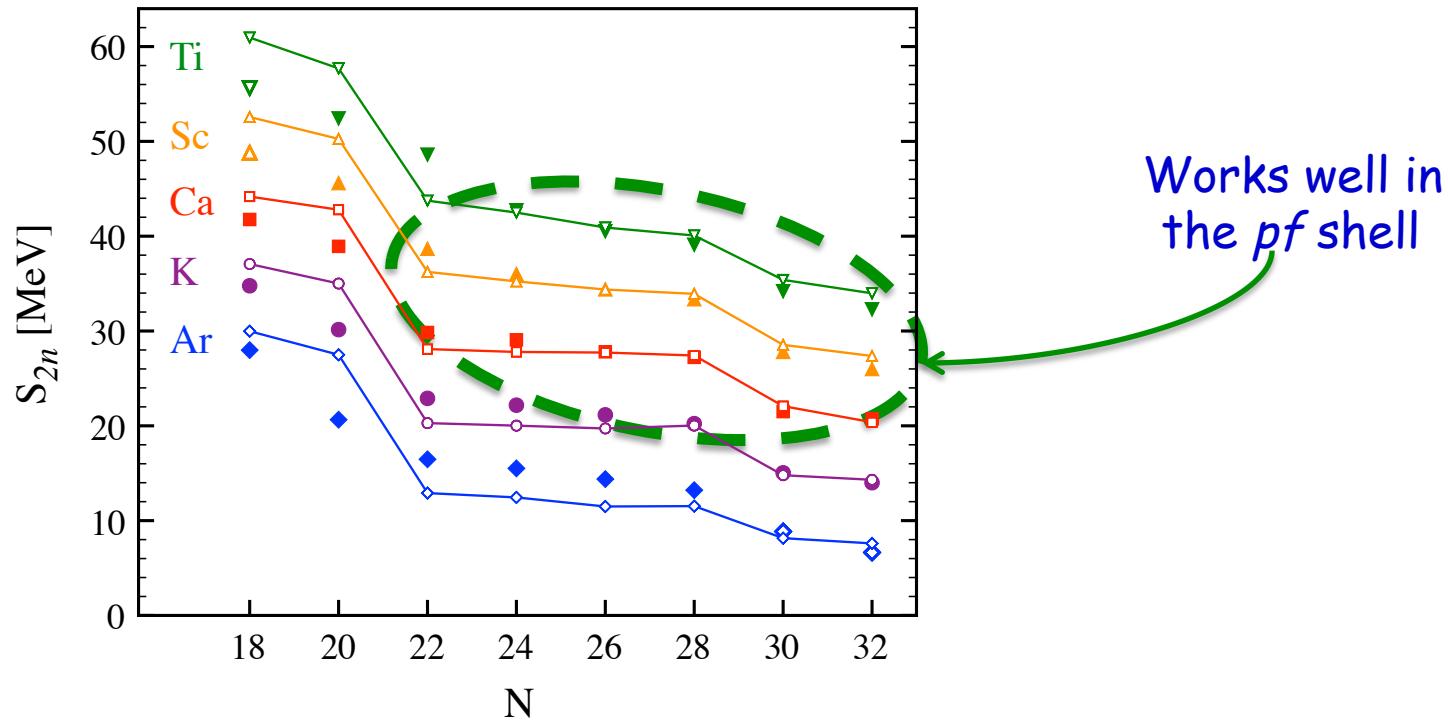


→ First *ab-initio* calculation over a contiguous portion of the nuclear chart—open shells are now possible through the Gorkov-GF formalism

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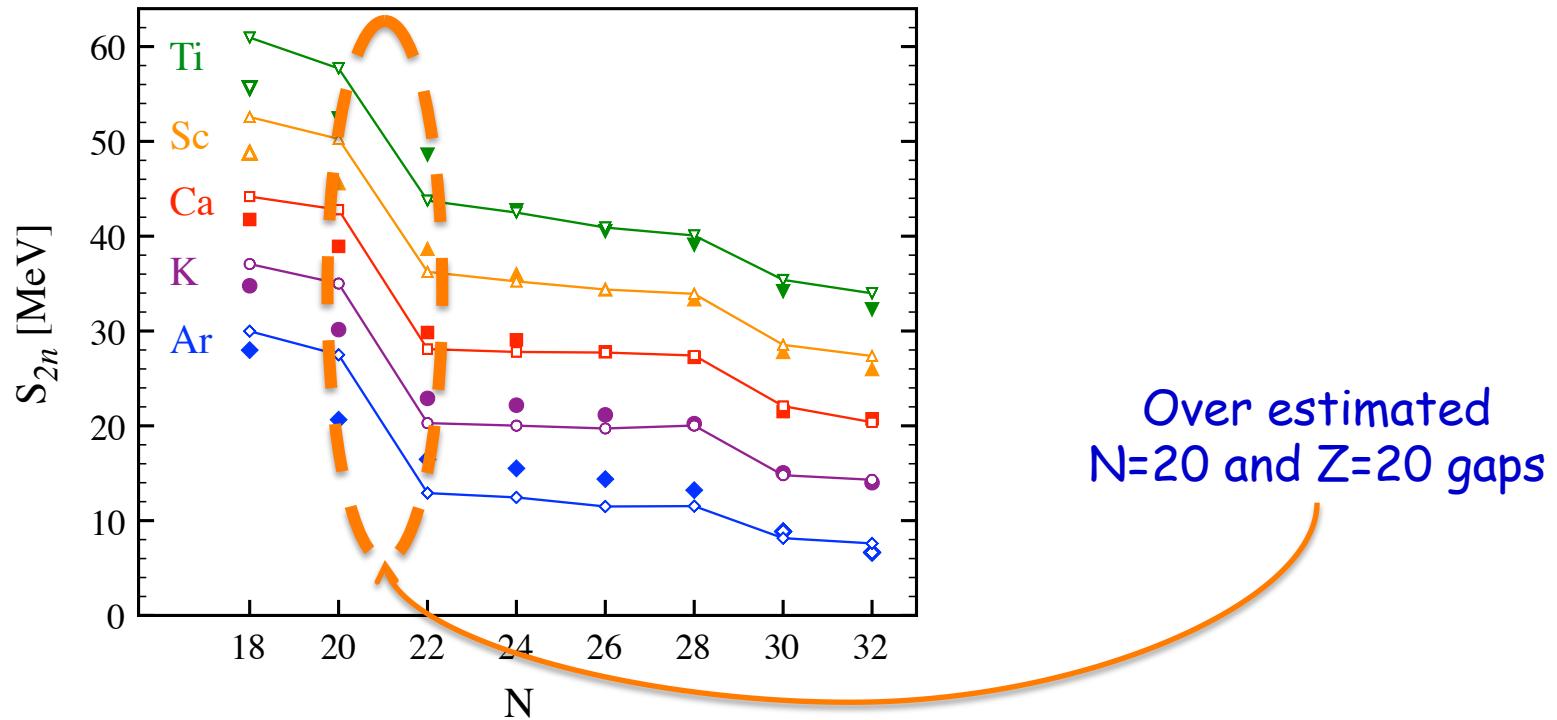


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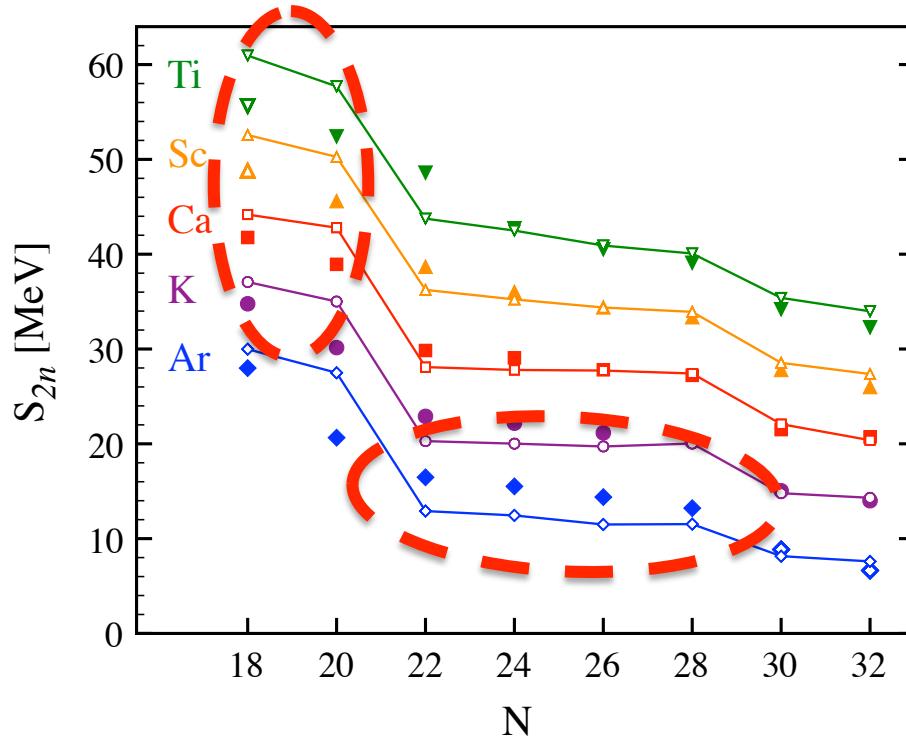


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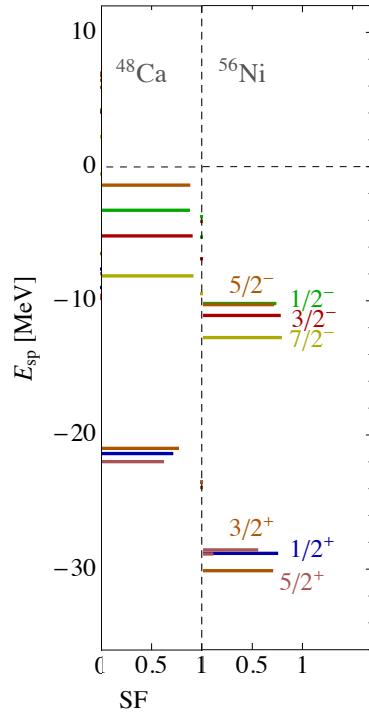
Lack of deformation due
to quenched cross-shell
quadrupole excitations

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

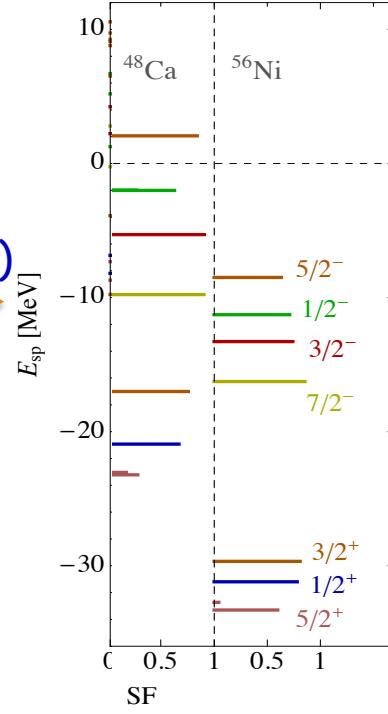
The *sd-pf* shell gap

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

2N + 3NF (induced)



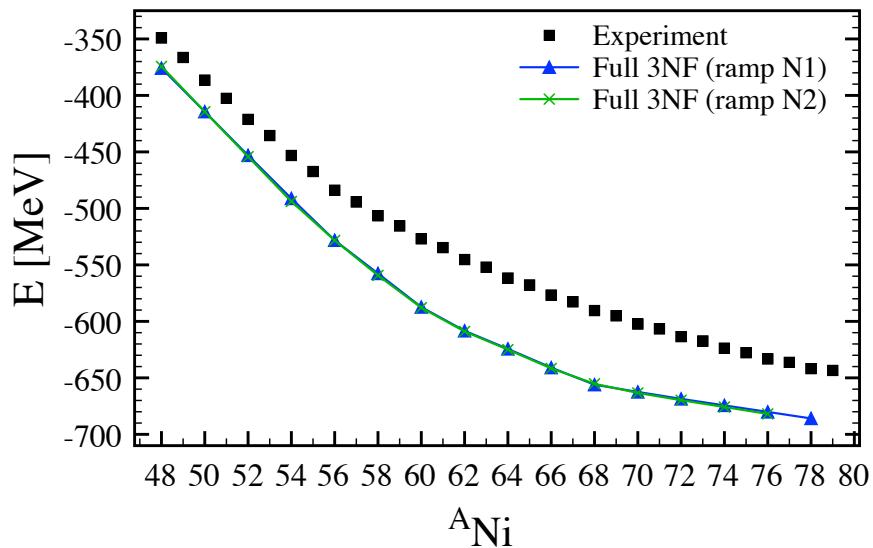
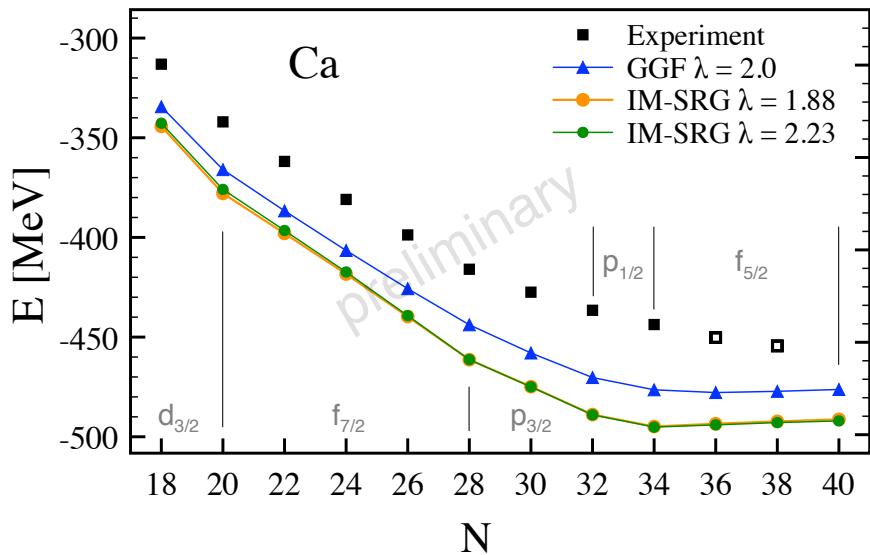
2N + 3NF (FULL)



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

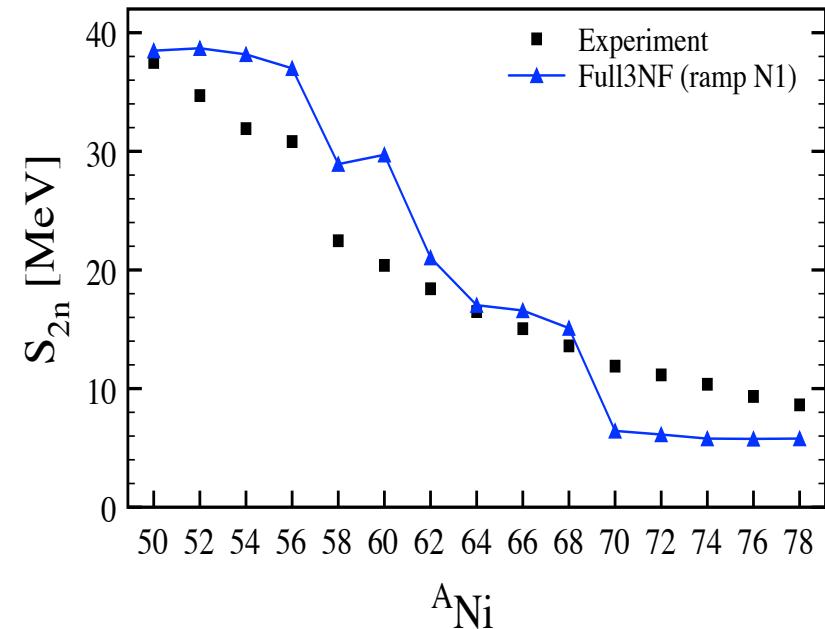
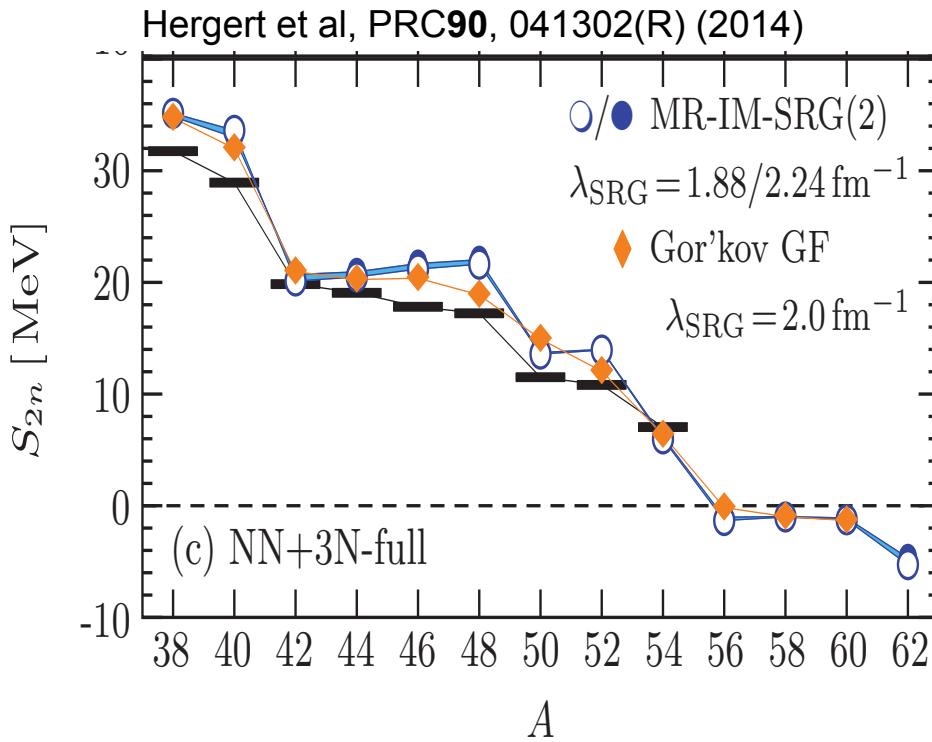
	2NF only	2+3NF(ind.)	2+3NF(full)	Experiment
^{16}O :	2.10	2.41	2.38	2.718 ± 0.210 [19]
^{44}Ca :	2.48	2.93	2.94	3.520 ± 0.005 [20]

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

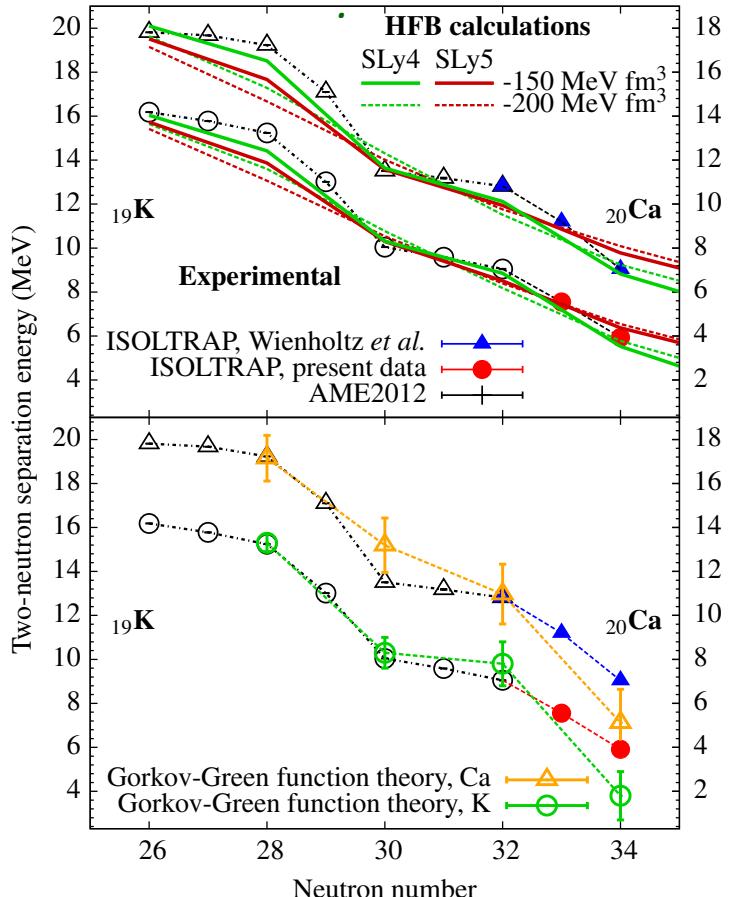
Ca and Ni isotopic chains



- 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 $N=28$

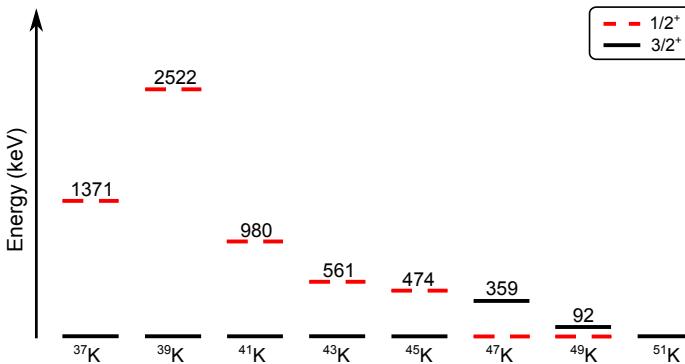
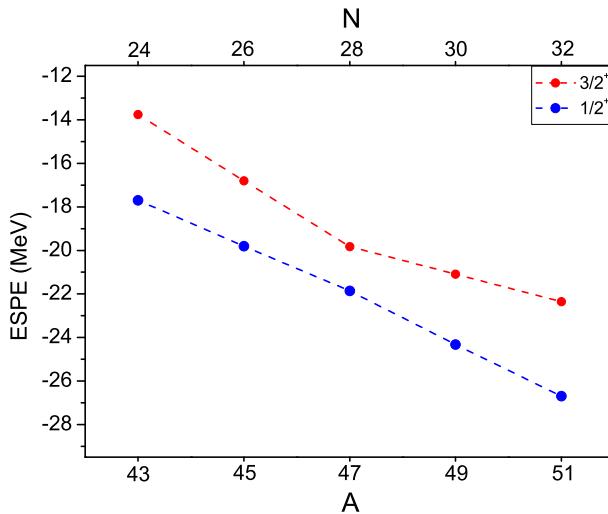


FIG. 1. (color online) Experimental energies for $1/2^+$ and $3/2^+$ states in odd- A K isotopes. Inversion of the nuclear spin is obtained in $^{47,49}\text{K}$ and reinversion back in ^{51}K . Results are

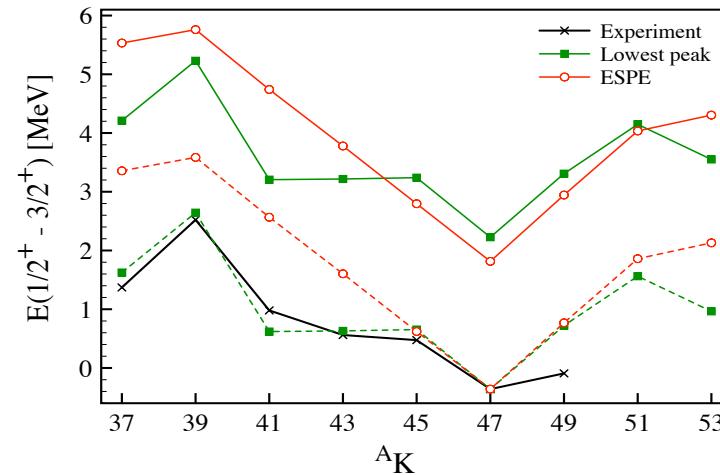
J. Papuga, et al., Phys. Rev. Lett. **110**, 172503 (2013);
Phys. Rev. C **90**, 034321 (2014)

^AK isotopes
Laser spectroscopy @ ISOLDE

Change in separation described by chiral NN+3NF:



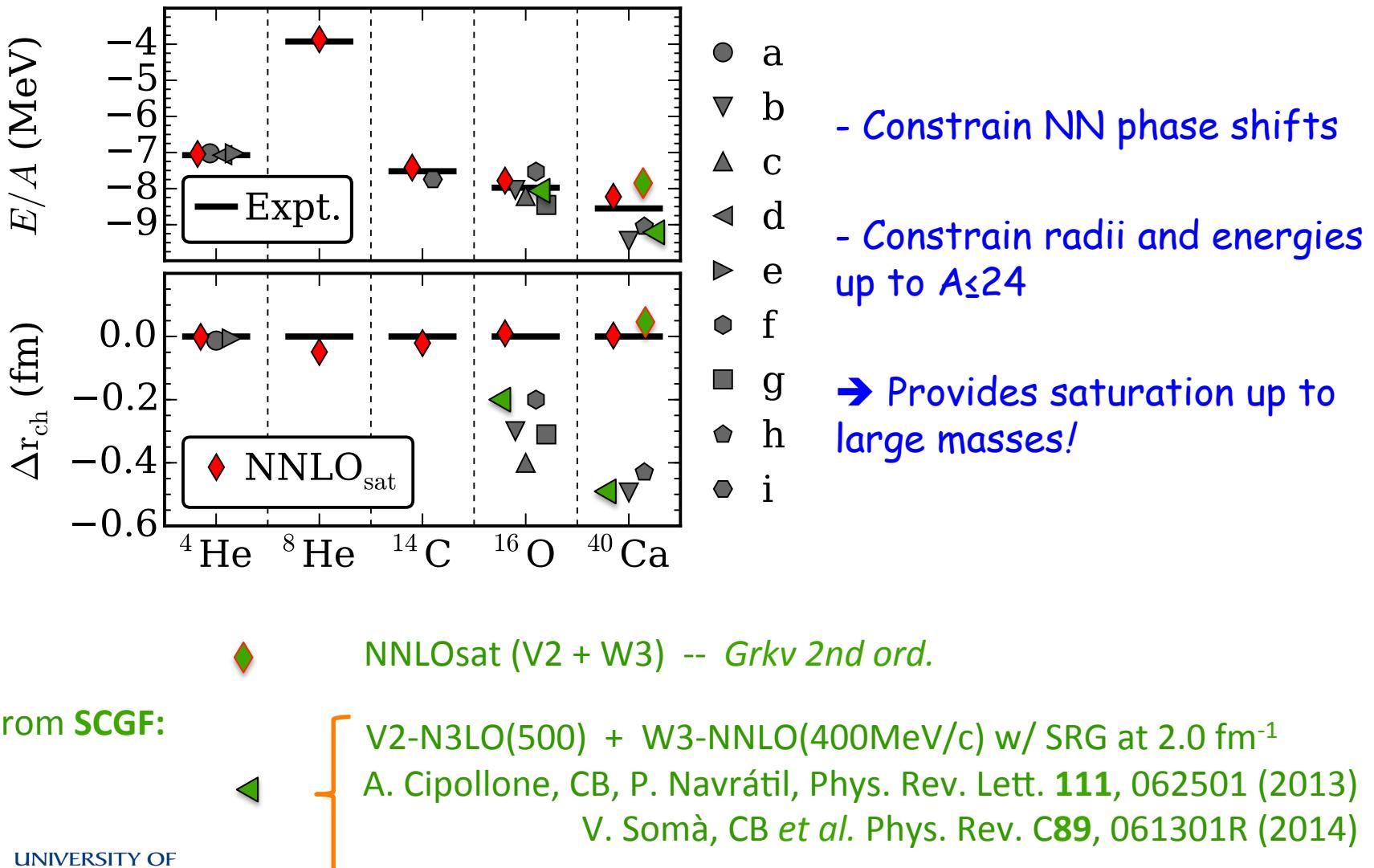
ESPE: "centroid" energies



(Gorkov calculations at 2nd order)

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

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



Collaborators



énergie atomique • énergies alternatives



TECHNISCHE
UNIVERSITÄT
DARMSTADT



Universitat de Barcelona



Washington
University in St. Louis



Center for
Molecular Modeling



UNIVERSITY OF
SURREY



A. Cipollone, A. Rios, F. Raimondi

V. Somà, T. Duguet

A. Carbone

P. Navratil

A. Polls

W.H. Dickhoff, S. Waldecker

D. Van Neck, M. Degroote

M. Hjorth-Jensen