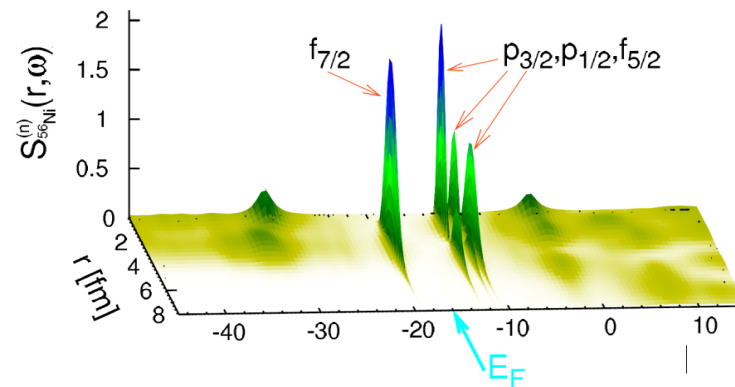
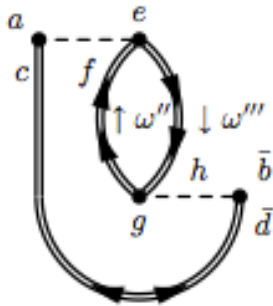


Toward ab-initio predictions for mid-mass open shells

C. Barbieri



Towards a unified description of nuclei

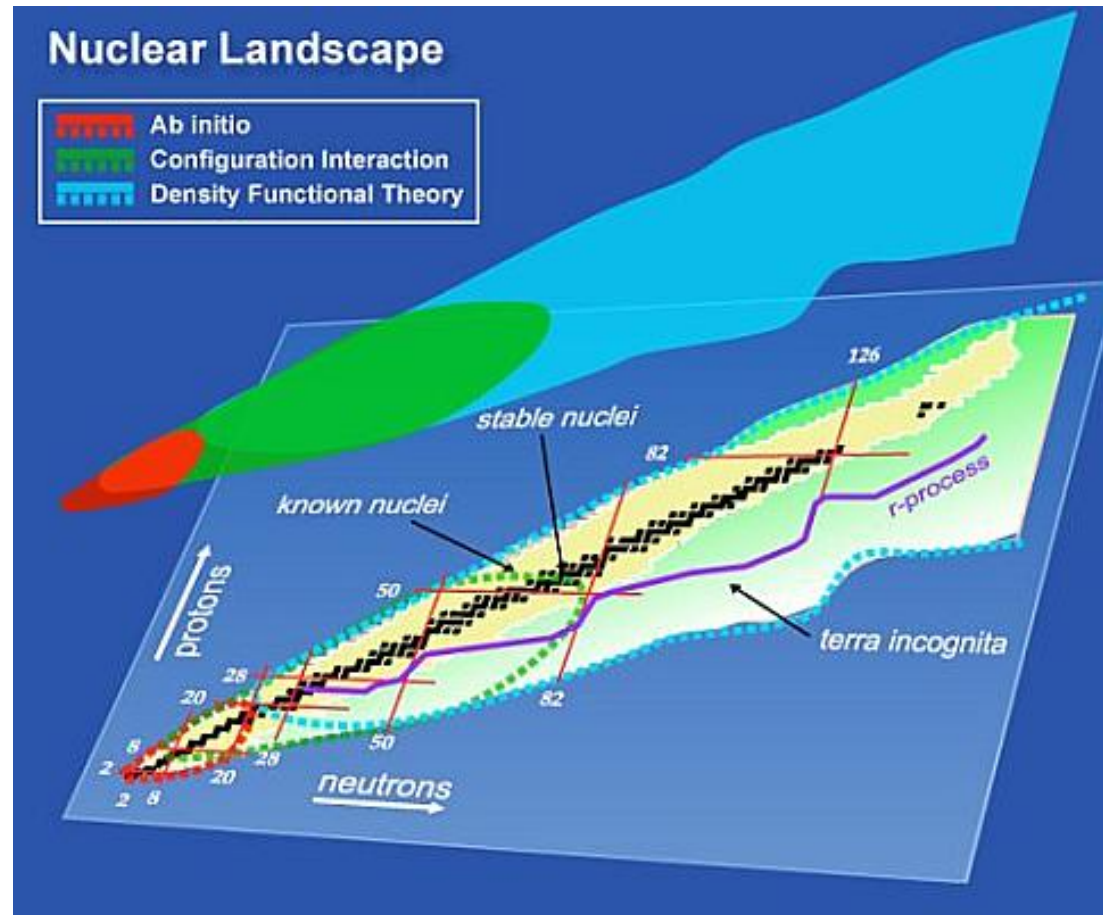
Open issues @ mid masses are:

→ Need of good nuclear Hamiltonians (3N forces mostly!)

→ Structure calculations are limited to closed-shells or $A \pm 1$, $A \pm 2$

→ Ab-Initio link between structure and reactions.

(BUT calculations are GOOD!!!)



Green's functions can be naturally extended to: Scattering observable
Open shell nuclei

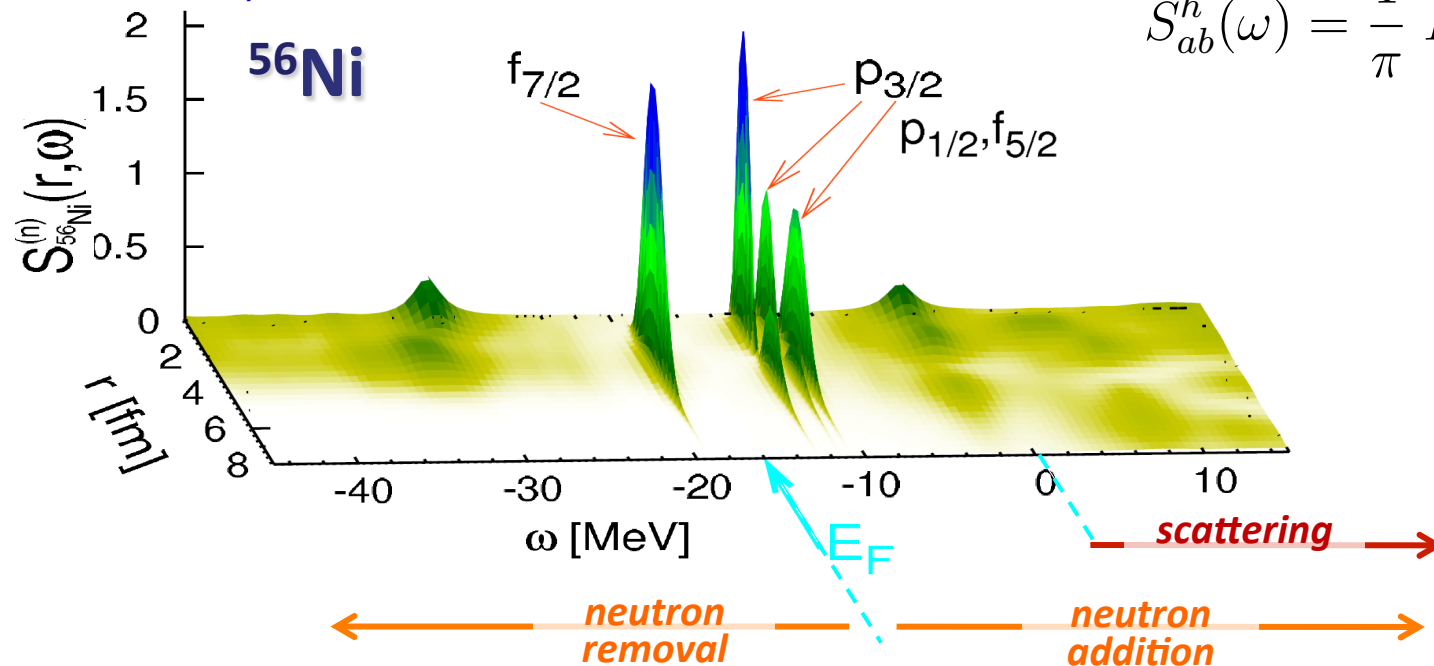
Green's functions in many-body theory

One-body Green's function (or propagator) describes the motion of quasi-particles and holes:

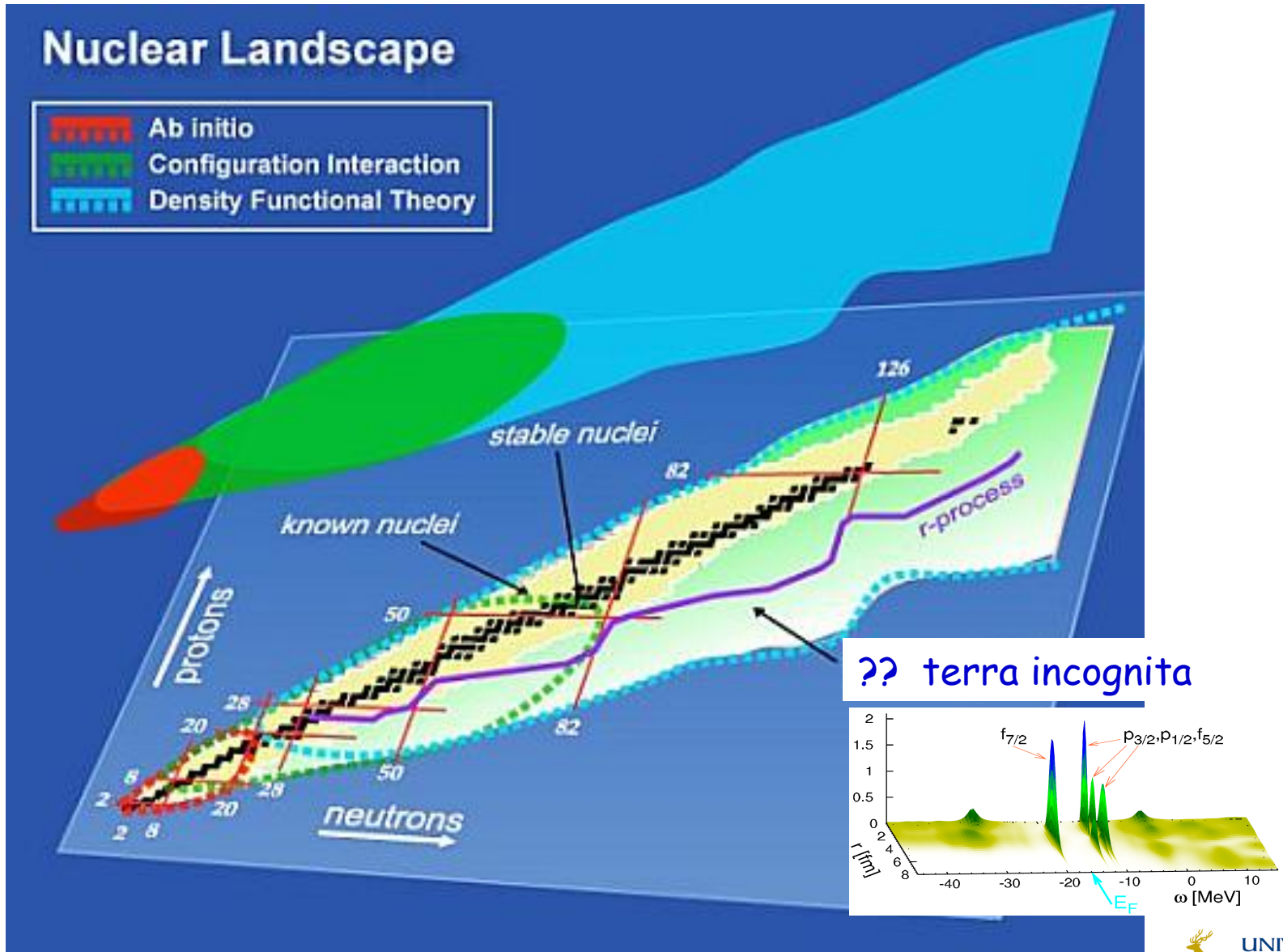
$$g_{\alpha\beta}(E) = \sum_n \frac{\langle \Psi_0^A | c_\alpha | \Psi_n^{A+1} \rangle \langle \Psi_n^{A+1} | c_\beta^\dagger | \Psi_0^A \rangle}{E - (E_n^{A+1} - E_0^A) + i\eta} + \sum_k \frac{\langle \Psi_0^A | c_\beta^\dagger | \Psi_k^{A-1} \rangle \langle \Psi_k^{A-1} | c_\alpha | \Psi_0^A \rangle}{E - (E_0^A - E_k^{A-1}) - i\eta}$$

...this contains all the structure information probed by nucleon transfer (spectral function):

$$S_{ab}^h(\omega) = \frac{1}{\pi} \text{Im} g_{ab}(\omega)$$



Towards a global description exotic structures...

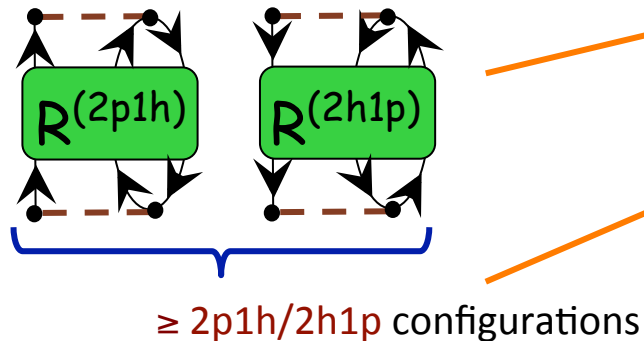
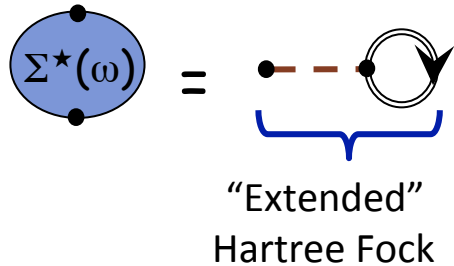


Calculating the spectral function:

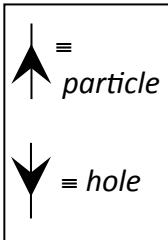
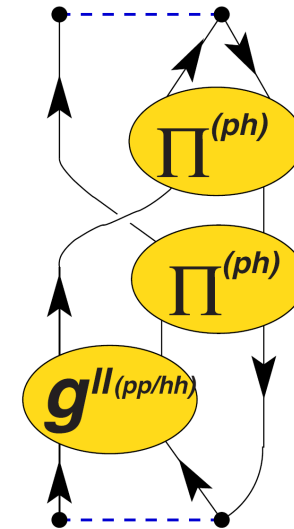
FRPA, ADC(3), and the like...

Faddeev-RPA in two words...

Self-energy
(optical potential):



Faddeev-RPA:

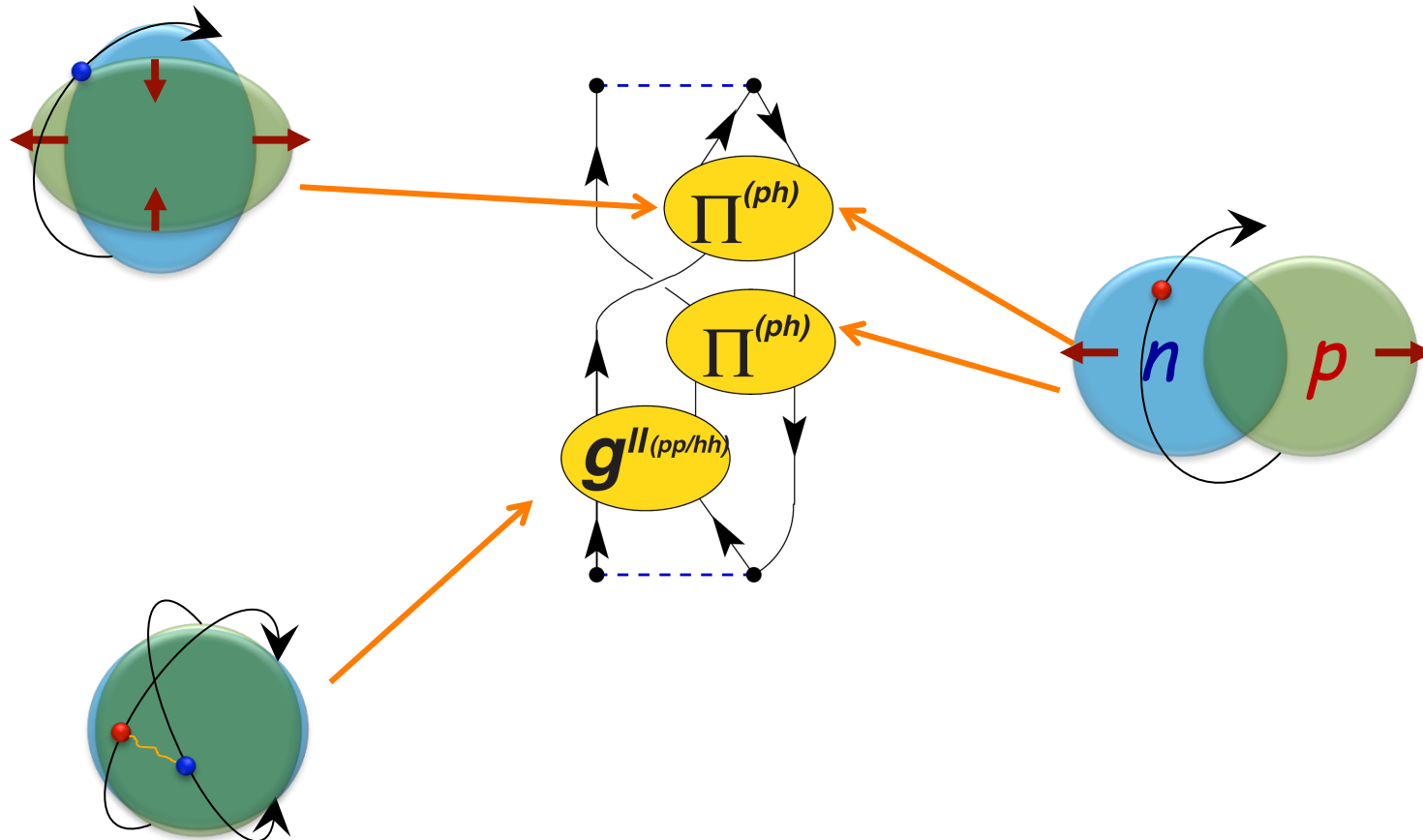
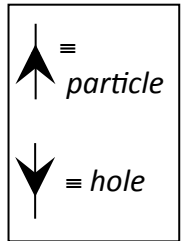


Phys.Rev.C63,
034313 (2001)
Phys.Rev.C65,
064313 (2002)
Phys.Rev.A76,
052503 (2007)

- 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

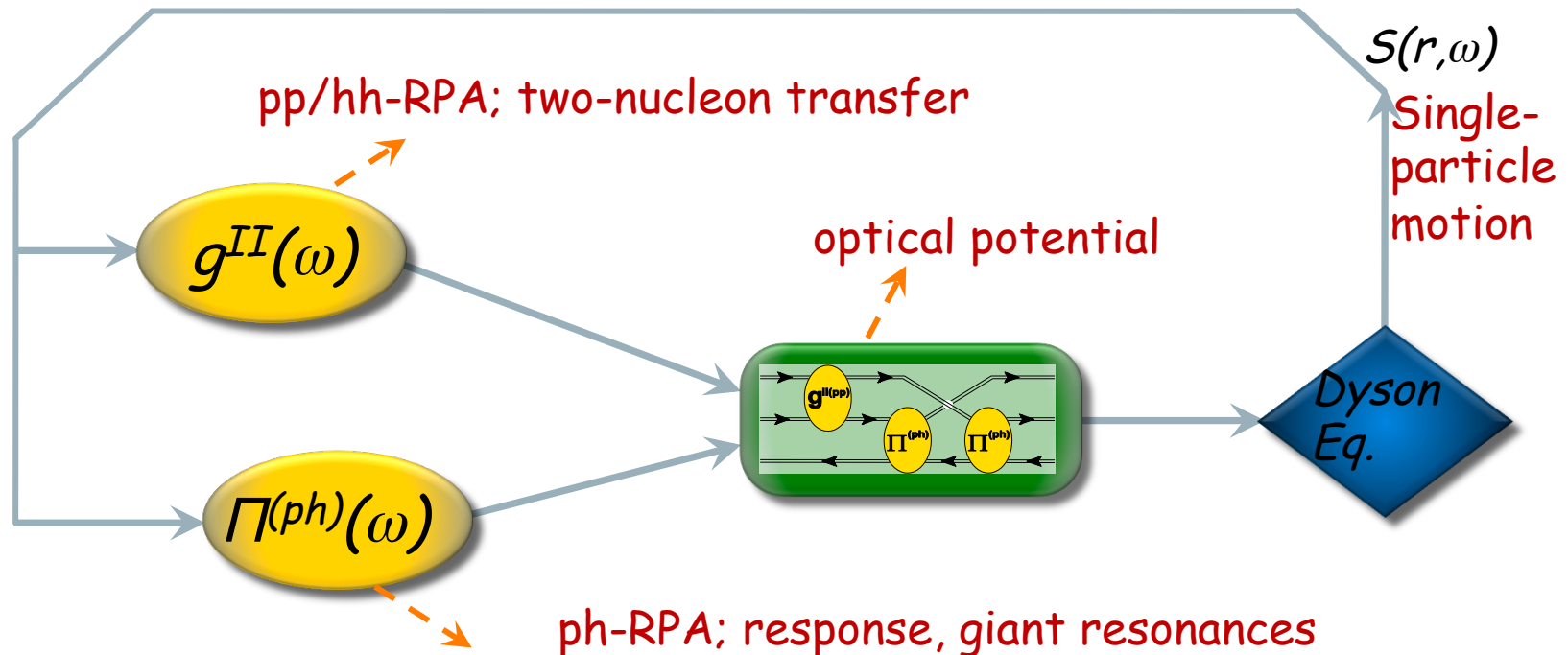
Faddeev-RPA in two words...

Particle vibration coupling is the main cause driving the distribution of particle strength—a least close to the Fermi surface...



Self-Consistent Green's Function Approach

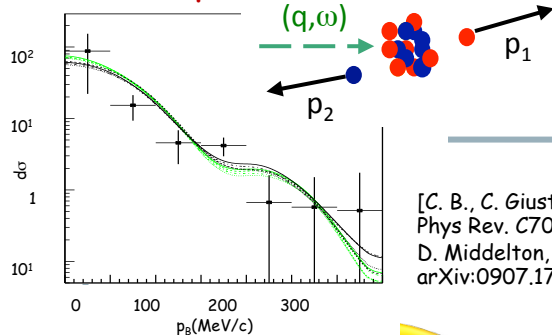
Why self-consistency ???



- Global picture of nuclear dynamics
- Reciprocal correlations among effective modes
- Guaranties *macroscopic conservation laws*

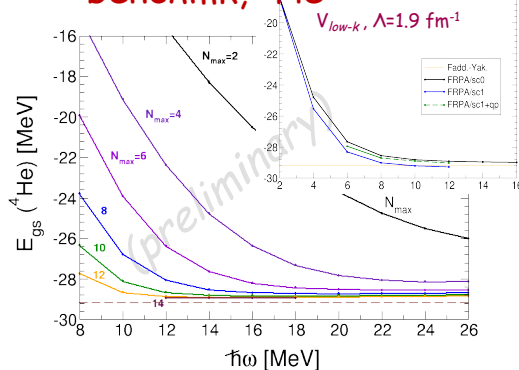
Self-Consistent Green's Function Approach

$^{16}\text{O}(e,e'pn)^{14}\text{N}$ @ MAINZ



[C. B., C. Giusti, et al. Phys Rev. C70, 014606 (2004)
D. Middleton, et al. arXiv:0907.1758; EPJA in print]

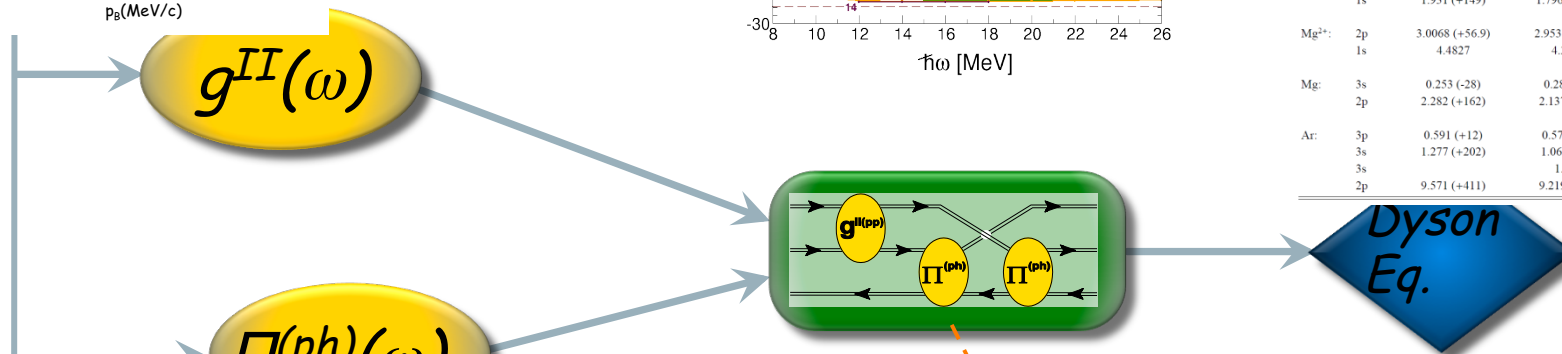
Binding energy benchmk, ^4He [C. B., arXiv:0909.0336]



Ionization energies/affinities, in atoms

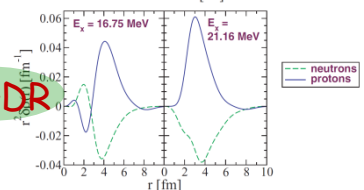
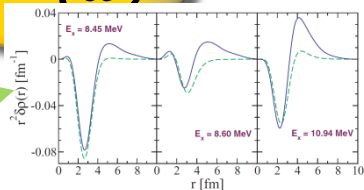
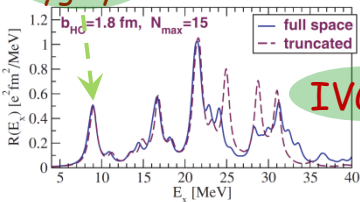
[CB, D. Van Neck, AIP Conf.Proc.1120,104 ('09) & in prep]

	Hartree-Fock	FRPAc	Experiment [16, 17]
He: 1s	0.918 (+14)	0.9008 (-2.9)	0.9037
Be ²⁺ : 1s	5.6672 (+116)	5.6551 (-0.5)	5.6556
Be: 2s	0.3093 (-34)	0.3224 (-20.2)	0.3426
1s	4.733 (+200)	4.5405 (+8)	4.533
Ne: 2p	0.852 (+57)	0.8037 (+11)	0.793
1s	1.931 (+149)	1.7967 (+15)	1.782
Mg ²⁺ : 2p	3.0068 (+56.9)	2.9537 (+3.8)	2.9499
1s	4.4827	4.3589	
Mg: 3s	0.253 (-28)	0.280 (-1)	0.281
2p	2.282 (+162)	2.137 (+17)	2.12
Ar: 3p	0.591 (+12)	0.579 (±0)	0.579
3s	1.277 (+202)	1.065 (-10)	1.075
3s		1.544	
2p	9.571 (+411)	9.219 (+59)	9.160



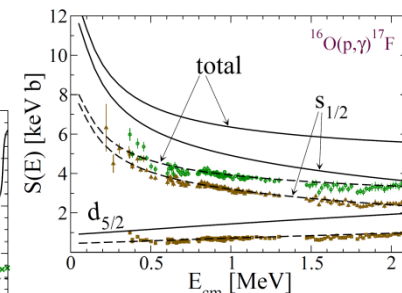
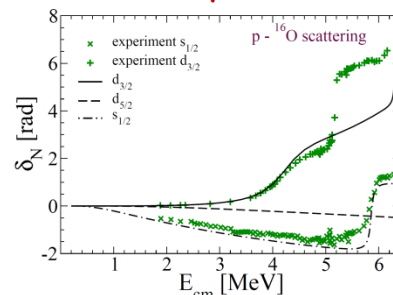
Isovector response for ^{32}Ar , ^{34}Ar

Proton Pygmy



[C. B., K. Langanke, et al., Phys Rev. C77, 024304 (2008)]

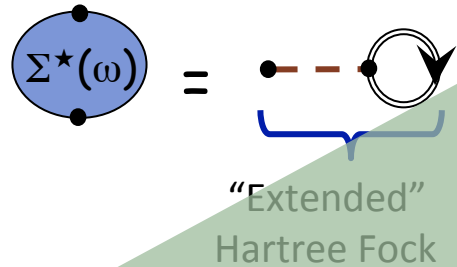
$^{16}\text{O}(p,\gamma)$



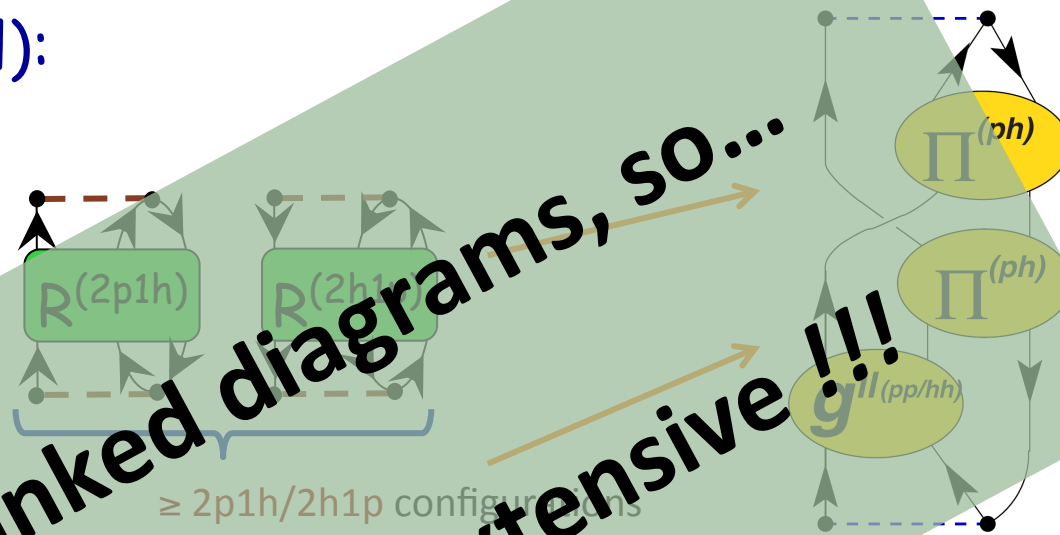
[C. B., B. K. Jennings Nucl. Phys A758, 395c (2005)
Phys Rev. C72, 014613 (2005)]

Faddeev-RPA in two words...

Self-energy
(optical potential):



Faddeev-RPA:



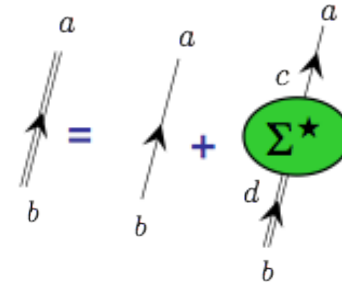
Phys.Rev.C63,
034313 (2001)
Phys.Rev.C65,
064313 (2002)
Phys.Rev.A76,
052503 (2007)

- 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

Dyson equation

* Propagators solves the Dyson equations

$$g_{ab}(\omega) = g_{ab}^0(\omega) + \sum_{cd} g_{ac}^0(\omega) \Sigma_{cd}(\omega) g_{db}(\omega)$$



* (Hole) single particle spectral function

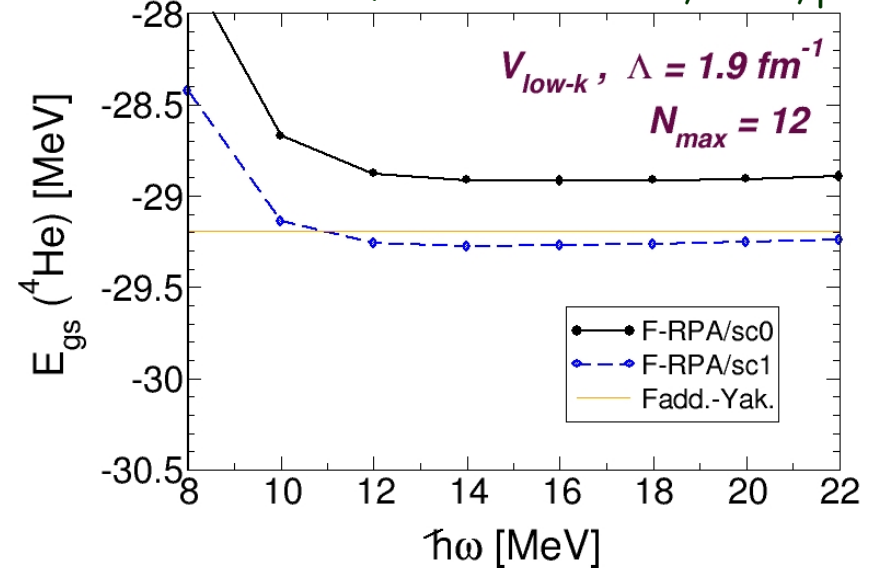
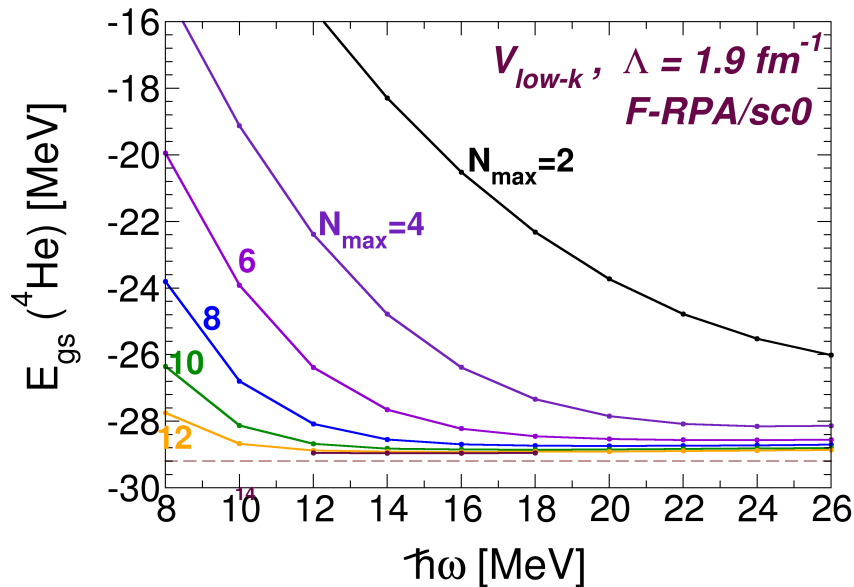
$$S_{ab}^h(\omega) = \frac{1}{\pi} \text{Im} g_{ab}(\omega) = \sum_k \langle \Psi_k^{A-1} | c_b | \Psi_0^A \rangle \langle \Psi_0^A | c_a^\dagger | \Psi_k^{A-1} \rangle \delta(\omega - (E_0^A - E_k^{A-1}))$$

* Koltun sum rule (for 2N interactions):

$$\frac{1}{2} \sum_{ab} \int_{-\infty}^{E_F} (t_{ab} + \delta_{ab}\omega) S_{ab}^h(\omega) d\omega = \langle T \rangle + \langle V^{NN} \rangle$$

Accuracy of FRPA - ^4He binding energy

[C. B., arXiv:0909.0336;
CERN Conf. Proc. -2010-001, Vol. 1, p. 137]



→ Self-consistent FRPA compares well with benchmark calculations on ^4He

	FRPA/sc0	FRPA/sc	Exact:
$V_{\text{low-k}}$:	-29.00(2)	-29.2 ± 0.15	-29.19(5) (Fadd.-Yak.)
			[Nogga et al., Phys. Rev. C70, 061002 (2004)]

self-consistency in the mean field only

estimates from different approx. to self-consistency

Accuracy of FRPA - simple atoms/molecules

binding, eq. bond distances, →
ionization energies (molecules)

98-99% of correlation
energy is recovered

[M. Degroote, D. van Neck, C. B.
Phys. Rev. A 83, 042517 (2011);
85, 012501 (2012)]

		FTDAc	FRPAc	CCSD(T)	FCI	Expt.
H ₂	E_0	-1.161	-1.161	-1.164	-1.164	-1.175
	r_{H-H}	0.757	0.757	0.761		0.741
	I	16.03	16.03	16.12		16.08
BeH ₂	E_0	-15.831	-15.832	-15.835	-15.836	-
	r_{Be-H}	1.337	1.337	1.339		1.340
	I	11.78	11.76	11.89		-
HCl	E_0	-460.256	-460.255	-460.254		-
	r_{H-Cl}	1.297	1.293	1.290		1.275
	I	12.24	12.24	12.26		-
HF	E_0	-100.224	-100.228	-100.228	-100.231	-
	r_{H-F}	0.916	0.913	0.920		0.917
	I	15.70	15.54	15.42		16.12
H ₂ O	E_0	-76.240	-76.236	-76.241		-
	r_{H-O}	0.964	0.962	0.967		0.958
	Λ_{O-H-O}	102	102	102		104
	I	12.15	12.21	11.94		12.61

		Hartree-Fock	Second order	FTDA	FRPA	Experiment [63,64]
He	1s	0.918(+14)	0.9012(-2.5)	0.9025(-1.2)	0.9008(-2.9)	0.9037
Be ²⁺	1s	5.6672(+116)	5.6542(-1.4)	5.6554(-0.2)	5.6551(-0.5)	5.6556
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	1s	4.733(+200)	4.5892(+56)	4.5439(+11)	4.5405(+8)	4.533
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Mg ²⁺	2p	3.0068(+56.9)	2.9217(-28.2)	2.9572(+7.3)	2.9537(+3.8)	2.9499
	2s	4.4827	4.3283	4.3632	4.3589	
Mg	3s	0.253(-28)	0.267(-14)	0.272(-9)	0.280(-1)	0.281
	2p	2.282(+162)	2.117(-3)	2.141(+21)	2.137(+17)	2.12
Ar	3p	0.591(+12)	0.563(-16)	0.581(+2)	0.579(≈ 0)	0.579
	3s	1.277(+202)	1.111(+36)	1.087(+12)	1.065(-10)	1.075
	3s		1.840	1.578	1.544	
σ_{rms} [mH]		81.4	29.3	13.7	10.6	

← ionization
energies (atoms)

Three-nucleon interactions

- Added to self-energy as an effective 1N plus 2N force.
- Correction to Koltun SR

A. Cipollone, P. Navratil, CB
arXiv:1211.3315 [nucl-th]

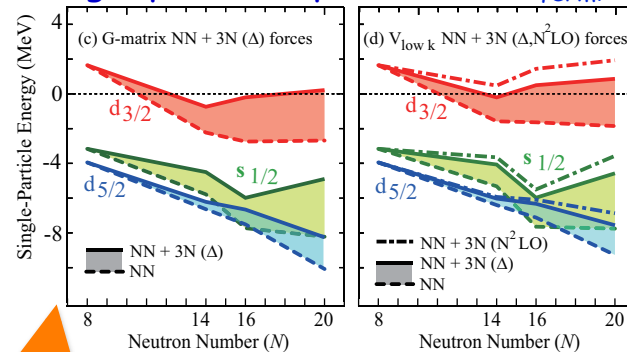
Modern realistic nuclear forces

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 ² LO $\mathcal{O}\left(\frac{Q^3}{\Lambda^3}\right)$			
N ³ LO $\mathcal{O}\left(\frac{Q^4}{\Lambda^4}\right)$			

(3NF arise naturally at N2LO)

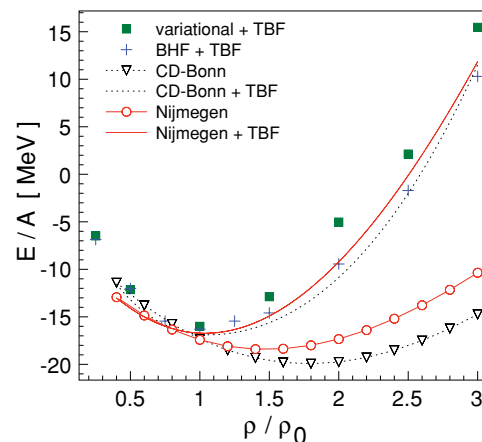
Single particle spectrum at E_{fermi} :



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

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

Saturation of nuclear matter:

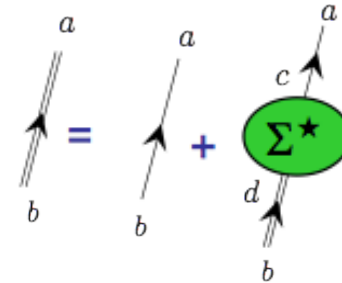


[V. Somà, Phys Rev. C **78**, 054003 (2008)]

Dyson equation

* Propagators solves the Dyson equations

$$g_{ab}(\omega) = g_{ab}^0(\omega) + \sum_{cd} g_{ac}^0(\omega) \Sigma_{cd}(\omega) g_{db}(\omega)$$



* (Hole) single particle spectral function

$$S_{ab}^h(\omega) = \frac{1}{\pi} \text{Im} g_{ab}(\omega) = \sum_k \langle \Psi_k^{A-1} | c_b | \Psi_0^A \rangle \langle \Psi_0^A | c_a^\dagger | \Psi_k^{A-1} \rangle \delta(\omega - (E_0^A - E_k^{A-1}))$$

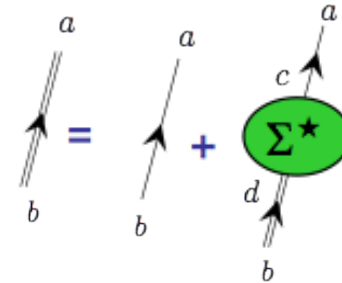
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$$\frac{1}{2} \sum_{ab} \int_{-\infty}^{E_F} (t_{ab} + \delta_{ab}\omega) S_{ab}^h(\omega) d\omega = \langle T \rangle + \langle V^{NN} \rangle$$

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* Koltun sum rule (with NNN interactions):

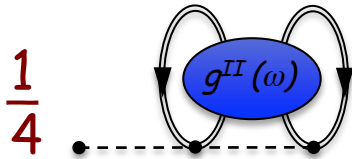
$$\frac{1}{2} \sum_{ab} \int_{-\infty}^{E_F} (t_{ab} + \delta_{ab}\omega) S_{ab}^h(\omega) d\omega = \langle T \rangle + \langle V^{NN} \rangle + \frac{3}{2} \langle V^{NNN} \rangle$$

$$\langle V^{NNN} \rangle \approx \frac{1}{6} \text{Diagram}$$

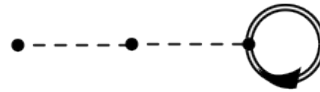
Inclusion of NNN forces

A. Carbone, A. Cipollone, CB, A. Rios, A Polls

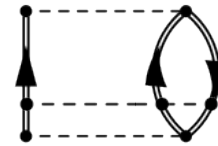
* NNN forces can enter diagrams in three different ways:



Correction to external
1-Body interaction



Correction to
non-contracted
2-Body interaction



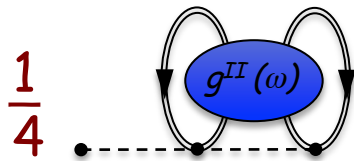
pure 3-Body
contribution

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

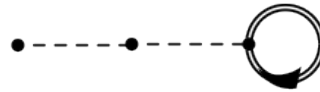
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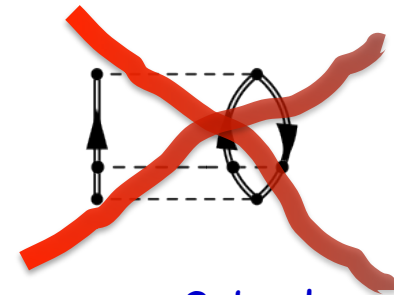
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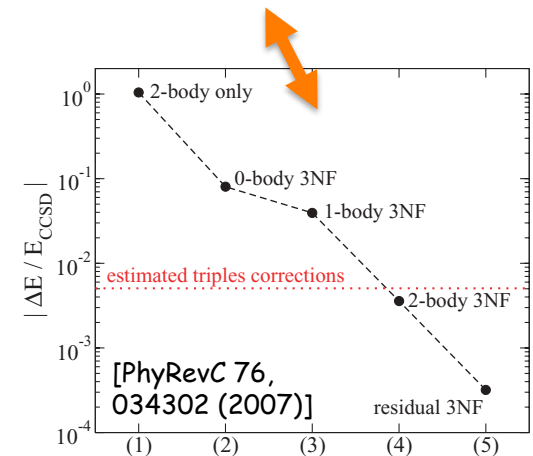


Correction to
non-contracted
2-Body interaction



pure 3-body
contribution (small)

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



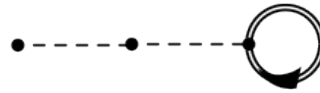
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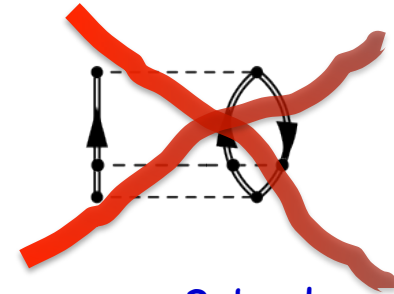
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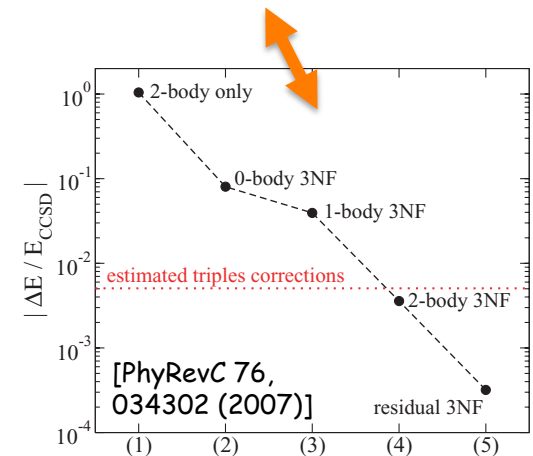


Correction to
non-contracted
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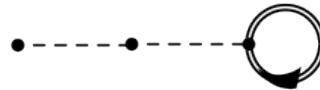
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A. Carbone, A. Cipollone, CB, A. Rios, A Polls

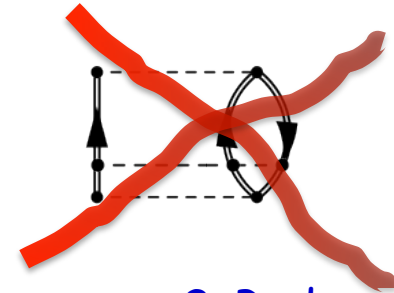
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Correction to external
1-Body interaction

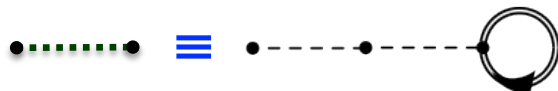


Correction to
non-contracted
2-Body interaction



pure 3-Body
contribution

BEWARE that defining:



and then:



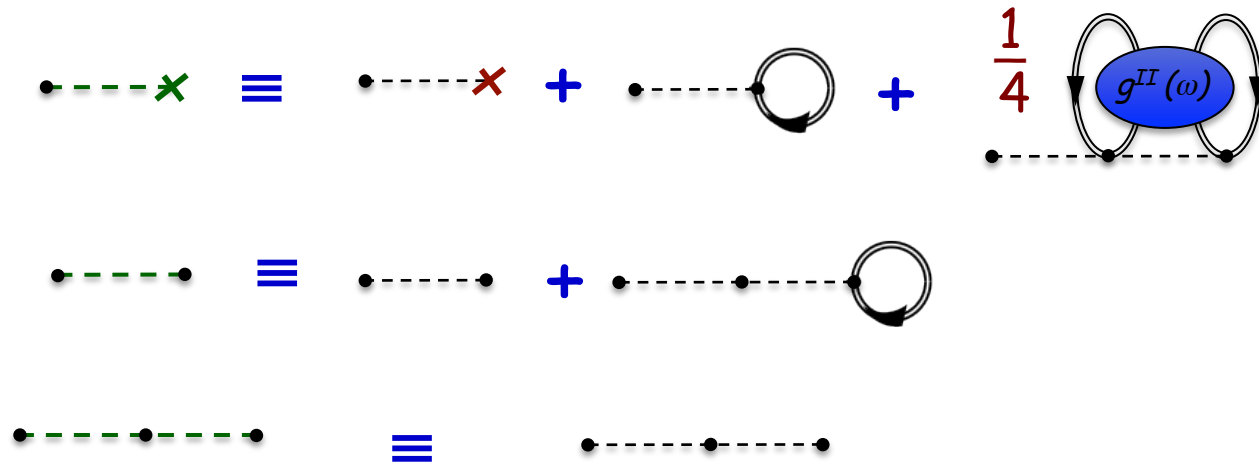
would double count the 1-body term.

Inclusion of NNN forces

A. Carbone, A. Cipollone, CB, A. Rios, A Polls

* NNN forces can enter diagrams in three different ways:

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

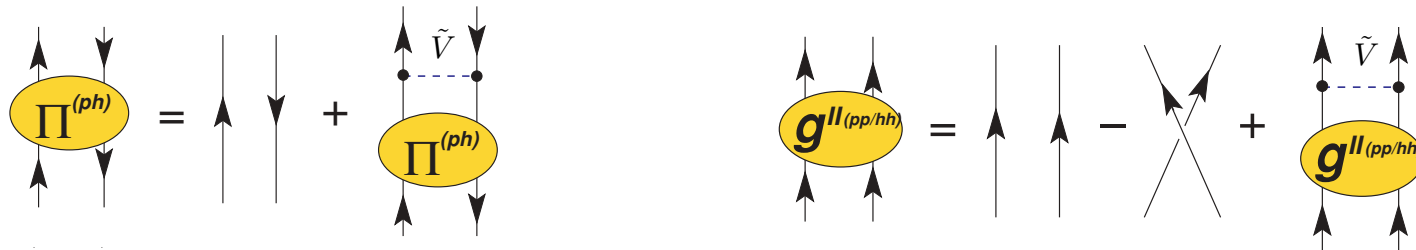


- Contractions are with fully correlated density matrices (BEYOND a normal ordering...)

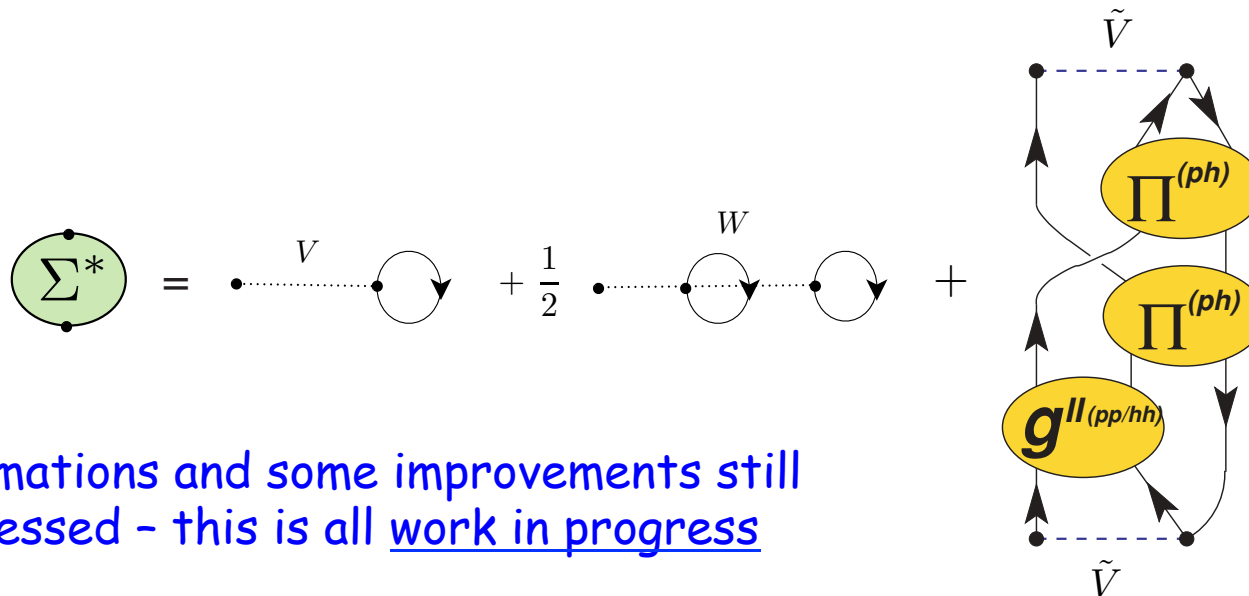
NNN forces in FRPA/FTDA formalism

A. Cipollone, CB, P. Navratil

Use: $\dots \tilde{V} \dots = \dots V \dots + \dots W \dots$ as 2-body potential in all V-irred. RPA/TDA summations



Then:



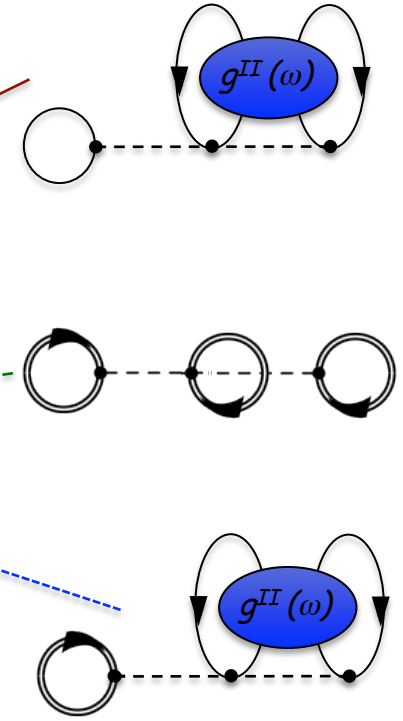
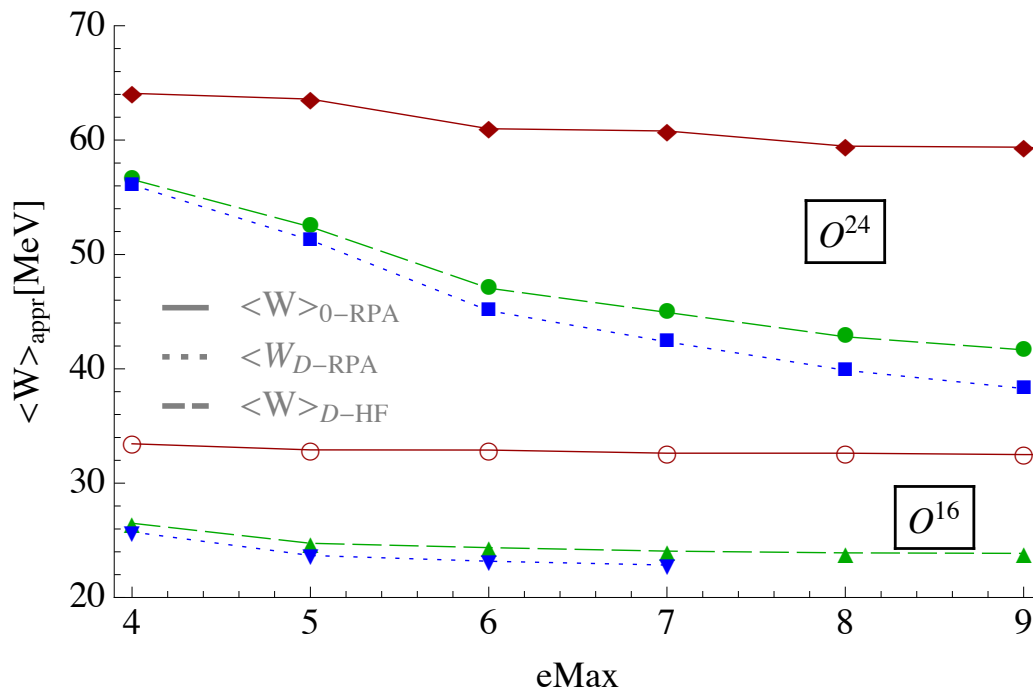
...approximations and some improvements still being assessed - this is all work in progress

NNN forces in FRPA/FTDA formalism

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Koltun sum rule requires a correction on the 3-body potential $\langle W \rangle$:

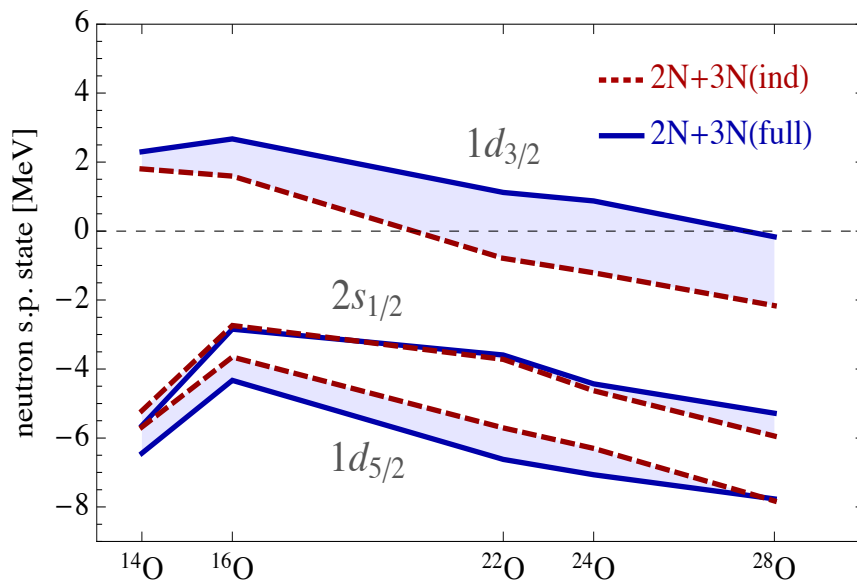
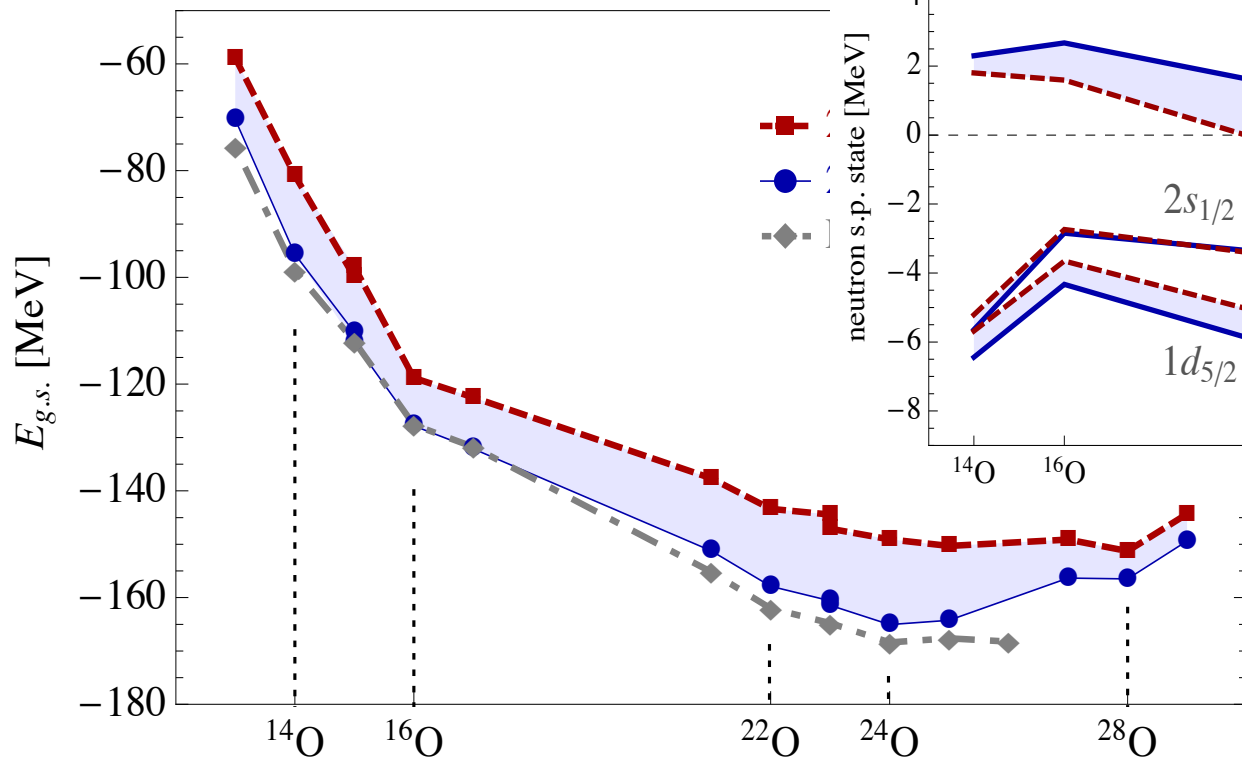
$$\langle H \rangle = \sum_{\alpha\beta} \frac{1}{4\pi i} \int_{C_{\uparrow}} d\omega [T_{\alpha\beta} + \omega \delta_{\alpha\beta}] g_{\alpha\beta}(\omega) - \frac{1}{2} \langle W \rangle$$



Oxygen isotopes with evolved chiral 3NF

A. Cipollone, CB, P. Navratil

Binding energy

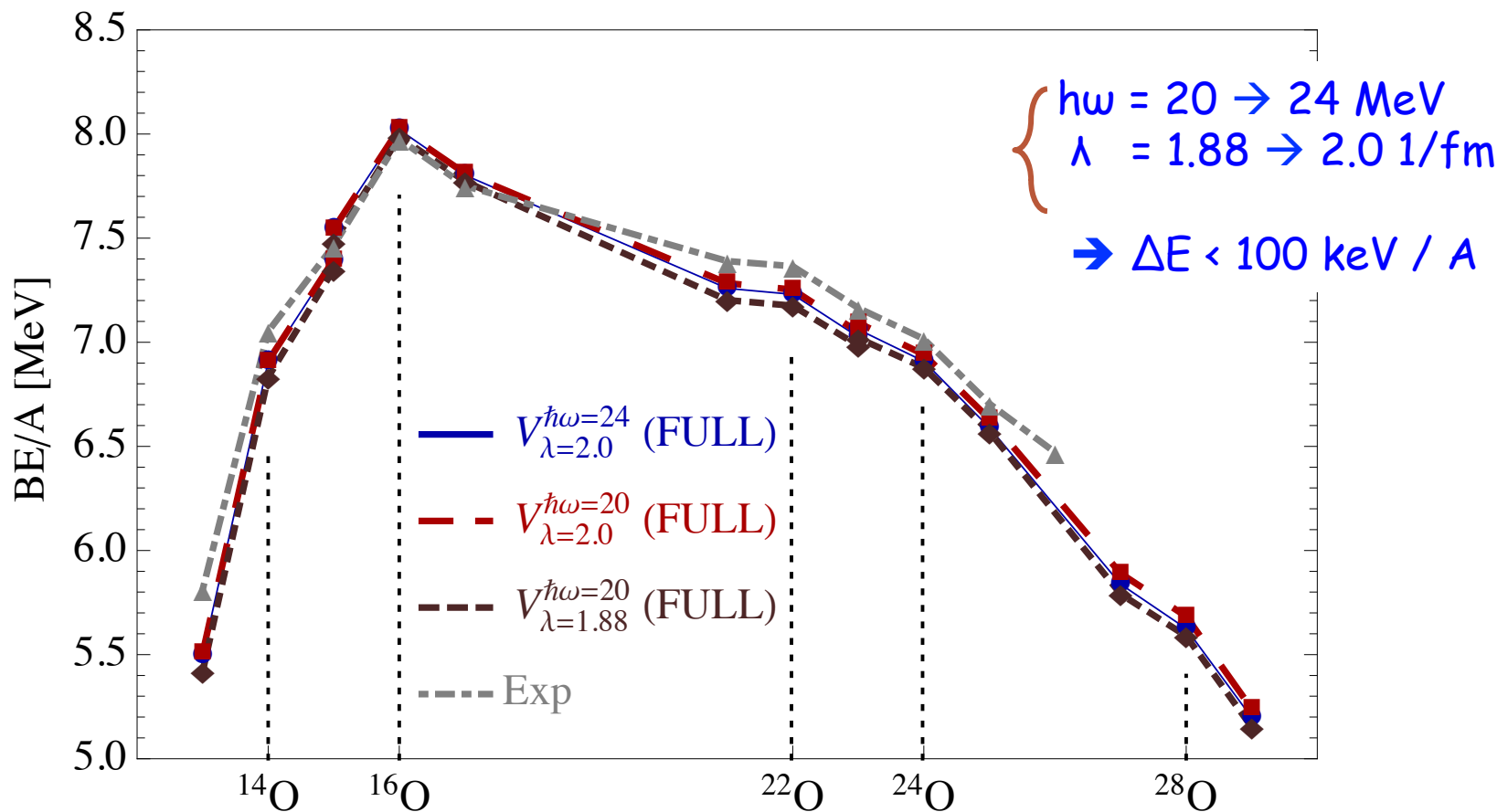


CB, A. Cipollone, *et al.*, arXiv:1211.3315 [nucl-th]

N3LO ($\Lambda = 500\text{MeV}/c$) chiral NN interaction evolved to 2N + 3N forces (1.8fm^{-1})
N2LO ($\Lambda = 400\text{MeV}/c$) chiral 3N interaction evolved (1.8fm^{-1})

Oxygen isotopes with evolved chiral 3NF

A. Cipollone, CB, P. Navratil



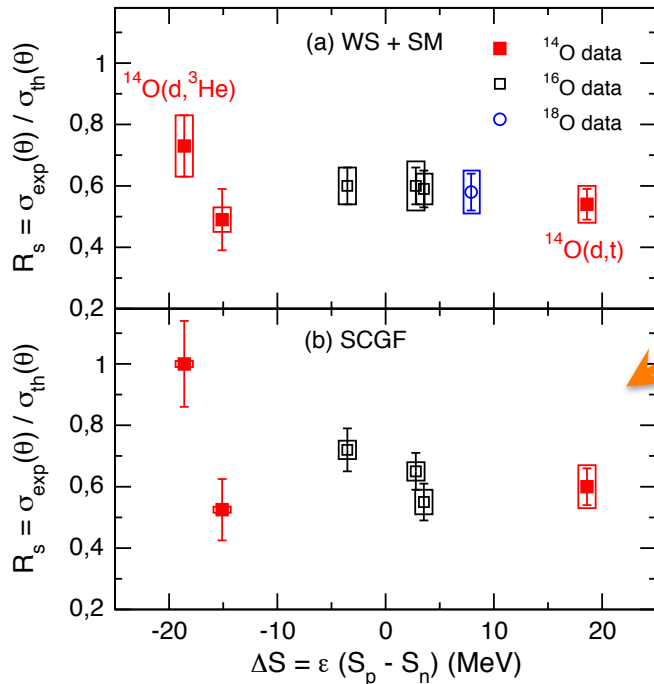
N3LO ($\Lambda = 500$ MeV/c) chiral NN interaction evolved to 2N + 3N forces
N2LO ($\Lambda = 400$ MeV/c) chiral 3N interaction evolved

Overlap functions and spect. factors in ^{14}O

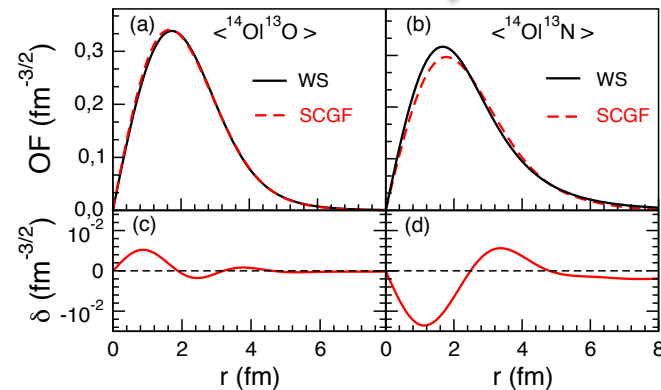
radii still too small !

TABLE 1. Predicted matter radii (in fm) for ^{16}O from SRG evolved 2N-only interactions and by including induced and full 3NF. Experiment are charge radii.

	2NF only	2+3NF(ind.)	2+3NF(full)	Experiment
^{16}O :	2.10	2.41	2.38	2.718 ± 0.210 [19]



After rescaling, the shape and results are the same as for phenomenological Woods-Saxon



F. Flavingny et al, CB, Phys. Rev. Lett. (2013)--in print

N3LO ($\Lambda = 500\text{MeV}/c$) chiral NN interaction evolved to 2N + 3N forces
 N2LO ($\Lambda = 400\text{MeV}/c$) chiral 3N interaction evolved

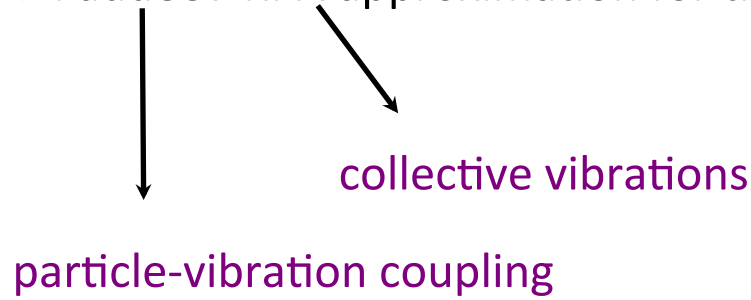
Approaching open-shells in the mid-mass region:

- Gorkov theory
- proof-of-principle results
at 2nd order

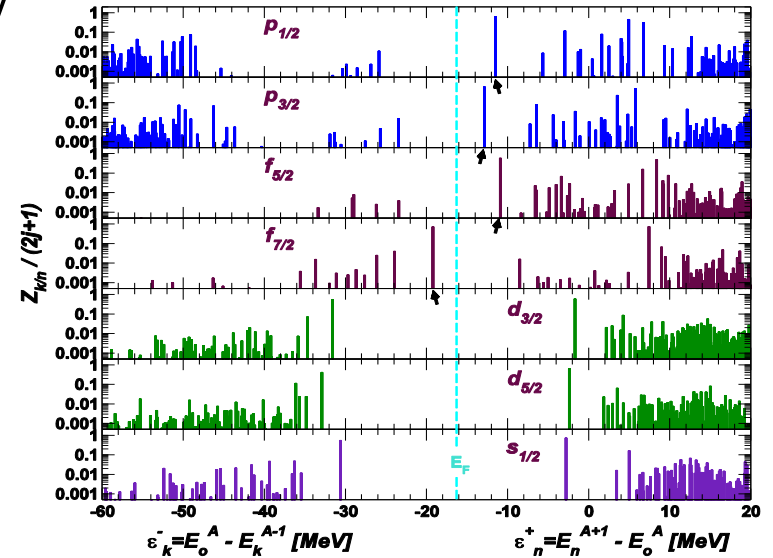
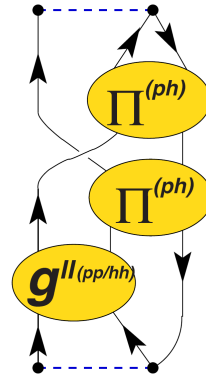
V. Somà, T. Duguet, CB, Phys. Rev. C84, 046317 (2011)
arXiv:1208.2472 [nucl-th]

Applications to doubly-magic nuclei

✱ Faddeev-RPA approximation for the self-energy



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



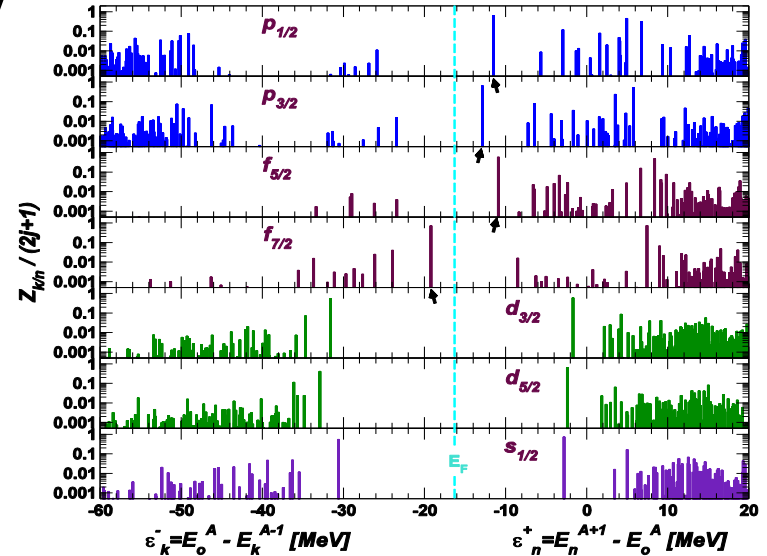
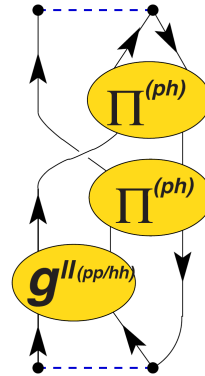
✱ Successful in medium-mass doubly-magic systems

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]



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

Gorkov equations

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

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

1st & 2nd order diagrams

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

✱ 1st order \Rightarrow energy-independent self-energy

$$\Sigma_{ab}^{11(1)} = \text{diagram with vertices } a, b, c, d \text{ and a loop with frequency } \omega'$$

$$\Sigma_{ab}^{12(1)} = \text{diagram with vertices } a, c, b, d \text{ and a loop with frequency } \omega'$$

✱ 2nd 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 \longrightarrow eigenvalue problem

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

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

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

unretarded ones, i.e.,

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

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

propagator one obtains

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

V. SOMÀ, T. DUGUET, AND C. BARBIERI

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

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

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

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

one obtains

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

where the block-diagonal normal density matrix is introduced through

$$\rho_{n_1 n_2}^{[a]} = \sum_{n_3} \mathcal{V}_{n_1 n_2}^{n_3}$$

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 $\Sigma^{22(1)}$

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

Let us consider the anomalous contributions to the first-order self-energies

$$\begin{aligned} \Sigma_{ab}^{21(1)} &= \frac{1}{2} \sum_{cd,k} \tilde{V}_{abcd} \tilde{V}_d^* \tilde{U}_c^* \\ &= -\frac{1}{2} \sum_{n_1, n_2, n_3} \sum_{\gamma} \sum_{JM} \sum_{M'} f_{n_1 n_2 n_3}^{n_1 n_2 n_4} \eta_a \eta_b C_{JM}^{JM'} \\ &= -\frac{1}{2} \sum_{n_1, n_2, n_3} \sum_{\gamma} \sum_{JM} f_{n_1 n_2 n_3}^{n_1 n_2 n_4} \eta_a \eta_b C_{JM}^{JM} \\ &= -\frac{1}{2} \sum_{n_1, n_2} \sum_{\gamma} f_{n_1 n_2}^{n_1 n_2 n_3} \eta_a \eta_b (-1)^{J_1} C_{JM}^{00} \\ &= \delta_{a\beta} \delta_{m_1 m_2} \frac{1}{2} \sum_{n_1, n_2} \sum_{\gamma} f_{n_1 n_2}^{n_1 n_2 n_3} \pi_a \pi_b (-1)^{J_1} \\ &= \delta_{a\beta} \delta_{m_1 m_2} \Sigma_{n_1 n_2}^{21(a)(1)} \\ &= \delta_{a\beta} \delta_{m_1 m_2} \tilde{K}_{n_1 n_2}^{[a]} \end{aligned}$$

where the block-diagonal anomalous density matrix is introduced through

$$\tilde{K}_{n_1 n_2}^{[a]} = \sum_{n_3} \tilde{U}_{n_1 n_2}^{n_3}$$

Block-diagonal forms of second-order angular momentum couplings of the three \mathcal{Q} , \mathcal{R} , and \mathcal{S} . One proceeds first coupling give J_{tot} . The recoupled \mathcal{M} term is computed

$$\begin{aligned} \mathcal{M}_{a(J_1 J_2)}^{b(k_1 k_2)} &= \sum_{m_1, m_2, m_3, M} C_{J_1 M_1}^{J_1 M_2} C_{J_2 M_2}^{J_2 M_3} C_{J_3 M_3}^{J_3 M} \\ &= \sum_{m_1, m_2, M} \sum_{J_1, J_2} C_{J_1 M_1}^{J_1 M_2} C_{J_2 M_2}^{J_2 M_3} C_{J_3 M_3}^{J_3 M} \\ &= \sum_{m_1, m_2, M} \sum_{J_1, J_2} \delta_{k_1 k_2} \delta_{m_1 m_2} \\ &\quad \times C_{J_1 M_1}^{J_1 M_2} C_{J_2 M_2}^{J_2 M_3} C_{J_3 M_3}^{J_3 M} \\ &= \sum_{m_1, m_2, M} \sum_{J_1, J_2} \eta_k f_{J_1 J_2}^{m_1 m_2 n_3} \\ &= \sum_{m_1, m_2, M} \sum_{J_1, J_2} \eta_k f_{J_1 J_2}^{m_1 m_2 n_3} \\ &= \delta_{J_1 J_2} \delta_{M_1 M_2} \sum_{n_1, n_2} \pi_k \\ &\quad \times \tilde{V}_{J_1 J_2}^{n_1 n_2 n_3} \tilde{U}_{n_1 n_2}^{n_3} \tilde{V}_{k_1 k_2}^{n_1 n_2} \\ &= \delta_{J_1 J_2} \delta_{M_1 M_2} \mathcal{R}_{n_1 n_2}^{n_3} \\ &= \delta_{J_1 J_2} \delta_{M_1 M_2} \mathcal{Q}_{n_1 n_2}^{n_3} \end{aligned}$$

where general properties of Clebsch-Gordan

$$\begin{aligned} \Lambda_{a(J_1 J_2)}^{b(k_1 k_2)} &= \delta_{J_1 J_2} \delta_{M_1 M_2} \sum_{n_1, n_2} \\ &= \delta_{J_1 J_2} \delta_{M_1 M_2} \mathcal{N}_{n_1 n_2} \end{aligned}$$

One can show that the same result is obtained

$$\begin{aligned} \mathcal{N}_{a(J_1 J_2)}^{b(k_1 k_2)} &= \sum_{m_1, m_2, M} C_{J_1 M_1}^{J_1 M_2} C_{J_2 M_2}^{J_2 M_3} C_{J_3 M_3}^{J_3 M} \\ &= \sum_{m_1, m_2, M} \sum_{J_1, J_2} C_{J_1 M_1}^{J_1 M_2} C_{J_2 M_2}^{J_2 M_3} C_{J_3 M_3}^{J_3 M} \\ &= \sum_{m_1, m_2, M} \sum_{J_1, J_2} \delta_{k_1 k_2} \delta_{m_1 m_2} \delta_{J_1 J_2} \delta_{M_1 M_2} \sum_{n_1, n_2} \pi_k \\ &\quad \times \tilde{V}_{J_1 J_2}^{n_1 n_2 n_3} \tilde{U}_{n_1 n_2}^{n_3} \tilde{V}_{k_1 k_2}^{n_1 n_2} \\ &= \delta_{J_1 J_2} \delta_{M_1 M_2} \mathcal{R}_{n_1 n_2}^{n_3} \\ &= \delta_{J_1 J_2} \delta_{M_1 M_2} \mathcal{Q}_{n_1 n_2}^{n_3} \end{aligned}$$

Expressions for 1st & 2nd order diagrams

Proceeding similarly for ... and defining

$$= \delta_{a\beta} \delta_{m_1 m_2} \frac{1}{2} \sum_{n_1, n_2, n_3} \sum_{\gamma} \left\{ \frac{\mathcal{M}_{n_1 n_2 n_3}^{n_1 n_2 n_4}}{\omega - (\omega_1 + \omega_2 + \omega_3) + i\eta} + \frac{\mathcal{M}_{n_1 n_2 n_3}^{n_1 n_2 n_4}}{\omega + (\omega_1 + \omega_2 + \omega_3) - i\eta} \right\} \quad (C42)$$

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

$$\mathcal{D}_{n_1 n_2 n_3}^{n_1 n_2 n_4} \equiv \frac{1}{\sqrt{6}} [\mathcal{M}_{n_1 n_2 n_3}^{n_1 n_2 n_4} + \mathcal{P}_{n_1 n_2 n_3}^{n_1 n_2 n_4} - \mathcal{R}_{n_1 n_2 n_3}^{n_1 n_2 n_4}] \quad (C43b)$$

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

$$\Sigma_{n_1 n_2}^{11(a)(2)} = \sum_{n_3, n_4} \sum_{\gamma} \sum_{JM} \left\{ \frac{C_{n_1 n_2 n_3}^{n_1 n_2 n_4}}{\omega - (\omega_1 + \omega_2 + \omega_3) + i\eta} + \frac{\mathcal{D}_{n_1 n_2 n_3}^{n_1 n_2 n_4}}{\omega + (\omega_1 + \omega_2 + \omega_3) - i\eta} \right\} \quad (C44a)$$

$$\Sigma_{n_1 n_2}^{12(a)(2)} = \sum_{n_3, n_4} \sum_{\gamma} \sum_{JM} \left\{ \frac{C_{n_1 n_2 n_3}^{n_1 n_2 n_4}}{\omega - (\omega_1 + \omega_2 + \omega_3) + i\eta} + \frac{\mathcal{D}_{n_1 n_2 n_3}^{n_1 n_2 n_4}}{\omega + (\omega_1 + \omega_2 + \omega_3) - i\eta} \right\} \quad (C44b)$$

$$\Sigma_{n_1 n_2}^{21(a)(2)} = \sum_{n_3, n_4} \sum_{\gamma} \sum_{JM} \left\{ \frac{\mathcal{R}_{n_1 n_2 n_3}^{n_1 n_2 n_4}}{\omega - (\omega_1 + \omega_2 + \omega_3) + i\eta} + \frac{\mathcal{D}_{n_1 n_2 n_3}^{n_1 n_2 n_4}}{\omega + (\omega_1 + \omega_2 + \omega_3) - i\eta} \right\} \quad (C44c)$$

$$\Sigma_{n_1 n_2}^{22(a)(2)} = \sum_{n_3, n_4} \sum_{\gamma} \sum_{JM} \left\{ \frac{\mathcal{R}_{n_1 n_2 n_3}^{n_1 n_2 n_4}}{\omega - (\omega_1 + \omega_2 + \omega_3) + i\eta} + \frac{\mathcal{D}_{n_1 n_2 n_3}^{n_1 n_2 n_4}}{\omega + (\omega_1 + \omega_2 + \omega_3) - i\eta} \right\} \quad (C44d)$$

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

$$T_{ab} - \mu \delta_{ab} \equiv \delta_{J_1 J_2} \delta_{M_1 M_2} [T_{n_1 n_2}^{[a]} - \mu \delta_{n_1 n_2}^{[a]}], \quad (C45)$$

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

$$\mathcal{W}_{k(J_1 J_2)}^{k_1 k_2} \equiv \delta_{J_1 J_2} \delta_{M_1 M_2} \mathcal{W}_{n_1 n_2}^{n_3 n_4}, \quad (C46a)$$

$$\mathcal{Z}_{k(J_1 J_2)}^{k_1 k_2} \equiv -\delta_{J_1 J_2} \delta_{M_1 M_2} \eta_k \mathcal{Z}_{n_1 n_2}^{n_3 n_4}, \quad (C46b)$$

with

$$(\omega_k - E_{k_1 k_2}) \mathcal{W}_{n_1 n_2}^{n_3 n_4} \equiv \sum_{n_5} [(T_{n_1 n_2}^{[a]} - \mu \delta_{n_1 n_2}^{[a]})^* U_{n_5}^{[a]} + (\mathcal{D}_{n_1 n_2}^{n_3 n_4})^* V_{n_5}^{[a]}], \quad (C47a)$$

$$(\omega_k + E_{k_1 k_2}) \mathcal{Z}_{n_1 n_2}^{n_3 n_4} \equiv \sum_{n_5} [\mathcal{R}_{n_1 n_2}^{n_3 n_4} U_{n_5}^{[a]} + C_{n_1 n_2}^{n_3 n_4} V_{n_5}^{[a]}], \quad (C47b)$$

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

$$\begin{aligned} \omega_k U_{n_1 n_2}^{[a]} &= \sum_{n_3} [(T_{n_1 n_2}^{[a]} - \mu \delta_{n_1 n_2}^{[a]}) U_{n_3}^{[a]} + A_{n_1 n_2}^{[a]} U_{n_3}^{[a]} + \tilde{K}_{n_1 n_2}^{[a]} U_{n_3}^{[a]}] \\ &\quad + \sum_{n_3, n_4} \sum_{\gamma} [C_{n_1 n_2}^{n_3 n_4} \mathcal{W}_{n_3 n_4}^{n_5 n_6} + (\mathcal{D}_{n_1 n_2}^{n_3 n_4})^* \mathcal{Z}_{n_3 n_4}^{n_5 n_6}], \end{aligned} \quad (C48a)$$

$$\begin{aligned} \omega_k V_{n_1 n_2}^{[a]} &= \sum_{n_3} [- (T_{n_1 n_2}^{[a]} - \mu \delta_{n_1 n_2}^{[a]}) V_{n_3}^{[a]} + A_{n_1 n_2}^{[a]} V_{n_3}^{[a]} + \tilde{K}_{n_1 n_2}^{[a]} V_{n_3}^{[a]}] \\ &\quad + \sum_{n_3, n_4} \sum_{\gamma} [\mathcal{D}_{n_1 n_2}^{n_3 n_4} \mathcal{W}_{n_3 n_4}^{n_5 n_6} + (C_{n_1 n_2}^{n_3 n_4})^* \mathcal{Z}_{n_3 n_4}^{n_5 n_6}]. \end{aligned} \quad (C48b)$$

064317-30

These terms are finally put together to form the different contributions to second-order self-energies. Let us consider Σ_{ab}^{11} as an example (see Eq. (75)). By inserting Eqs. (C35) and (C36) and summing over all possible total and intermediate angular momenta, one has

$$\Sigma_{ab}^{11(2)} = \frac{1}{2} \sum_{m_1, m_2, k_1, k_2} \left\{ \frac{\mathcal{M}_{a(J_1 J_2)}^{b(k_1 k_2)} (\mathcal{M}_{b(J_1 J_2)}^{a(k_1 k_2)})^*}{\omega - (\omega_1 + \omega_2 + \omega_3) + i\eta} + \frac{\mathcal{M}_{a(J_1 J_2)}^{b(k_1 k_2)} (\mathcal{M}_{b(J_1 J_2)}^{a(k_1 k_2)})^*}{\omega + (\omega_1 + \omega_2 + \omega_3) - i\eta} \right\}$$

064317-29



$$\begin{aligned} & \frac{1}{2} \sum_{cdefgh} G_{cd}^{11(a)}(a'') G_{ef}^{11(b)}(a' - \omega) \\ & - \frac{1}{2} \sum_{cdefghk_1 k_2} \tilde{V}_{cfae} \tilde{V}_{ghdb} \left\{ \frac{V_c^{\omega} U_c^{a'} U_c^{b'} \tilde{V}_d^{a''} U_d^{b''} \tilde{V}_e^{a''} U_e^{b''} \tilde{V}_f^{a''} U_f^{b''}}{\omega - (\omega_1 + \omega_2 + \omega_3) + i\eta} + \frac{\tilde{U}_c^{a'} \tilde{V}_d^{a''} \tilde{V}_e^{a''} \tilde{U}_f^{b''} \tilde{V}_g^{a''} U_g^{b''}}{\omega + (\omega_1 + \omega_2 + \omega_3) - i\eta} \right\}. \end{aligned} \quad (B32)$$

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

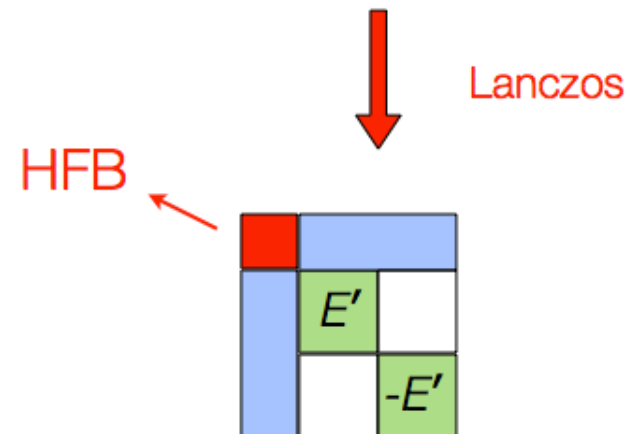
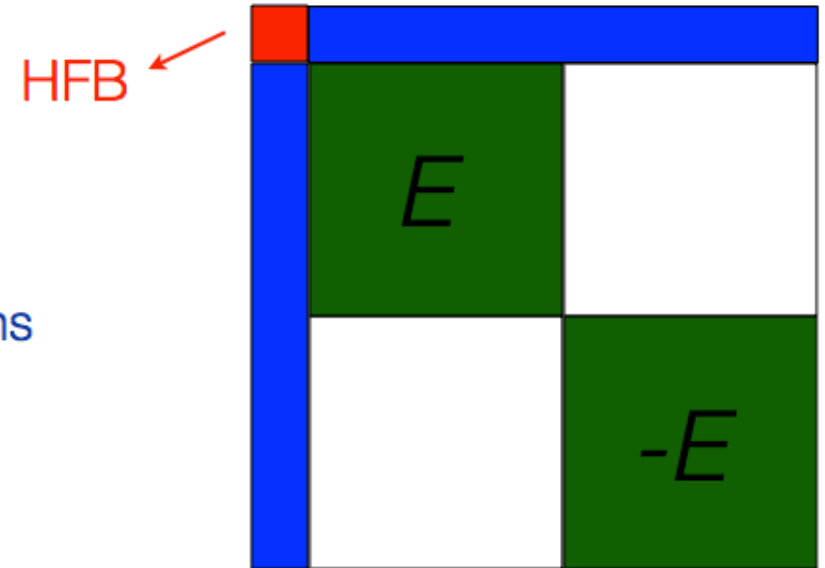
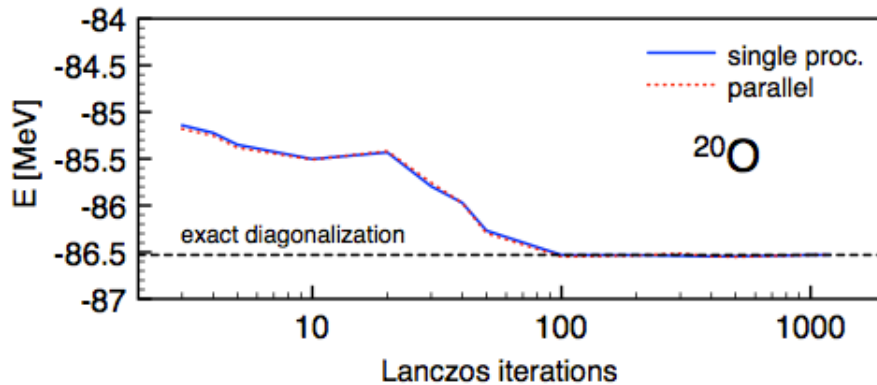
$$\sum_a \left[|\mathcal{U}_a^k|^2 + |\mathcal{V}_a^k|^2 \right] + \sum_{k_1 k_2 k_3} \left[|\mathcal{W}_k^{k_1 k_2 k_3}|^2 + |\mathcal{Z}_k^{k_1 k_2 k_3}|^2 \right] = 1$$

Lanczos reduction of self-energy

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

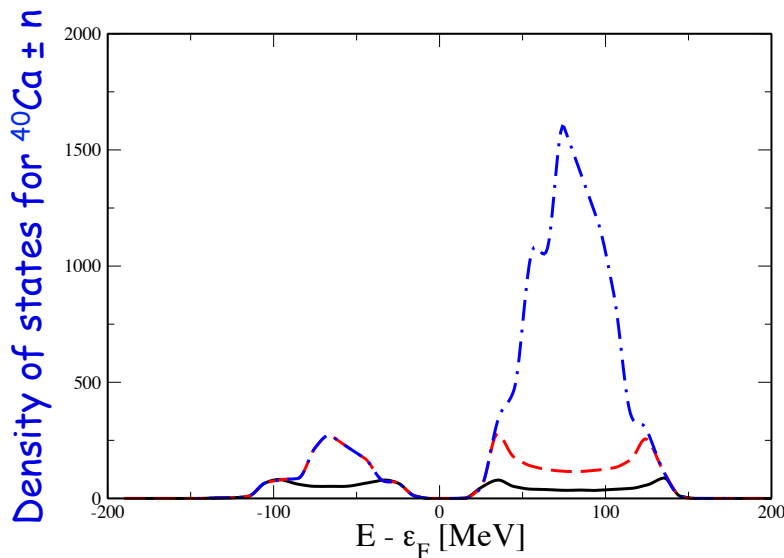
→ Conserves moments of spectral functions

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

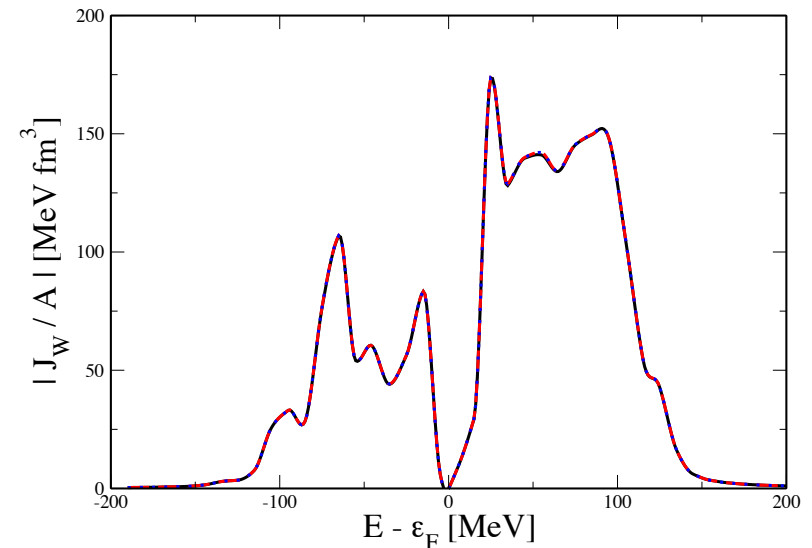


Application of Lanczos (example)

→ # of poles of the self-energy (= optical potential) are reduced without altering spectroscopic strength.



Volume integral of $^{40}\text{Ca} \pm n$
optical potential in $f_{7/2}$ part. wave



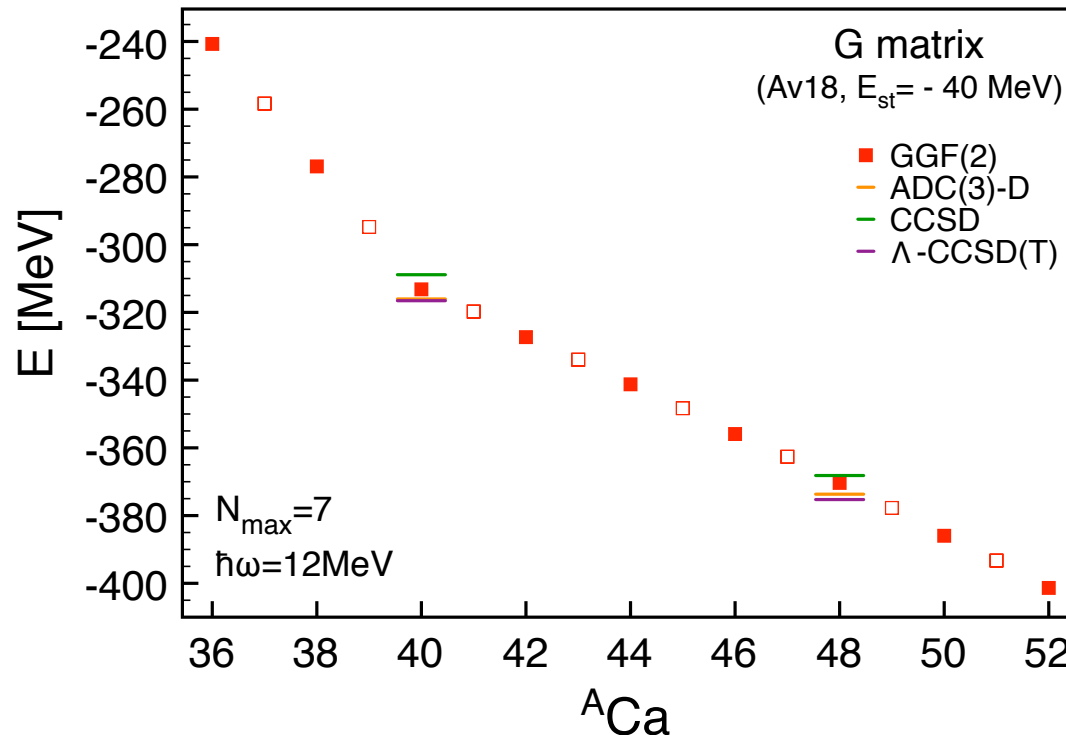
— 200 vectors
- - - 600 vectors
- . - . 8,837 vectors (full basis)

→ Ground state energies converge with ≥ 200 Lanczos vectors (10 osc. shells).

Binding energies

Somà, CB, Duguet, arXiv:1208.2472

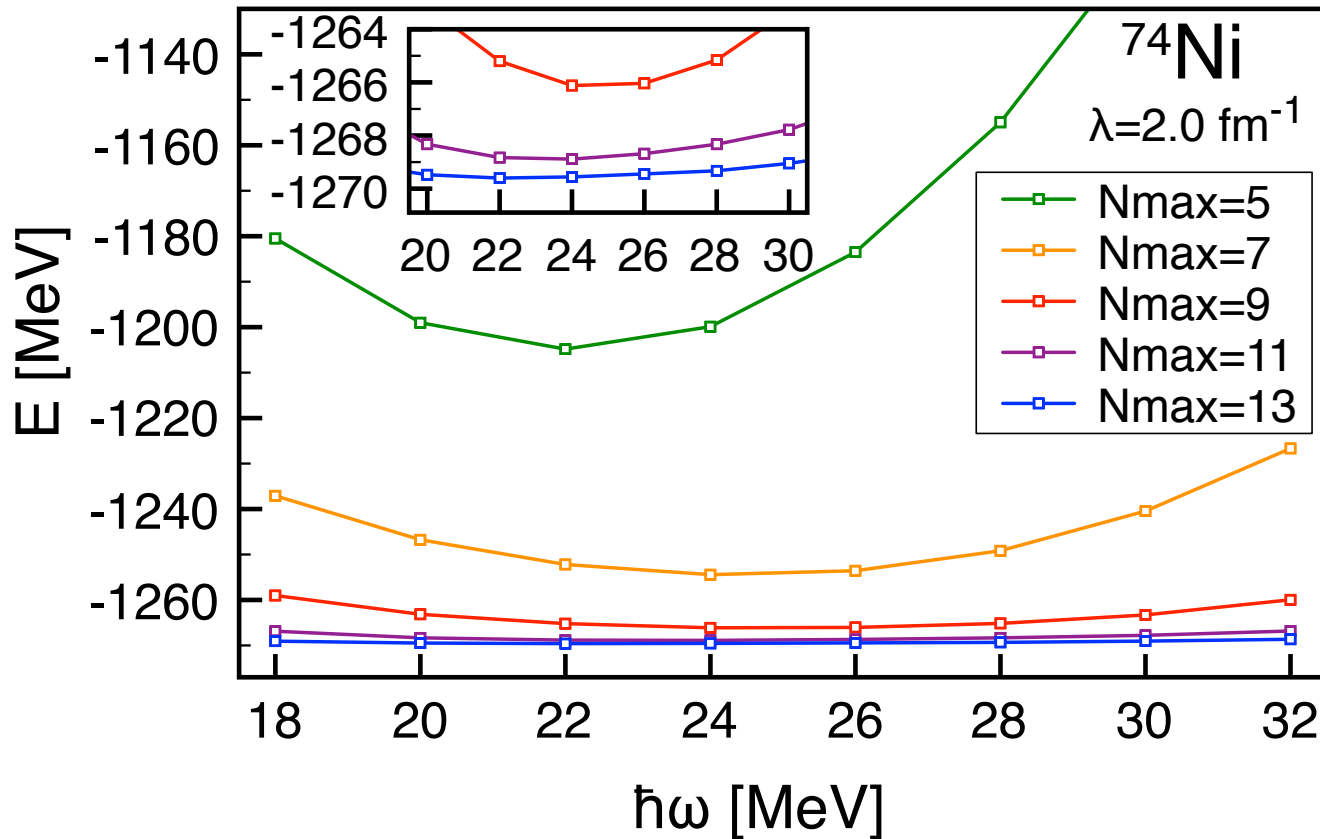
- * Systematic along isotopic/isotonic chains has become available



- 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...

Binding energies

Somà, CB, Duguet, arXiv:1208.2472



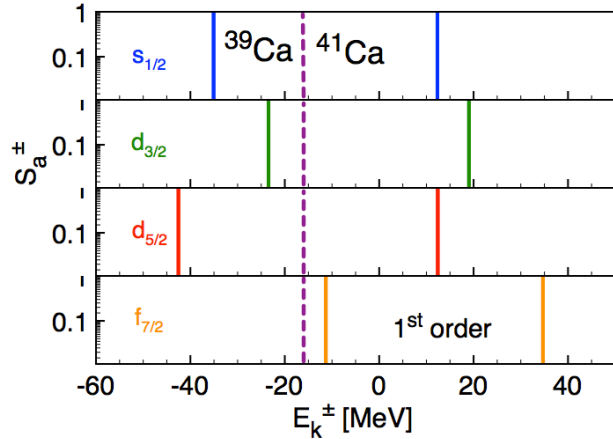
✳ Systematic along isotopic/isotonic chains has become possible

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

➡ Effect of self-consistency is relevant; i.e. less bound than MBPT2

Spectral distribution

Dyson 1st order (HF)

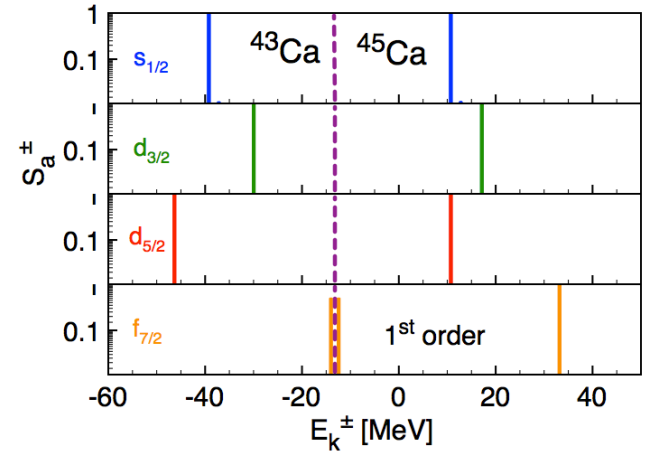


Fragmentation

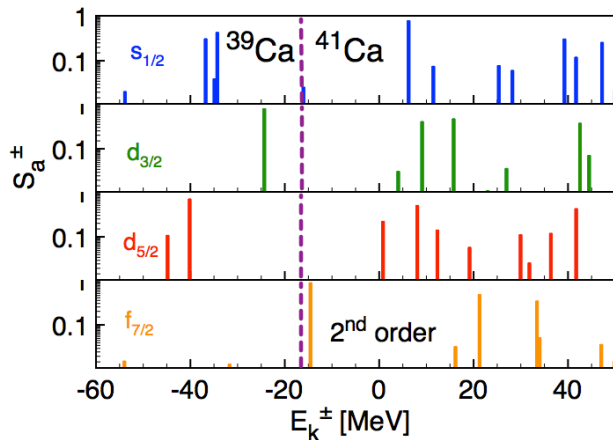
Static pairing



Gorkov 1st order (HFB)



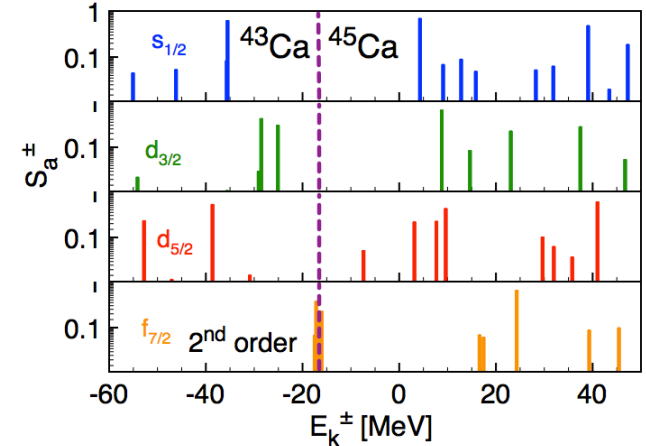
Dyson 2nd order



Dynamical fluctuations

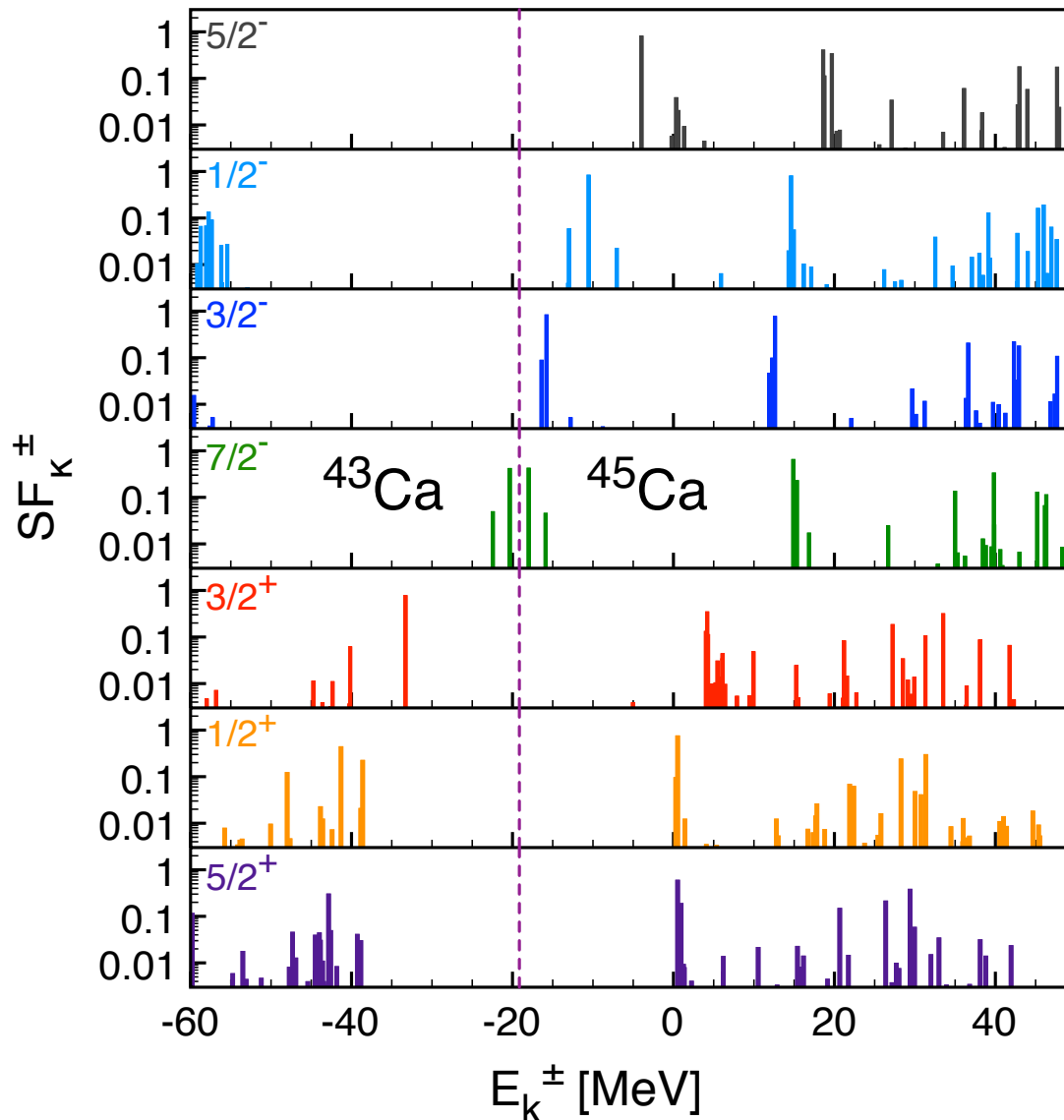


Gorkov 2nd order



Spectral distribution

Somà, CB, Duguet, arXiv:1208.2472



→ Gorkov-GF at 2nd order [or ADC(2)]

Evolved chiral 3NF and the Ca isotopes

A. Cipollone, CB, V.Somà, P. Navratil

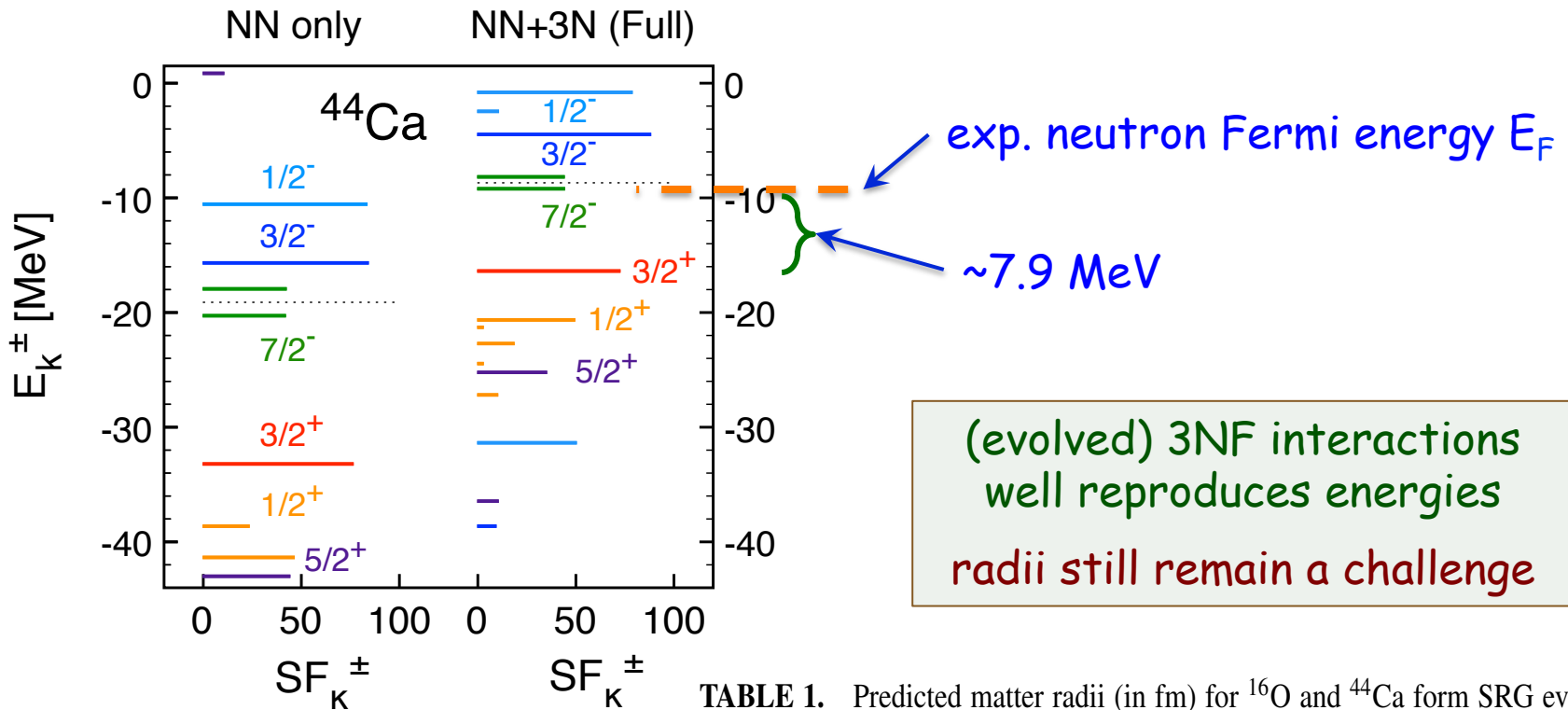


TABLE 1. Predicted matter radii (in fm) for ^{16}O and ^{44}Ca from SRG evolved 2N-only interactions and by including induced and full 3NF. Experiment are charge radii.

	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]

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

Collaborators



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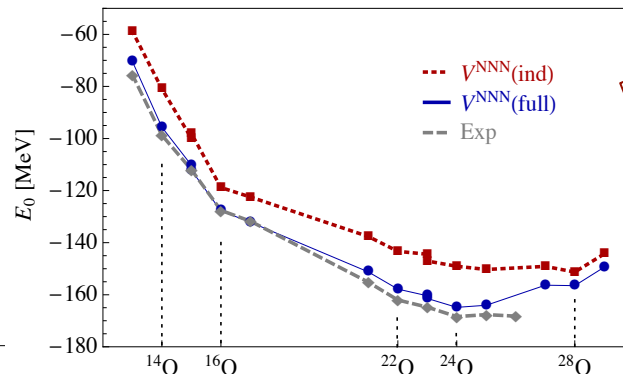
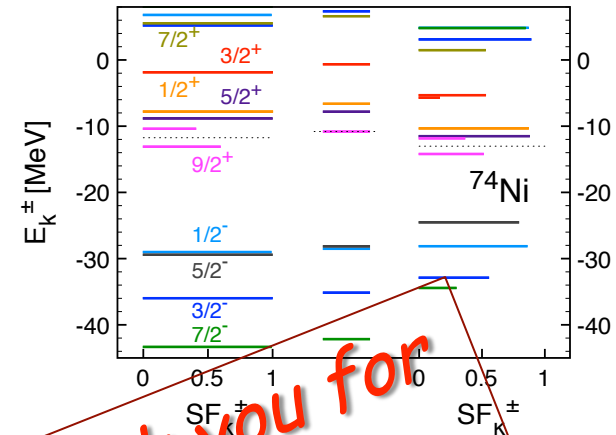
W.H. Dickhoff, S. Waldecker

D. Van Neck, M. Degroote

M. Hjorth-Jensen

Conclusions

- Self-Consistent Green's Functions (SCGF), is a microscopic *ab-initio* method applicable to medium mass nuclei. *Greatest advantage* is the link to several (experimentally accessible) information.
- Proof of principle calculations *Gorgov theory* are successful at 2nd order. This de facto show that the approach is viable and opens a whole new path:
 - Open-shell nuclei (*many, not* previously approachable otherwise!).
 - Reactions at driplines.
 - structure of next generation EDF.
- Addition of three nucleon forces (3NF) are feasible and underway.
 - This implies a step up in the accuracy of "ab-initio" calculations.



Thank you for
your
attention!!!