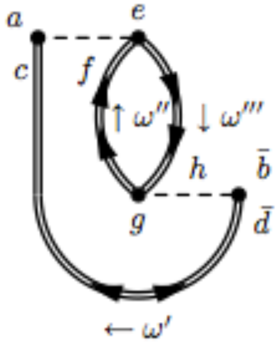
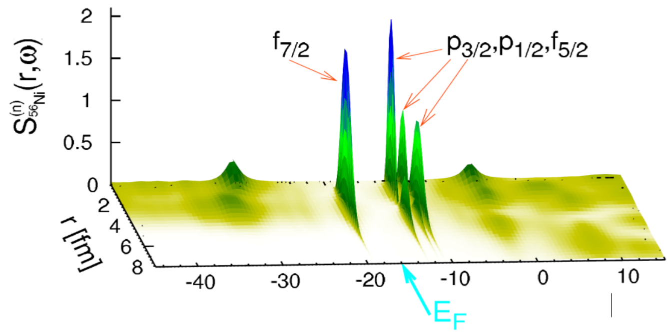
“Shell Model as a Unified View of Nuclear Structure”
in honour of Etienne Caurier, Alfredo Poves and Andres Zuker
Strasburg, Oct. 8-10, 2012

Towards predictive theory for the mid-mass region: Gorkov and 3NF



C. Barbieri



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Towards a unified description of nuclei

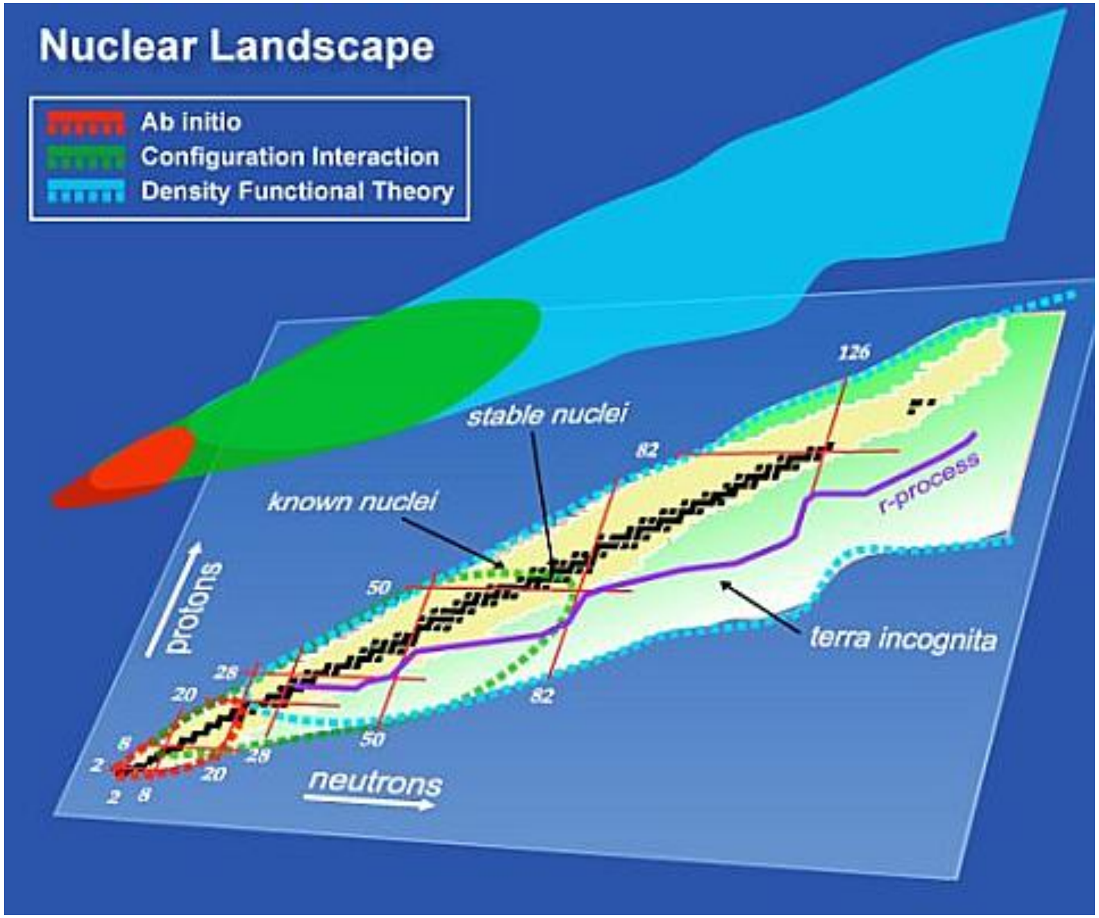
Open issues @ mid masses are:

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

→ Structure calculations are limited to closed-shells or A±1, A±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

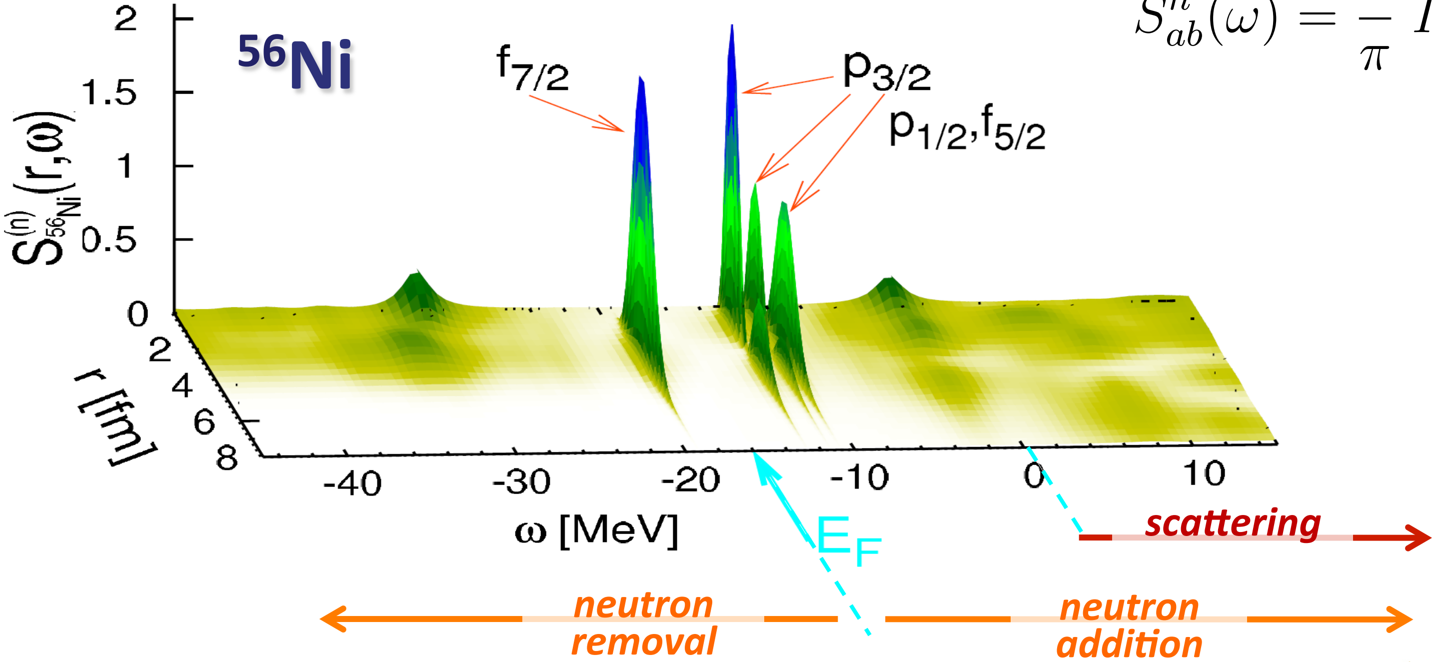
Green's functions in many-body theory

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

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

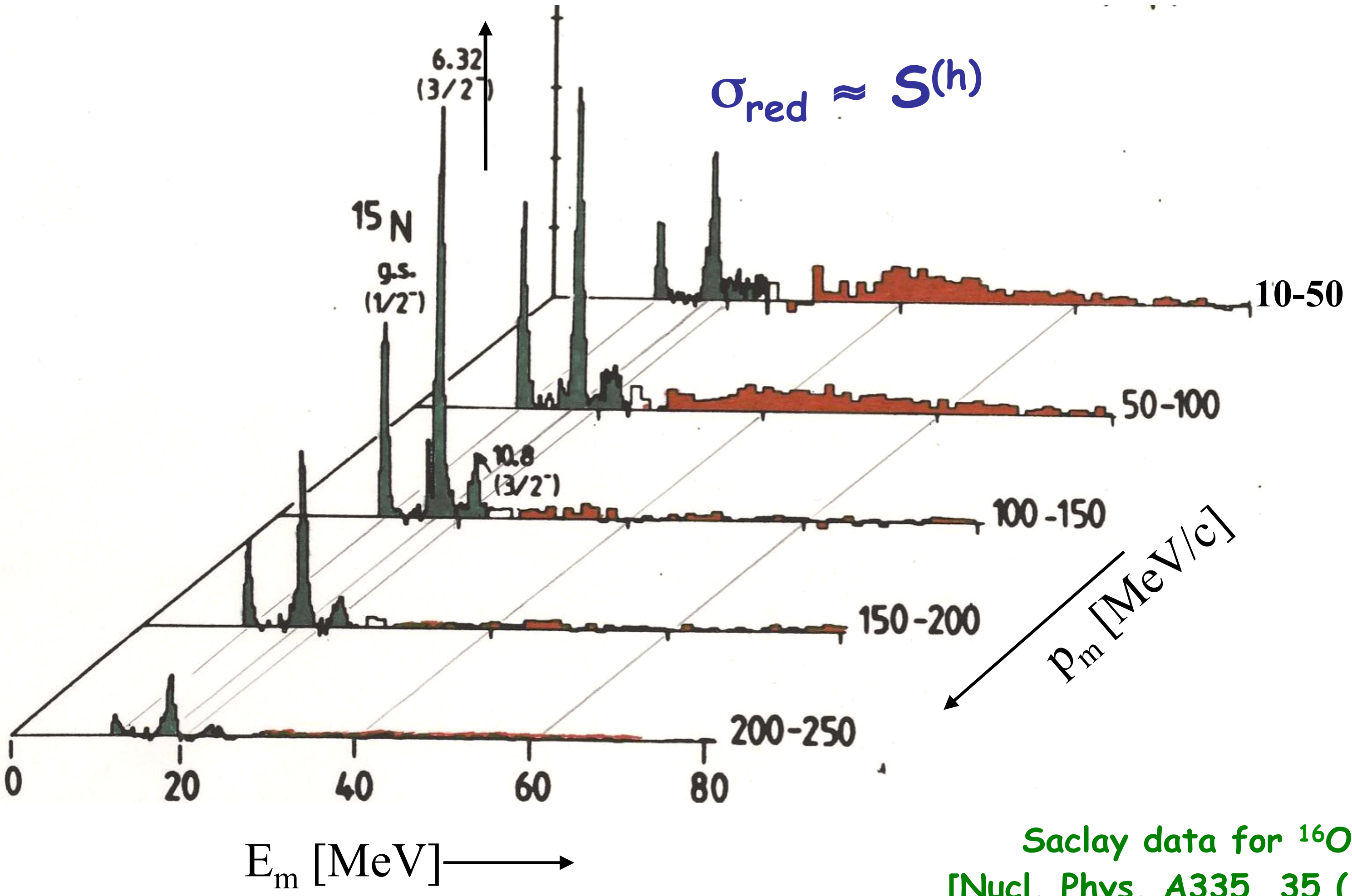
…this contains <u>all the structure information</u> probed by nucleon transfer (spectral function):

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



[CB, M.Hjorth-Jensen, Pys. Rev. C**79**, 064313 (2009); CB, Phys. Rev. Lett. **103**, 202502 (2009)]

One-hole spectral function from experiment



$\sigma_{red} \approx S^{(h)}$

Saclay data for $^{16}O(e,e'p)$
[Nucl. Phys. A335, 35 (1980)]

→ distribution of nucleons in momentum (**p_m**) and energies (**E_m**)

Dependence of Spect. Fact. from p-h gap

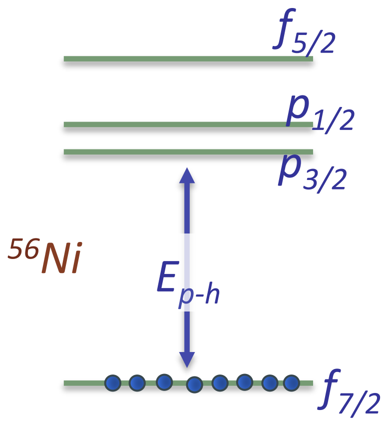
N3LO needs a monopole correction to fix the p-h gap:
[A.P.Zuker (2003), Phys. Rev. Lett. **90**, 042502]

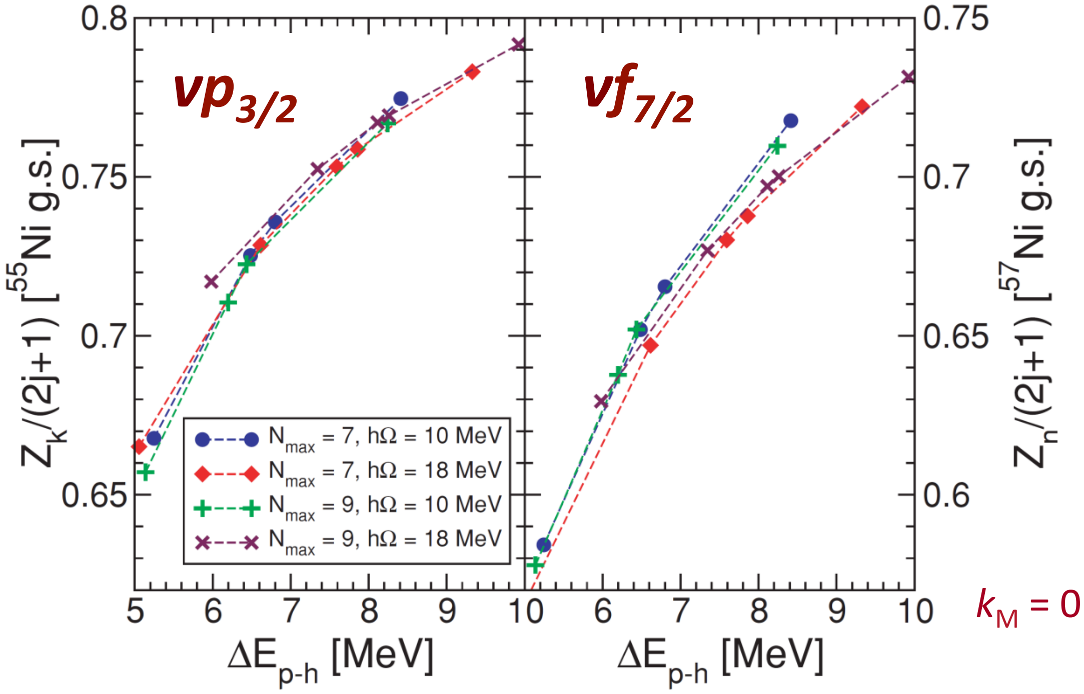
$$\begin{cases} \Delta V^T_{fr} \to \Delta V^T_{fr} - (-1)^T \kappa_M \,, \\ \Delta V^T_{ff} \to \Delta V^T_{ff} - 1.5(1-T)\kappa_M \,, \end{cases}$$

$r \equiv p_{3/2}, p_{1/2}, f_{5/2}$

$f \equiv f_{7/2}$

Experimental Eph is found for k_M =0,57





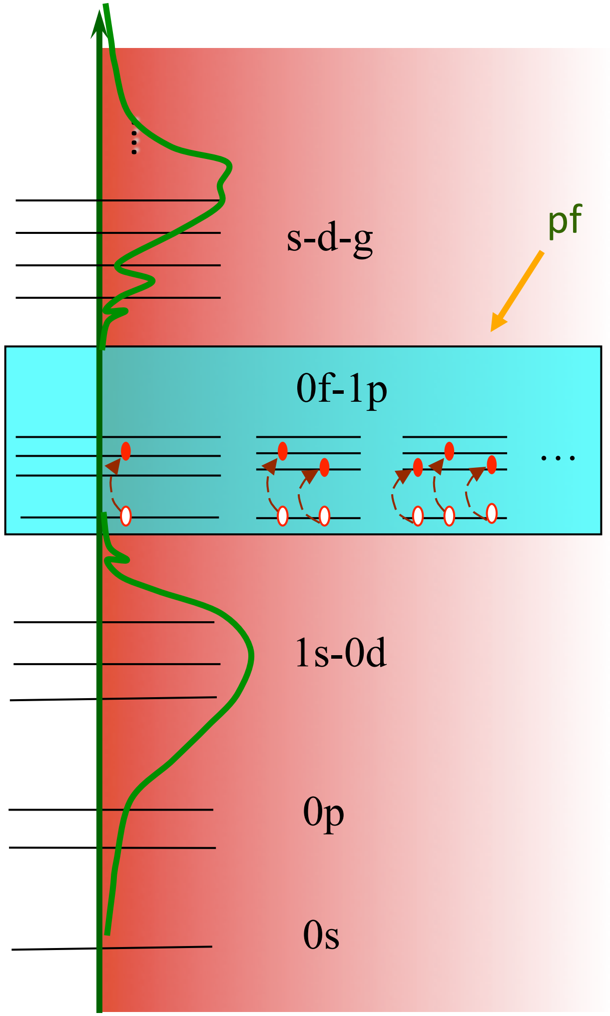
k_M = 0.4-0.7 MeV

small k_M ← → large k_M

N3LO interaction + monopole corr.

[CB, M.Hjorth-Jensen, Pys.Rev.C79, 064313 (2009)]

Correlations & model space (RPA and SM)



Quenching of absolute spectroscopic factors

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

Overall quenching of *spectroscopic factors* is driven by:
SRC → *~10%*
part-vibr. coupling → *dominant*
"shell-model" → *in open shell*

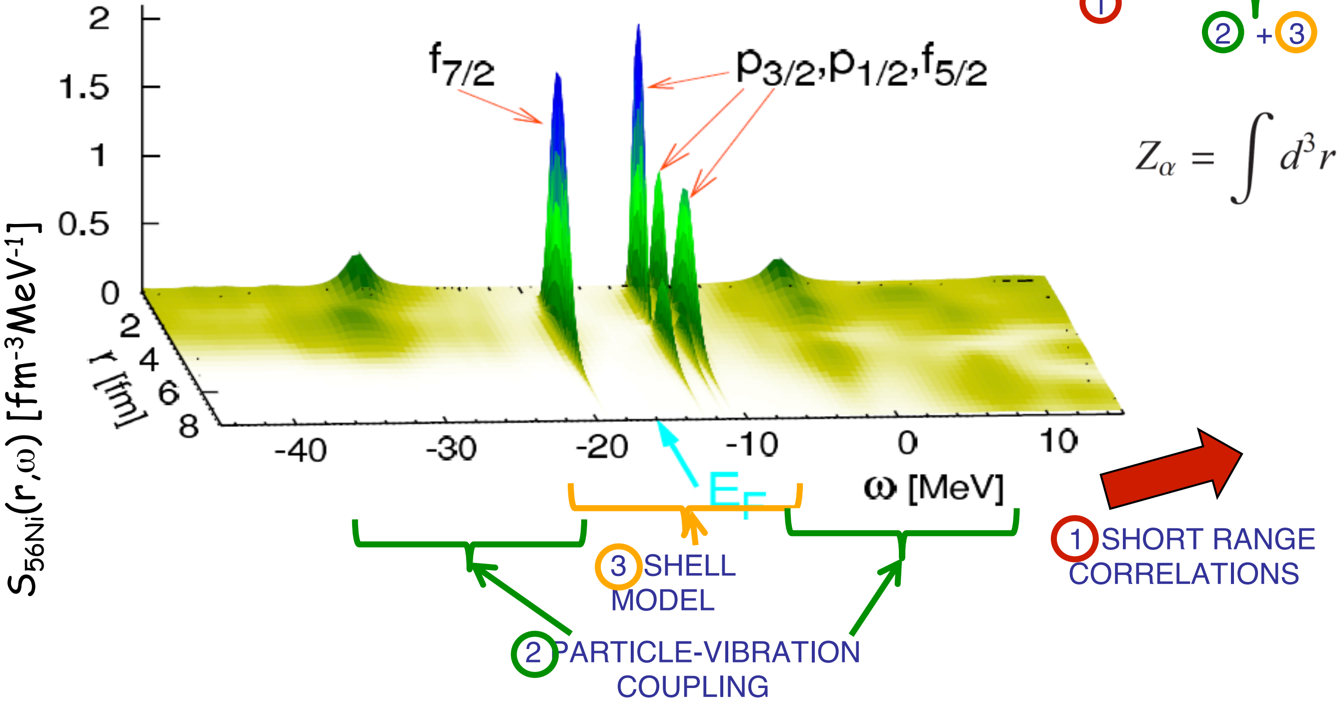
…with analogous conclusions for ^{48}Ca

	10 osc. shells			Exp. [30]	1p0f space		
	FRPA (SRC)	full FRPA	FRPA $+\Delta Z_\alpha$		FRPA	SM	ΔZ_α
^{57}Ni:							
$\nu 1p_{1/2}$	0.96	0.63	0.61		0.79	0.77	-0.02
$\nu 0f_{5/2}$	0.95	0.59	0.55		0.79	0.75	-0.04
$\nu 1p_{3/2}$	0.95	0.65	0.62	0.58(11)	0.82	0.79	-0.03
^{55}Ni:							
$\nu 0f_{7/2}$	0.95	0.72	0.69		0.89	0.86	-0.03
	①	② + ③			③		

^{57}Ni

^{55}Ni

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

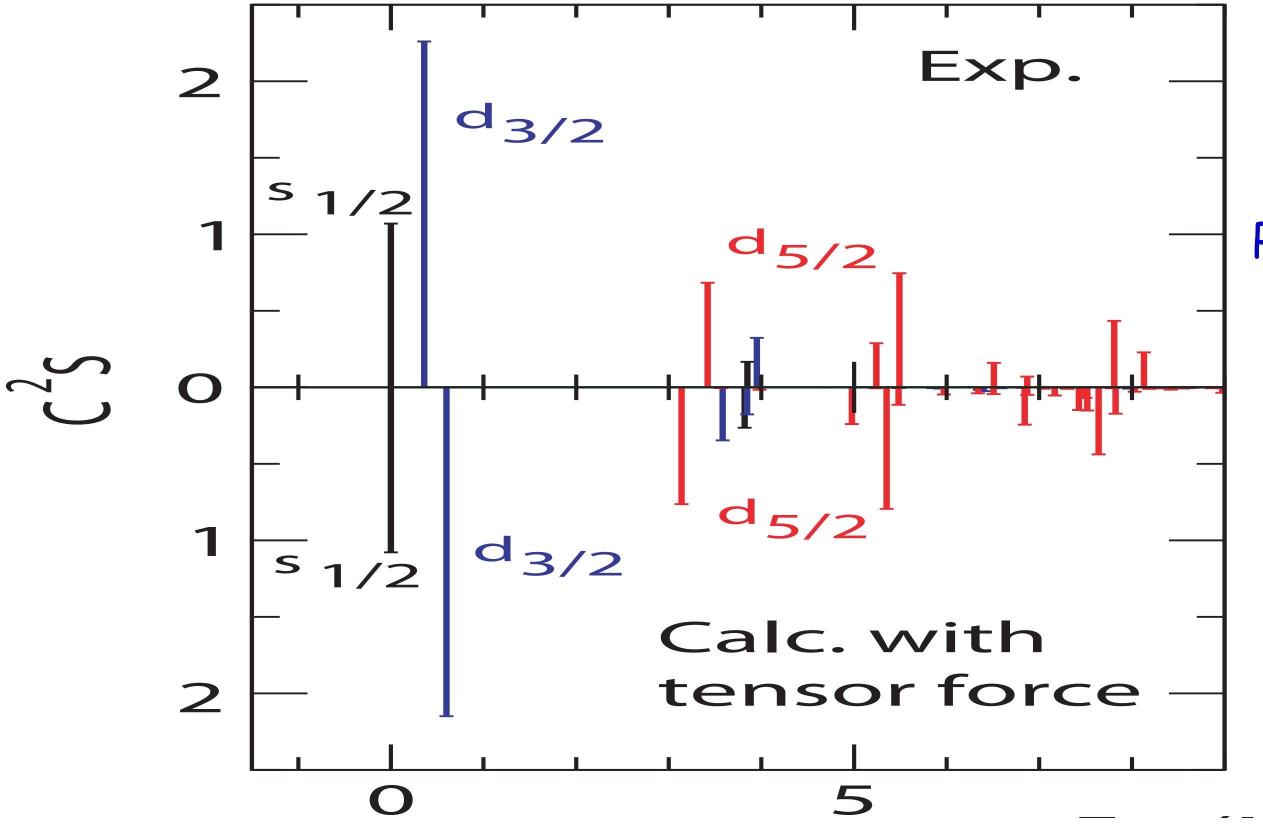


③ SHELL MODEL

② PARTICLE-VIBRATION COUPLING

① SHORT RANGE CORRELATIONS

BUT still need shell-model (configuration mixing) to understand low energy fragmentation !



Proton 'holes' in ^{48}Ca
($\equiv{}^{48}$Ca(e,e'p)^{47}K)

Y. Utsuno et al., arXiv:1201.4077v1 [nucl-th]

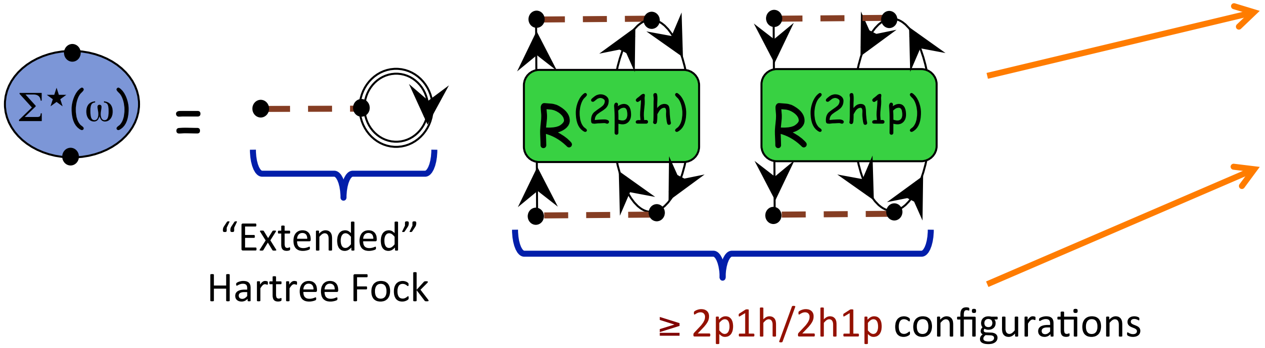
Calculating the spectral function:

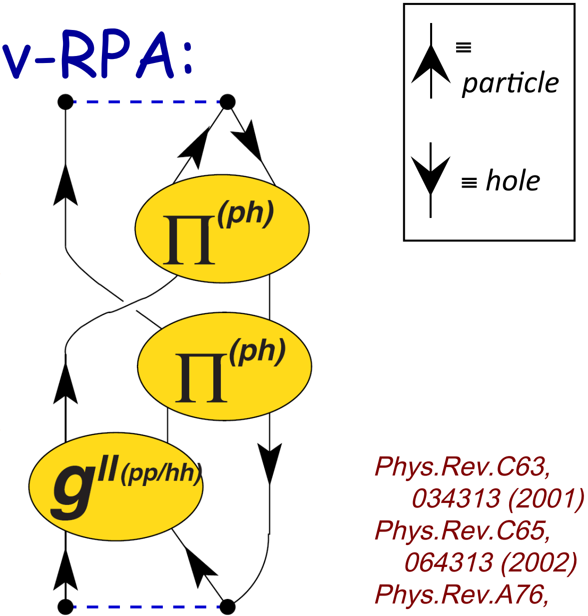
FRPA, ADC(3), and the like…

Faddeev-RPA in two words…

Self-energy
(optical potential):

Faddeev-RPA:





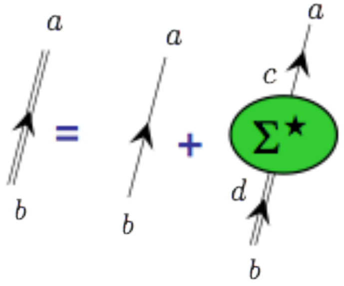
Phys.Rev.C63, 034313 (2001)
Phys.Rev.C65, 064313 (2002)
Phys.Rev.A76, 052503 (2007)

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

Dyson equation

- Propagators solves the Dyson equations

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



- (Hole) single particle spectral function

$$S^h_{ab}(\omega) = \frac{1}{\pi}\, Im\, g_{ab}(\omega) = \sum_k \langle \Psi^{A-1}_k | c_b | \Psi^A_0 \rangle \langle \Psi^A_0 | c^\dagger_a | \Psi^{A-1}_k \rangle\ \delta(\omega - (E^A_0 - E^{A-1}_k))$$

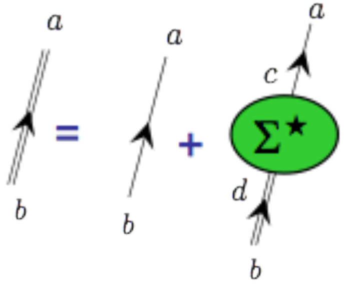
- Koltun sum rule (for 2N interactions):

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

Dyson equation

- Propagators solves the Dyson equations

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



- (Hole) single particle spectral function

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

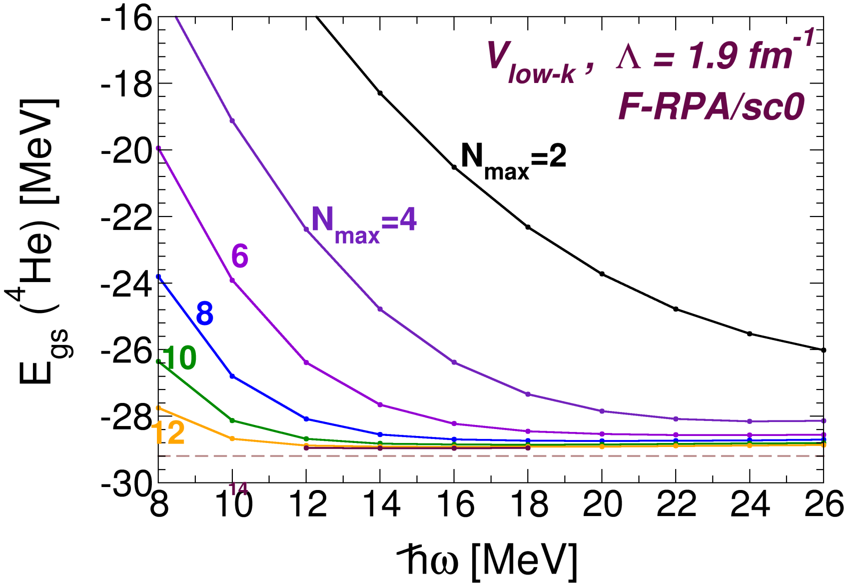
- Koltun sum rule (with NNN interactions):

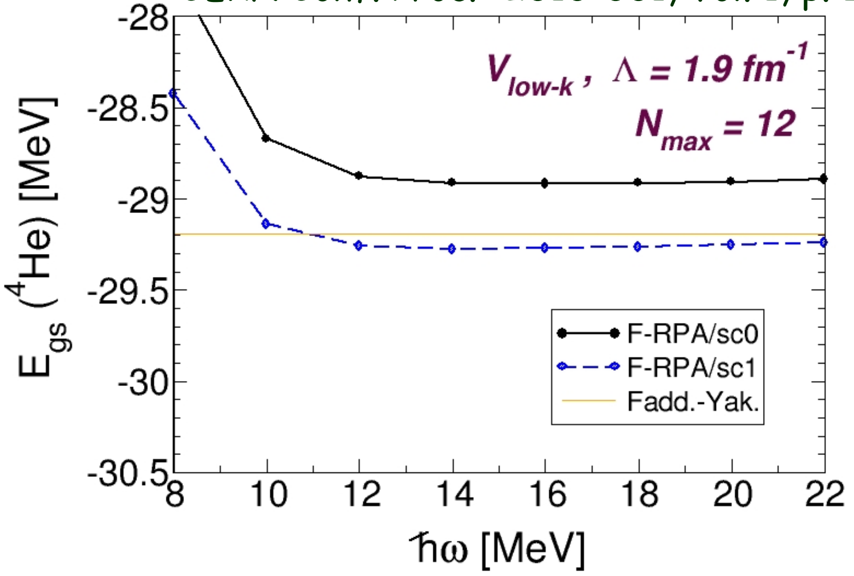
$$\frac{1}{2}\sum_{ab}\int_{-\infty}^{E_F} (t_{ab} + \delta_{ab}\omega) S^h_{ab}(\omega)\ d\omega = \langle T\rangle + \langle V^{NN}\rangle + \frac{3}{2}\langle V^{NNN}\rangle$$

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

Binding Energy – ^{4}He Case

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





➔Self-consistent FRPA *compares well* with benchmark calculations on ^{4}He

	FRPA/sc0	FRPA/sc	Exact:
V_{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

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]

Going to open-shells: Gorkov ansatz

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

✷ Ansatz $\boxed{\ldots \approx E_0^{N+2} - E_0^N \approx E_0^N - E_0^{N-2} \approx \ldots \approx 2\mu}$

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

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

Gorkov Green's functions and equations

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

- Set of 4 Green's functions

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

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

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

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

[Gorkov 1958]

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

Gorkov equations

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

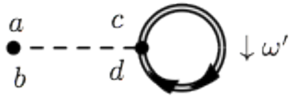
$$\mathbf{\Sigma}^\star_{ab}(\omega) \equiv \mathbf{\Sigma}_{ab}(\omega) - \mathbf{U}_{ab}$$

1st & 2nd order diagrams

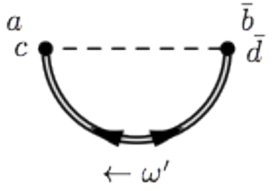
[V. Somà, T. Duguet, CB, Pys. Rev. C84, 046317 (2011)]

- 1st order ➡ energy-independent self-energy

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

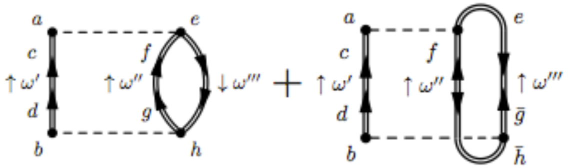


$\Sigma^{12\,(1)}_{ab} =$

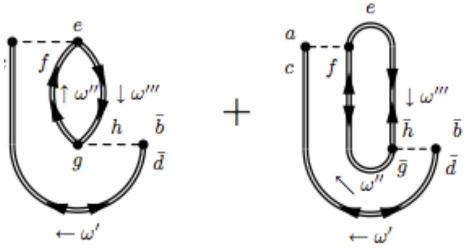


- 2nd order ➡ energy-dependent self-energy

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



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



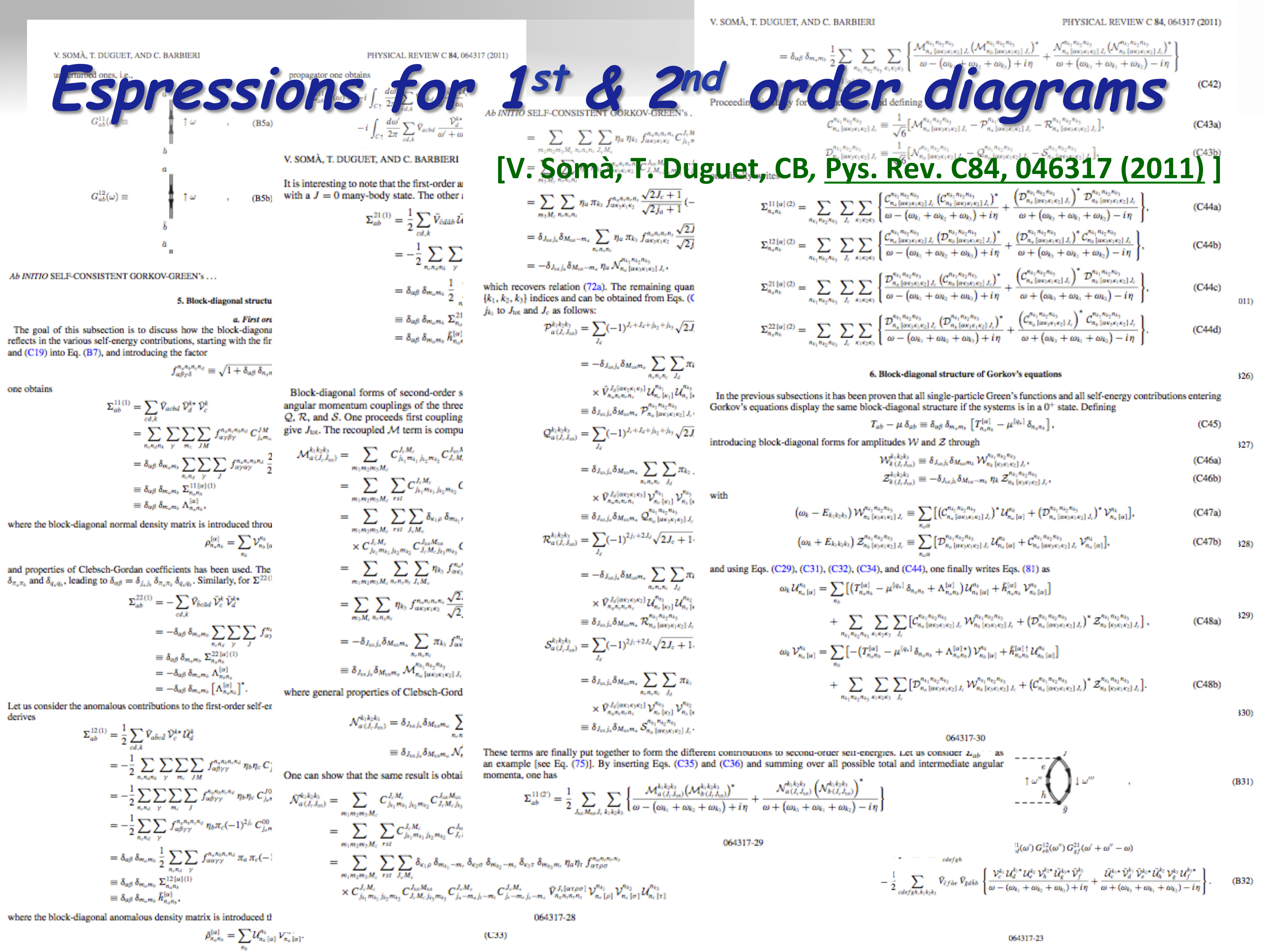
- Gorkov equations ⟶ eigenvalue problem

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

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

Espressions for 1st & 2nd order diagrams

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



Gorkov equations

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

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

↓

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

Energy *independent* eigenvalue problem

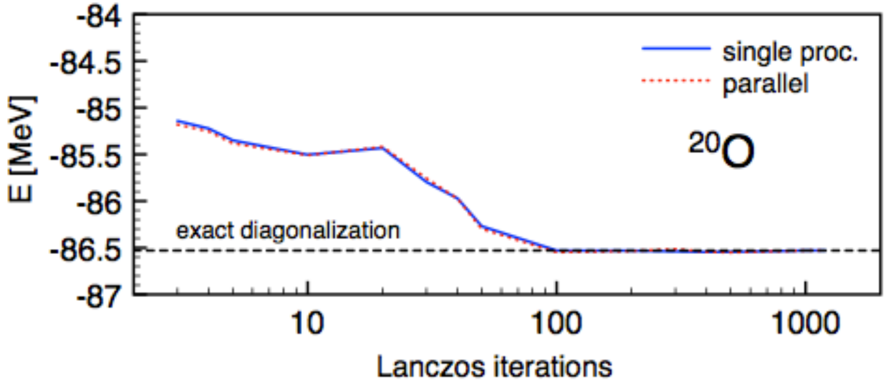
with the normalization condition $\sum_a \left[\left|\mathcal{U}^k_a\right|^2 + \left|\mathcal{V}^k_a\right|^2 \right] + \sum_{k_1 k_2 k_3} \left[\left|\mathcal{W}^{k_1 k_2 k_3}_k\right|^2 + \left|\mathcal{Z}^{k_1 k_2 k_3}_k\right|^2 \right] = 1$

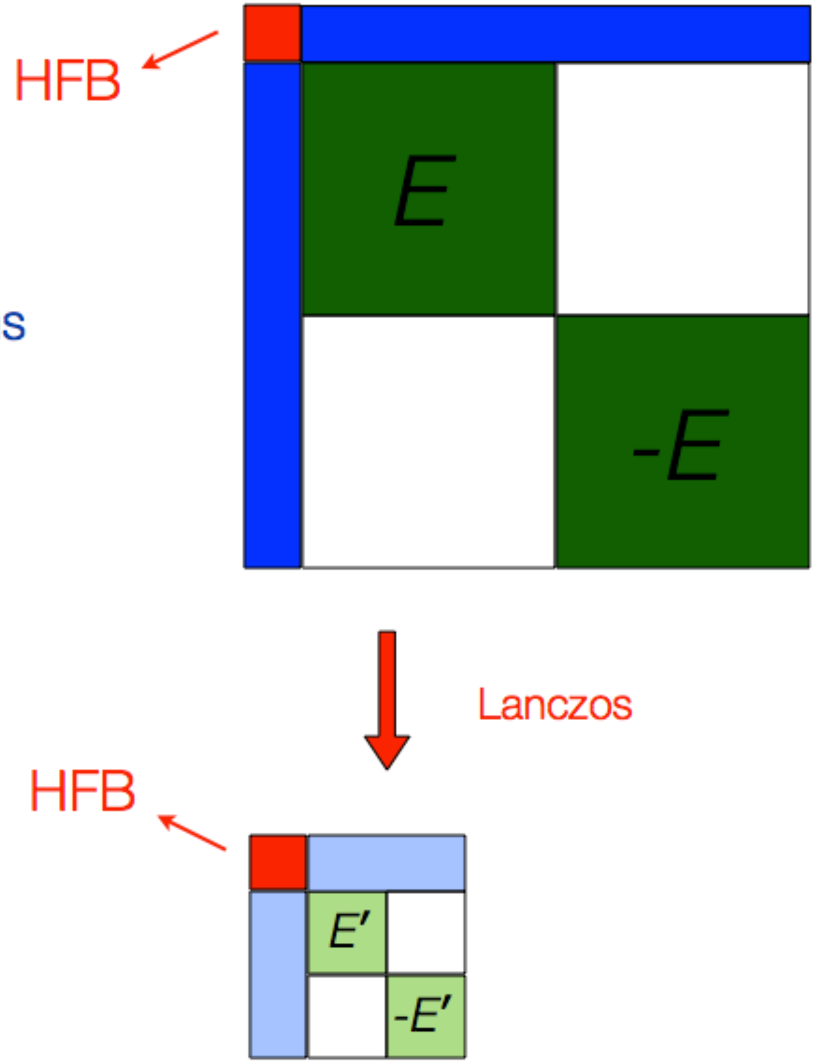
Lanczos reduction of self-energy

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

➟ Conserves moments of spectral functions

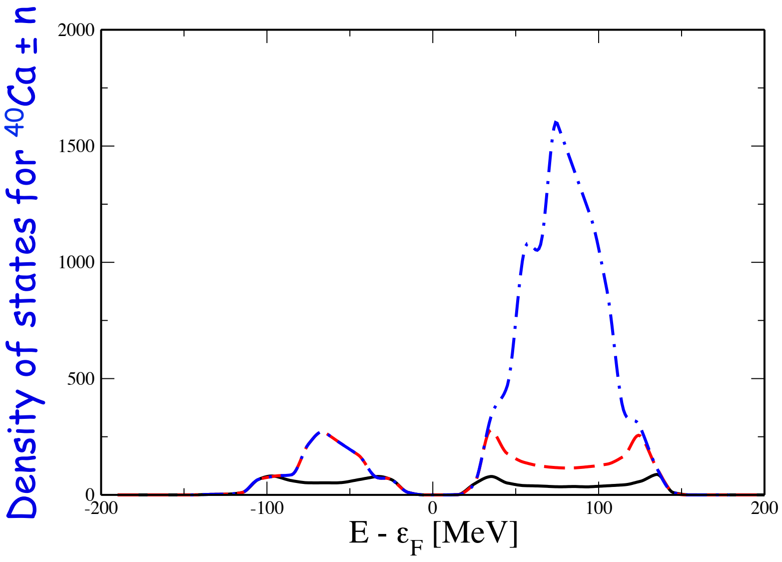
➟ Equivalent to exact diagonalization for $N_L \rightarrow \dim(E)$



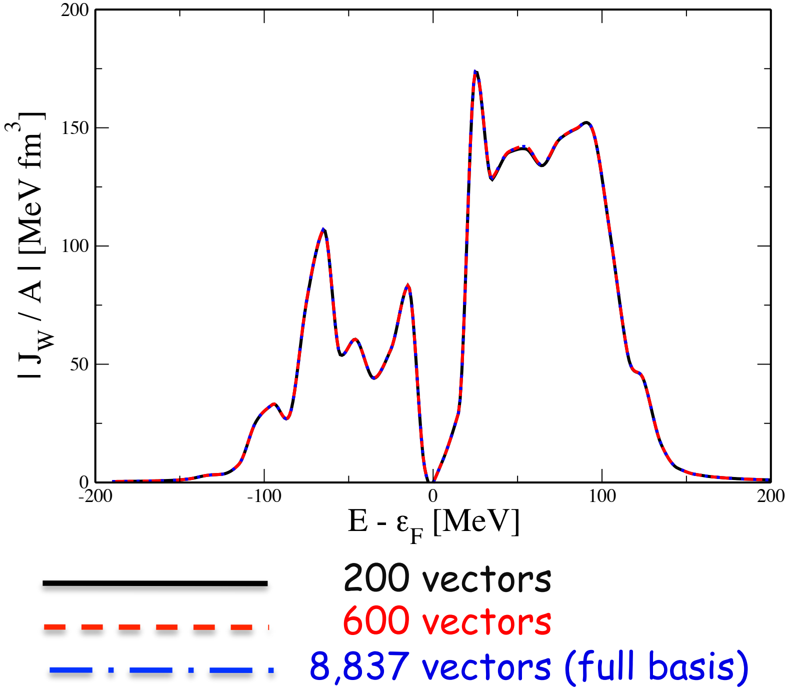


Application of Lanczos (example)

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



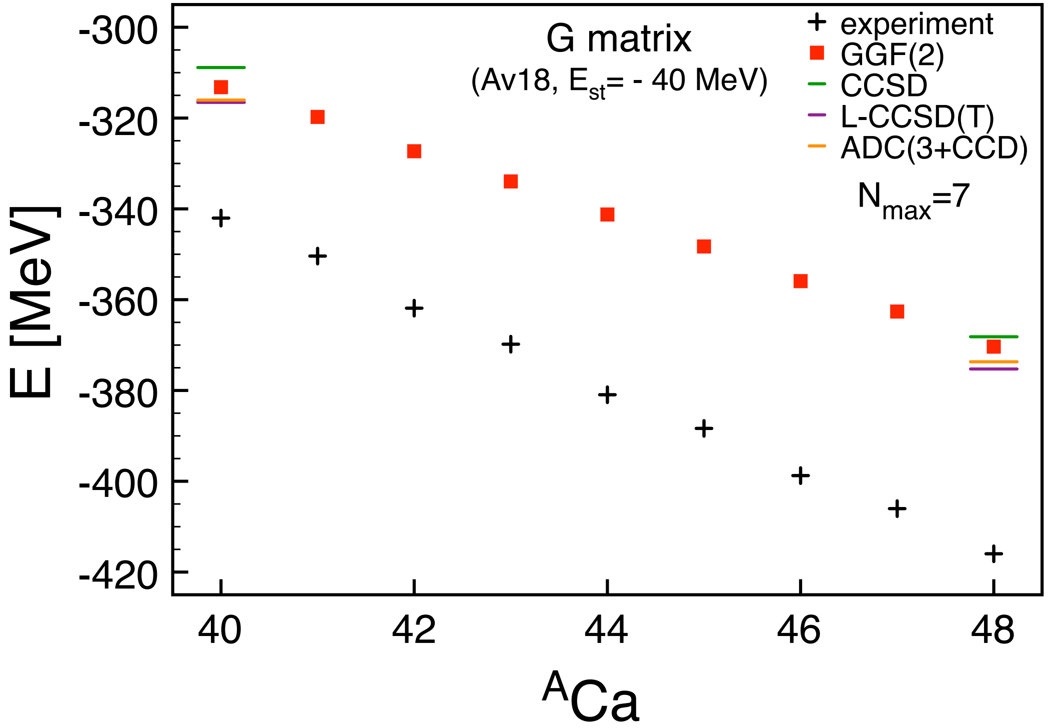
Volume integral of ^{40}**Ca ± n** optical potential in $f_{7/2}$ part. wave



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

Binding energies

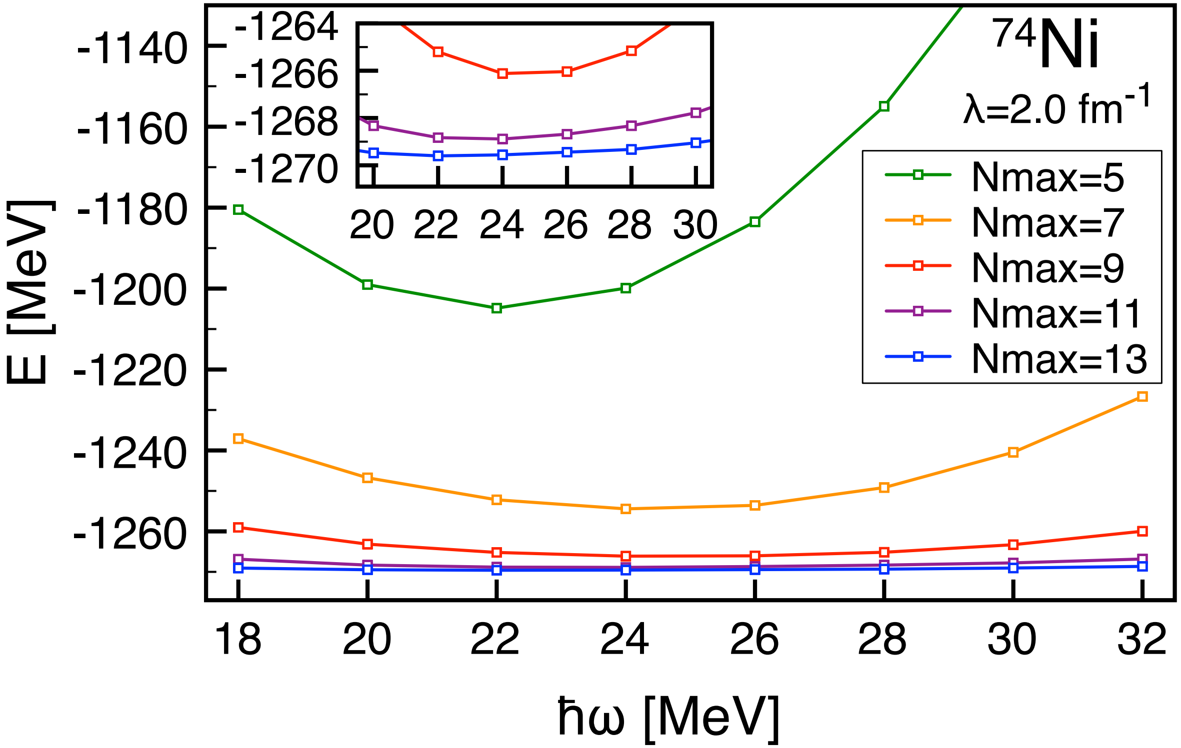
- Systematic along isotopic/isotonic chains has become available



➡ Correlation energy close to CCSD and FRPA (thorough comparison needed)

➡ Need for (at least) NNN forces

Binding energies

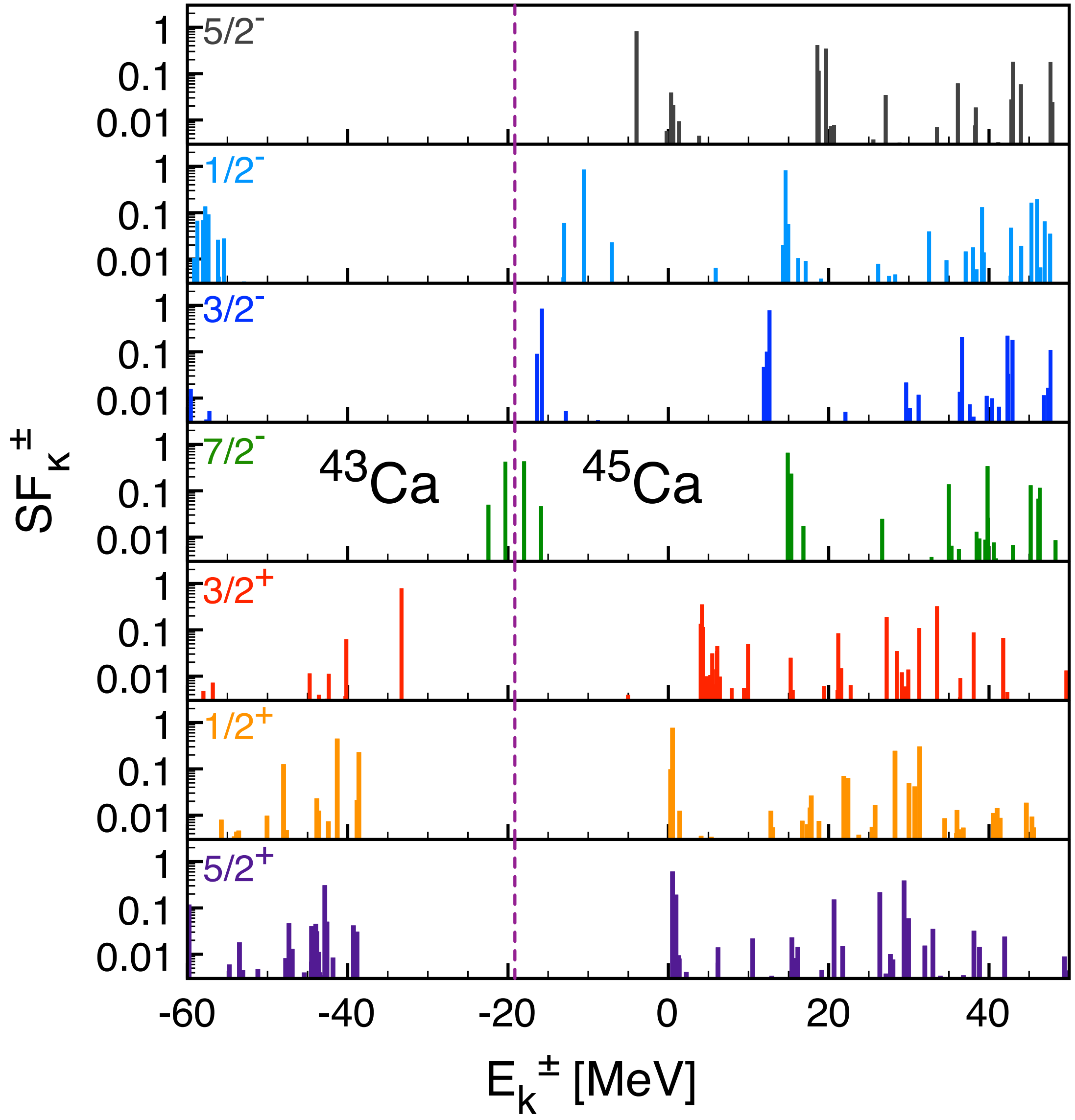


✳ Systematic along isotopic/isotonic chains has become available

- ➟ Correlation energy close to CCSD and FRPA (thorough comparison needed)
- ➟ Overbinding with A: traces need for (at least) NNN forces
- ➟ Effect of self-consistency significant; i.e. less bound than MBPT2

Spma, CB, Duguet, arXiv:1208.2472

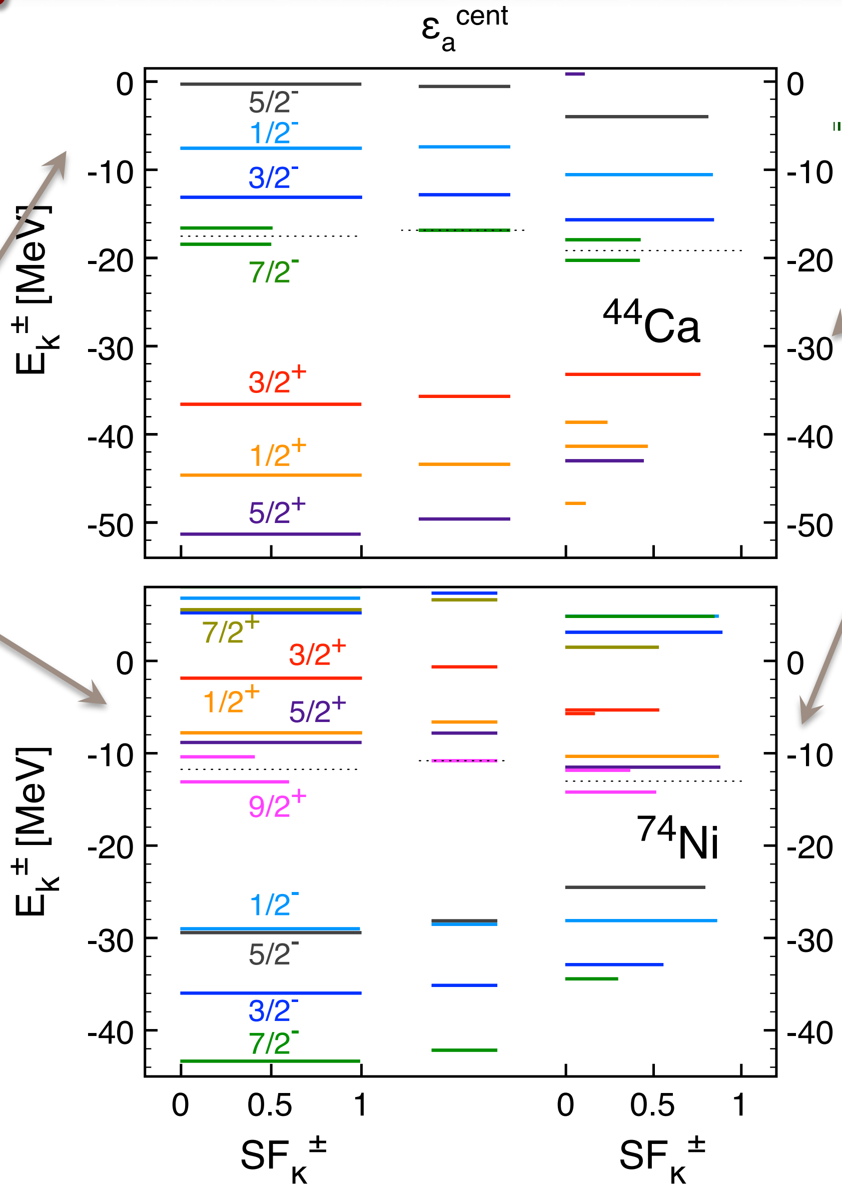
Spectral distribution



➡ Gorkov-GF at 2nd order [or ADC(2)]

Spma, CB, Duguet, arXiv:1208.2472

Spectral distribution



Gorkov-GF at 2nd order [or ADC(2)]

Gorkov-GF at 1st order [HFB]

Spma, CB, Duguet, arXiv:1208.2472

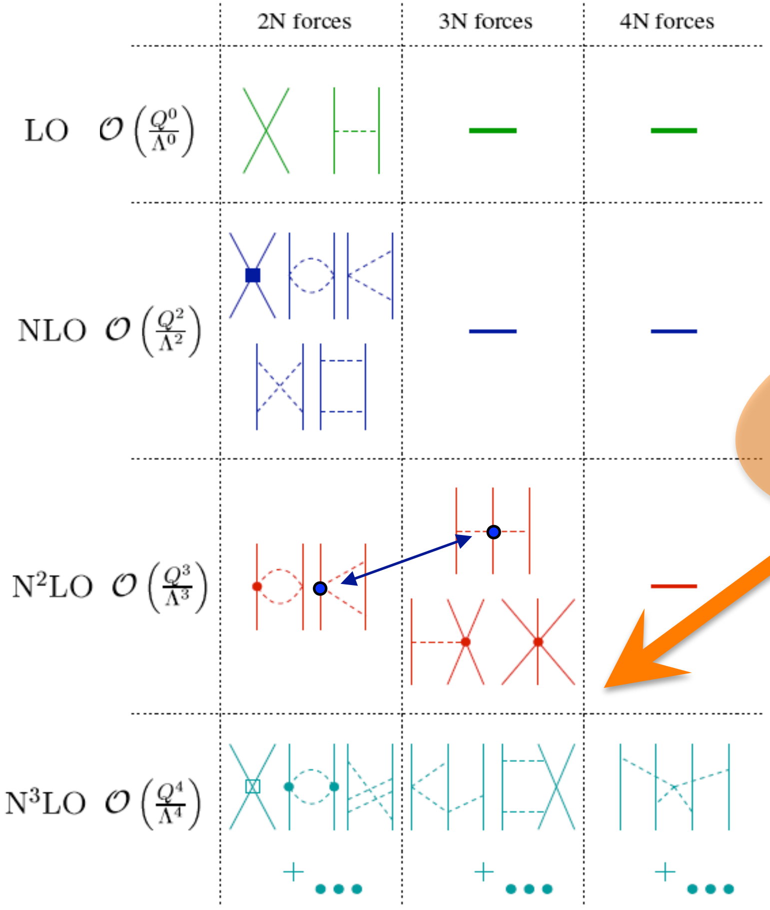
Three-nucleon interactions

→ application to nuclei
→ need new formalism?

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

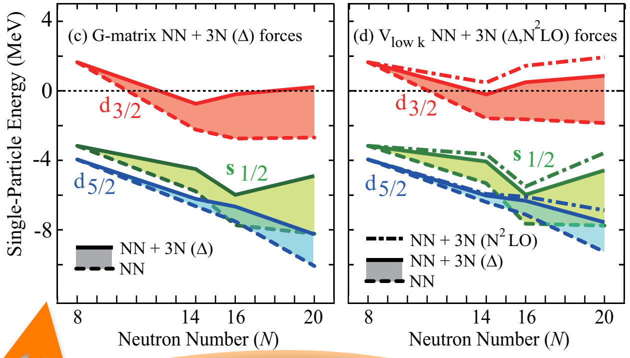
Modern realistic nuclear forces

Chiral EFT for nuclear forces:



(3NF arise naturally at N2LO)

Single particle spectrum at E_{fermi}:

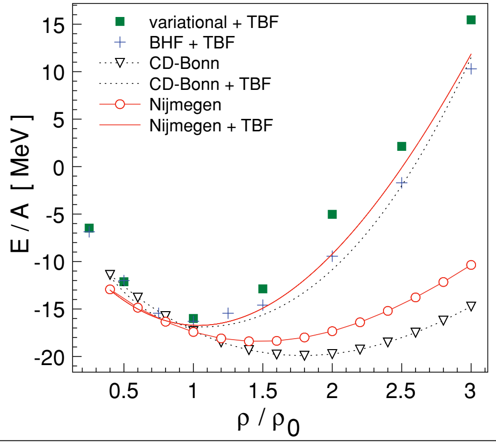


[T. Otsuka et al., Phys Rev. Lett **105**, 32501 (2010)]

Need at LEAST 3NF!!!

("cannot" do RNB physics without...)

Saturation of nuclear matter:

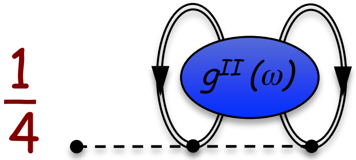


[V. Somà, Phys Rev. C **78**, 054003 (2008))]

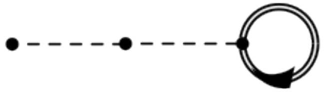
Inclusion of NNN forces

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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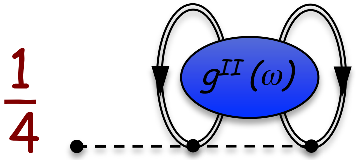

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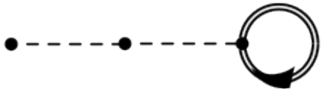

Correction to
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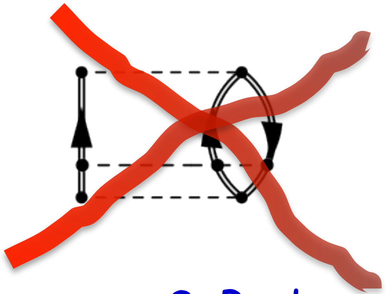
2-Body interaction



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$\frac{1}{2}$

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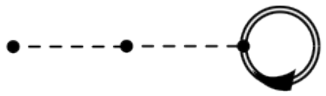
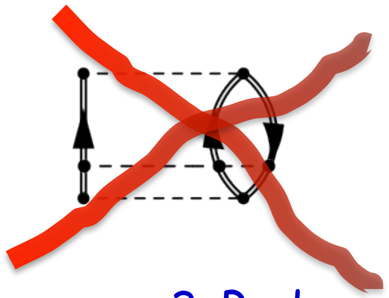


Correction to
<u>*non-contracted*</u>
2-Body interaction

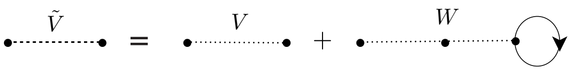


pure 3-Body
contribution

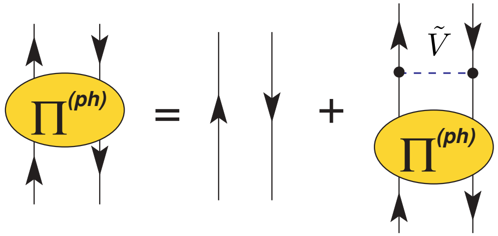
NNN forces in FRPA/FTDA formalism

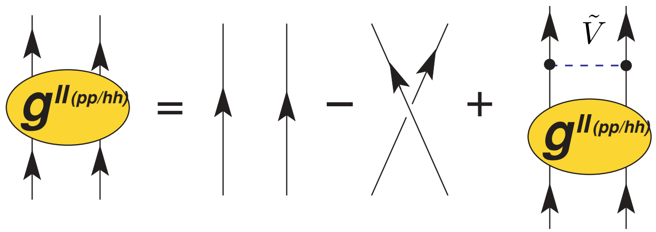
A. Cipollone, CB, P. Navratil

Use:

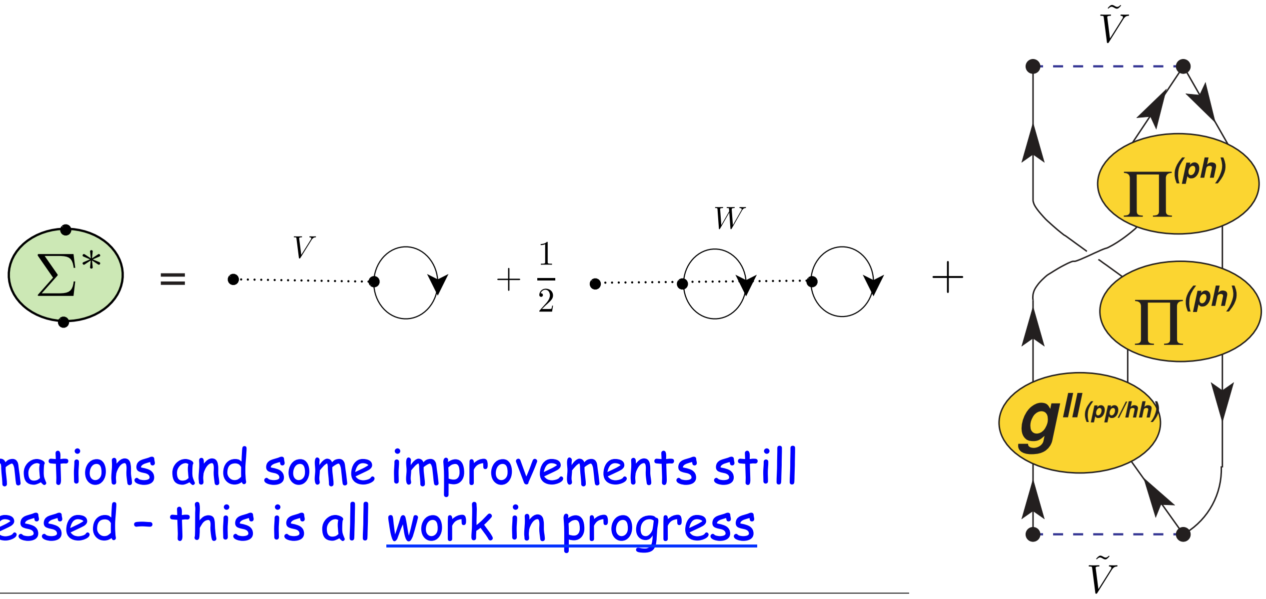


as 2-body potential in all V-irred.
RPA/TDA summations





Then:

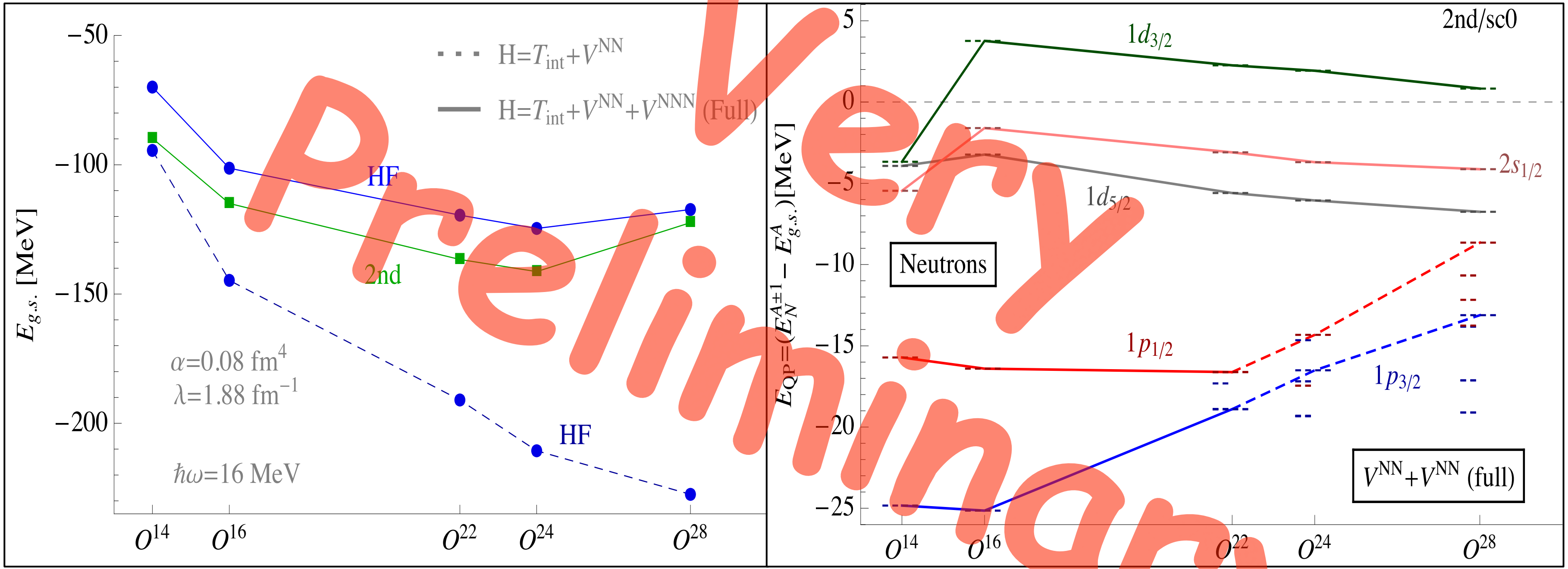


…approximations and some improvements still being assessed – this is all work in progress

Oxygen isotopes with evolved chiral 3NF

Binding energy

Single particle spectrum



Very Preliminary

Summary

Thank you for your attention!!!

- 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.