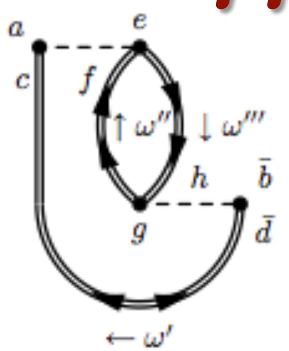
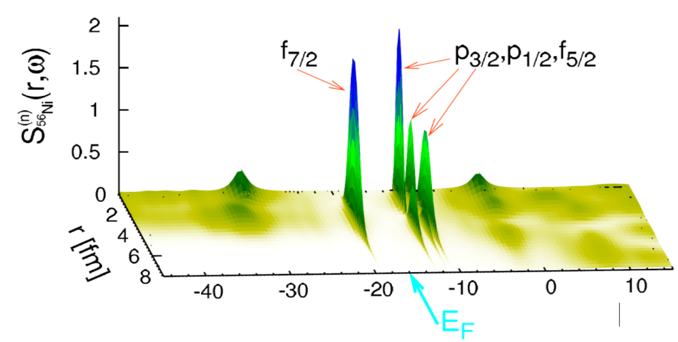
Green's function theory in the mid mass region: toward an ab-initio approach for the open shells



C. Barbieri



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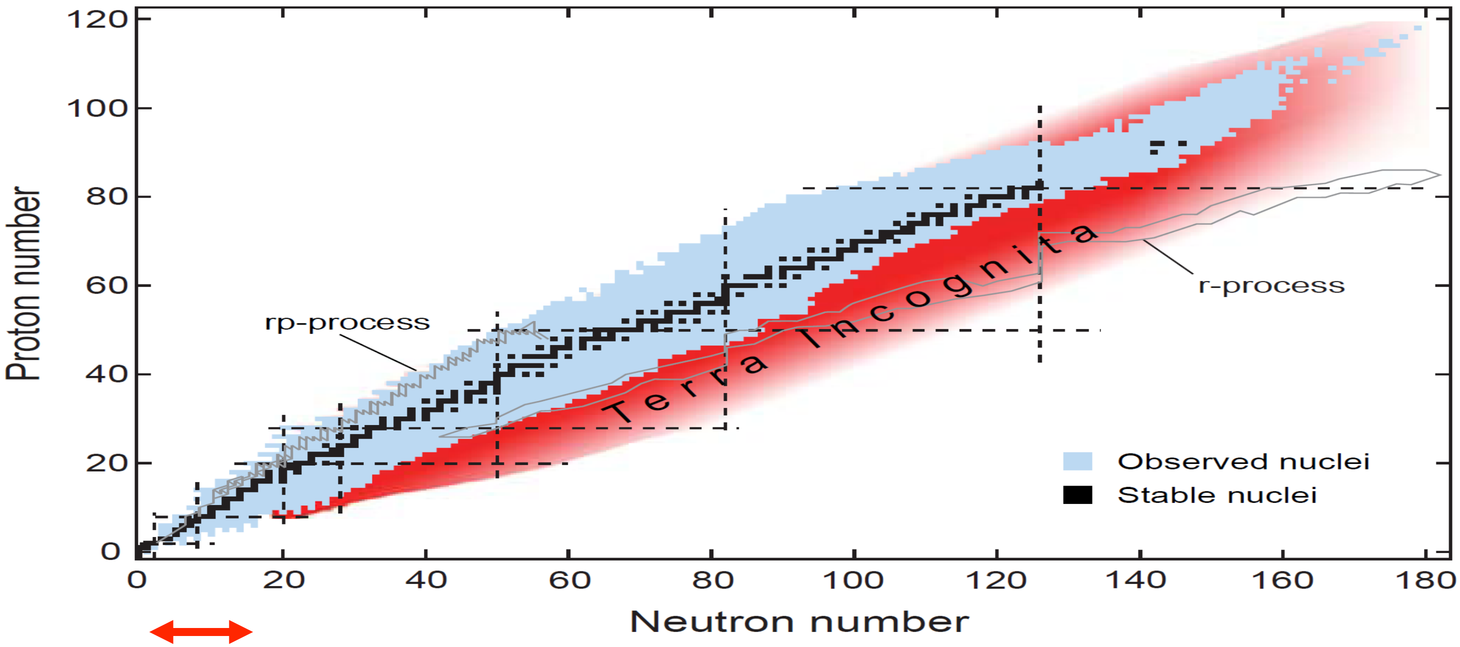
Towards a unified description of nuclei



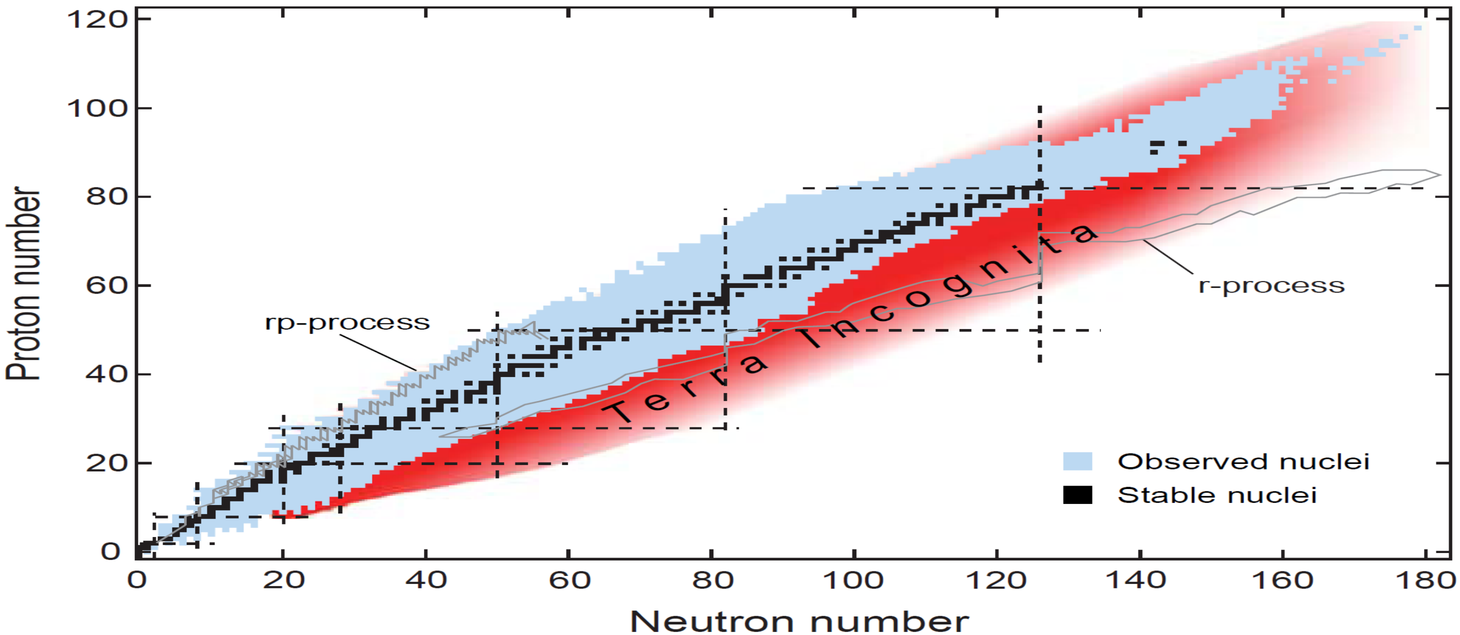
"Exact" methods (GFMC, NCSM, ...)

Ab-initio approaches (CC, SCGF, IM-SRG)

Shell model

SR and MR energy density functionals

Towards a unified description of nuclei



The present status @ mid masses is:

→Still in need of good nuclear Hamiltonians (3N forces mostly!)

→Only structure calculations and limited to closed-shells or A±1, A±2 (BUT calculations are GOOD!!!)

→ However, Green's functions can be extended to: Scattering observables
<u>*Open shell nuclei*</u>

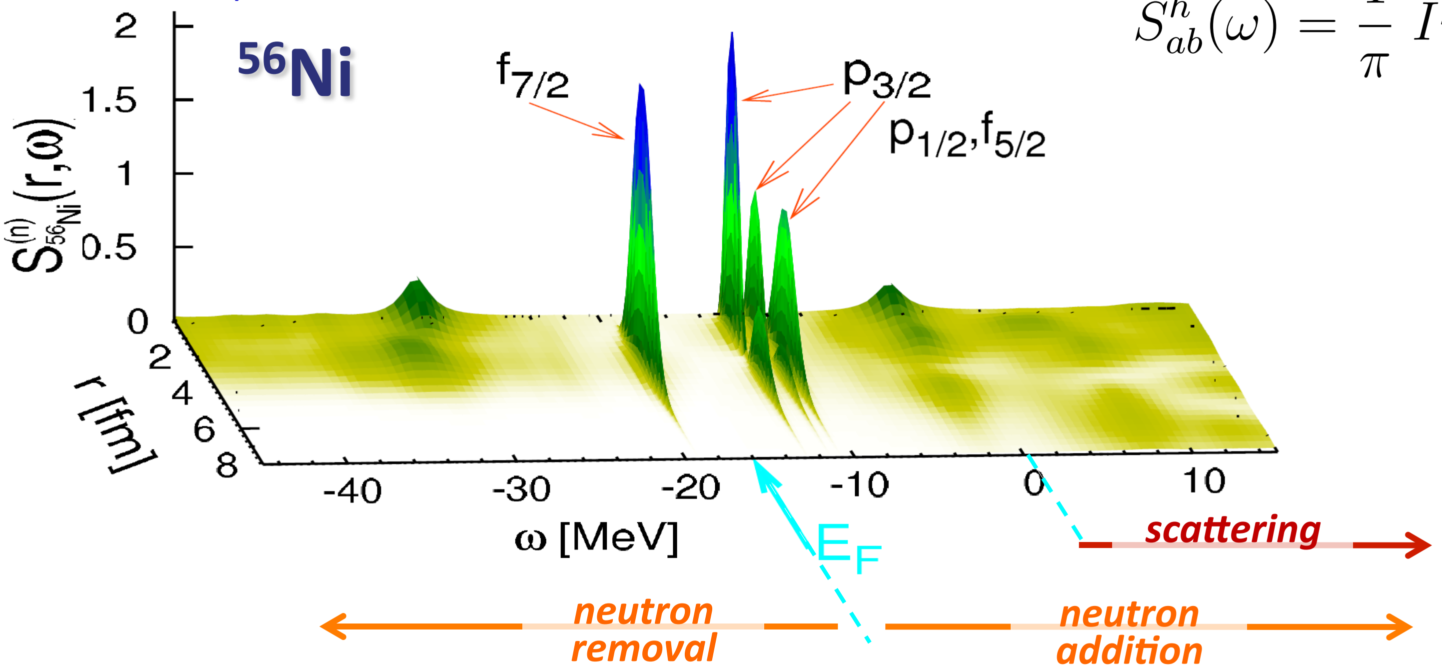
Green's functions in many-body theory

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):

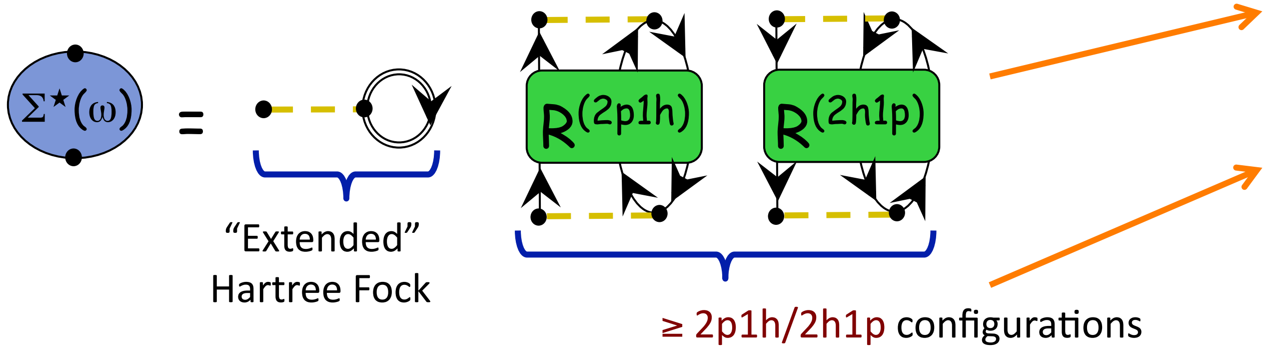
$$S_{ab}^h(\omega) = \frac{1}{\pi}\, Im\, g_{ab}(\omega)$$



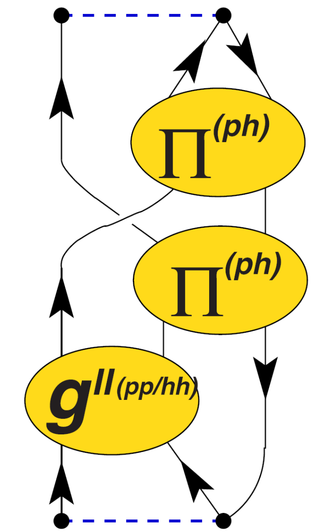
[CB, M.Hjorth-Jensen, Pys. Rev. C**79**, 064313 (2009); CB, Phys. Rev. Lett. **103**, 202502 (2009)]

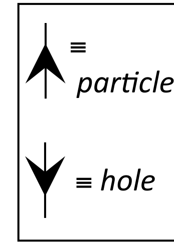
Faddeev-RPA in two words…

Self-energy (optical potential):



Faddeev-RPA:





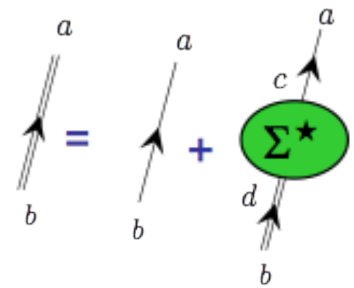
Phys.Rev.C63, 034313 (2001)
Phys.Rev.C65, 064313 (2002)
Phys.Rev.A76, 052503 (2007)

- A complete expansion requires <u>*all types*</u> 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

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

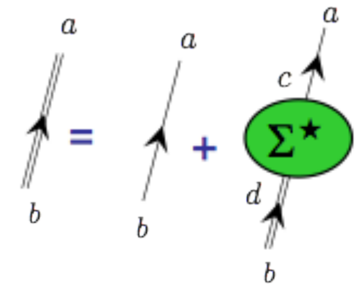
- Koltun sum rule (for 2N interactions):

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

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

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

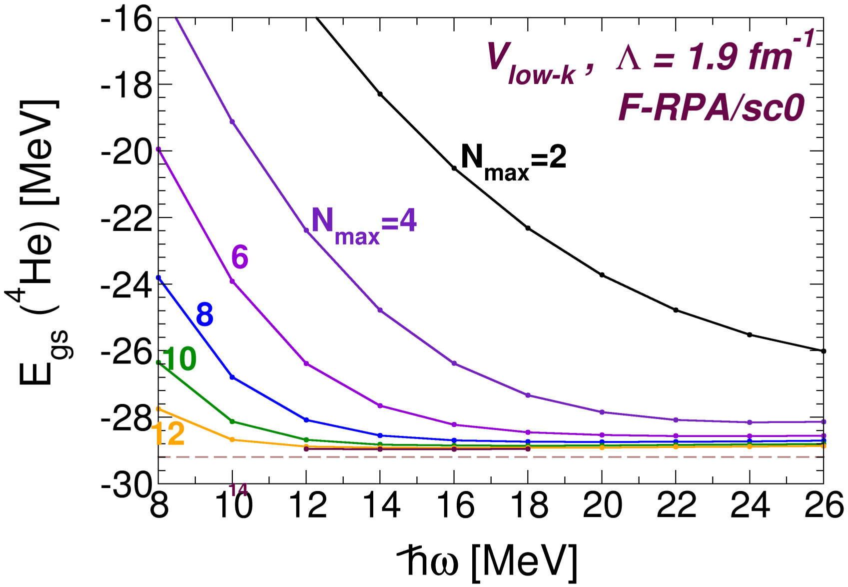
✺ Koltun sum rule (with NNN interactions):

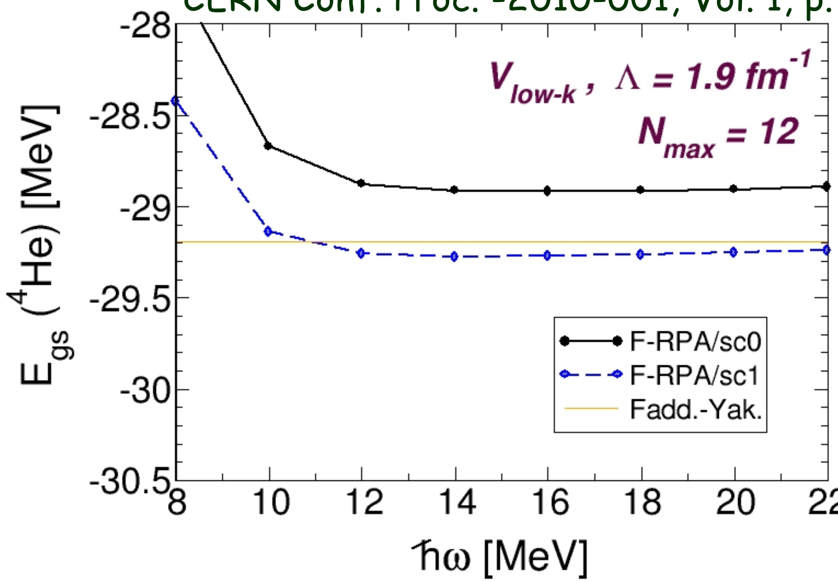
$$\frac{1}{2} \sum_{ab} \int_{-\infty}^{E_F} (t_{ab} + \delta_{ab}\omega) S^h_{ab}(\omega)\ d\omega = \langle T \rangle + \langle V^{NN} \rangle + \frac{3}{2} \langle V^{NNN} \rangle$$

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

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

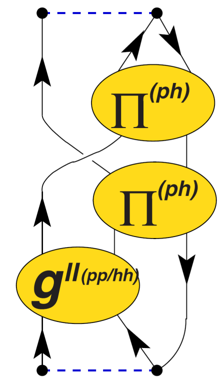
Applications to doubly-magic nuclei

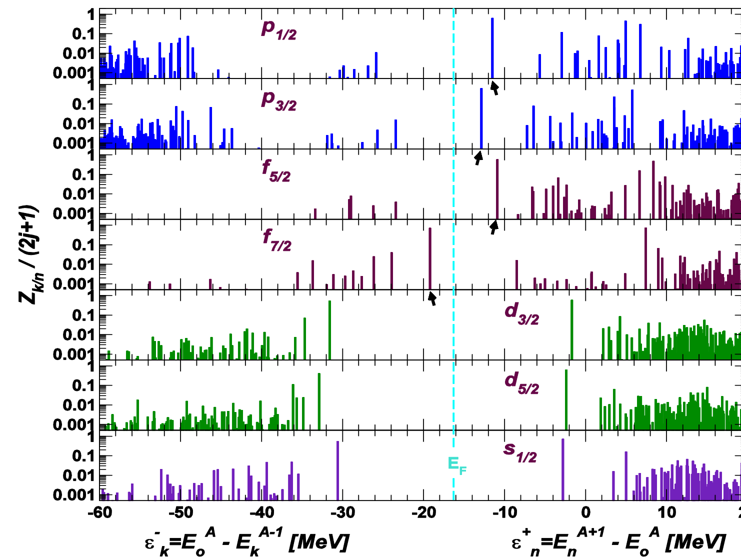
- Faddeev-RPA approximation for the self-energy

collective vibrations

particle-vibration coupling

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





- Successful in medium-mass doubly-magic systems

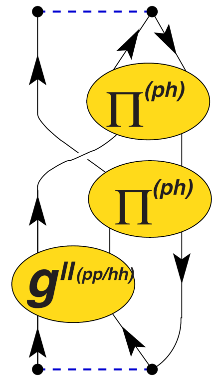
Applications to doubly-magic nuclei

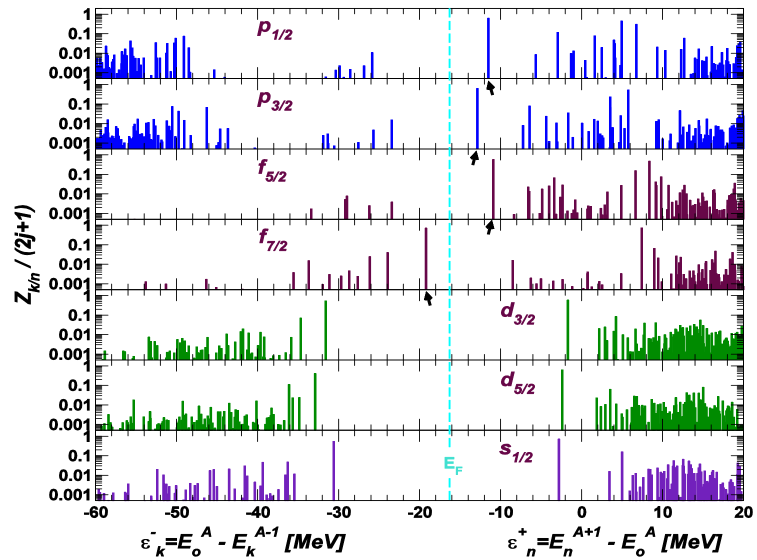
✳ Faddeev-RPA approximation for the self-energy

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

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

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

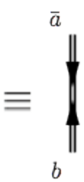
Gorkov Green's functions and equations

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

✳ Set of 4 Green's functions

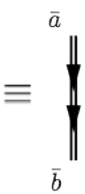
$$i\,G^{11}_{ab}(t,t') \equiv \langle\Psi_0|T\left\{a_a(t)a^{\dagger}_b(t')\right\}|\Psi_0\rangle \quad \equiv$$

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



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

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



[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

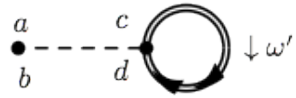
$$\mathbf{\Sigma}^{\star}_{ab}(\omega) \equiv \begin{pmatrix} \Sigma^{\star\,11}_{ab}(\omega) & \Sigma^{\star\,12}_{ab}(\omega) \\ \Sigma^{\star\,21}_{ab}(\omega) & \Sigma^{\star\,22}_{ab}(\omega) \end{pmatrix}$$

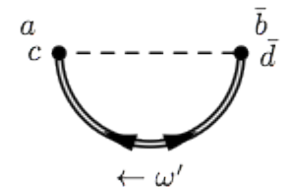
$$\mathbf{\Sigma}^{\star}_{ab}(\omega) \equiv \mathbf{\Sigma}_{ab}(\omega) - \mathbf{U}_{ab}$$

1st & 2nd order diagrams

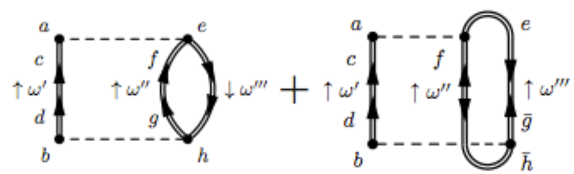
[V. Somà, T. Duguet, CB, Pys. Rev. C84, 046317 (2011)]

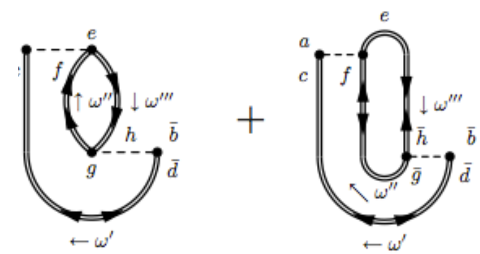
- 1[st] order ➟ energy-independent self-energy

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

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

- 2[nd] order ➟ energy-dependent self-energy

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

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

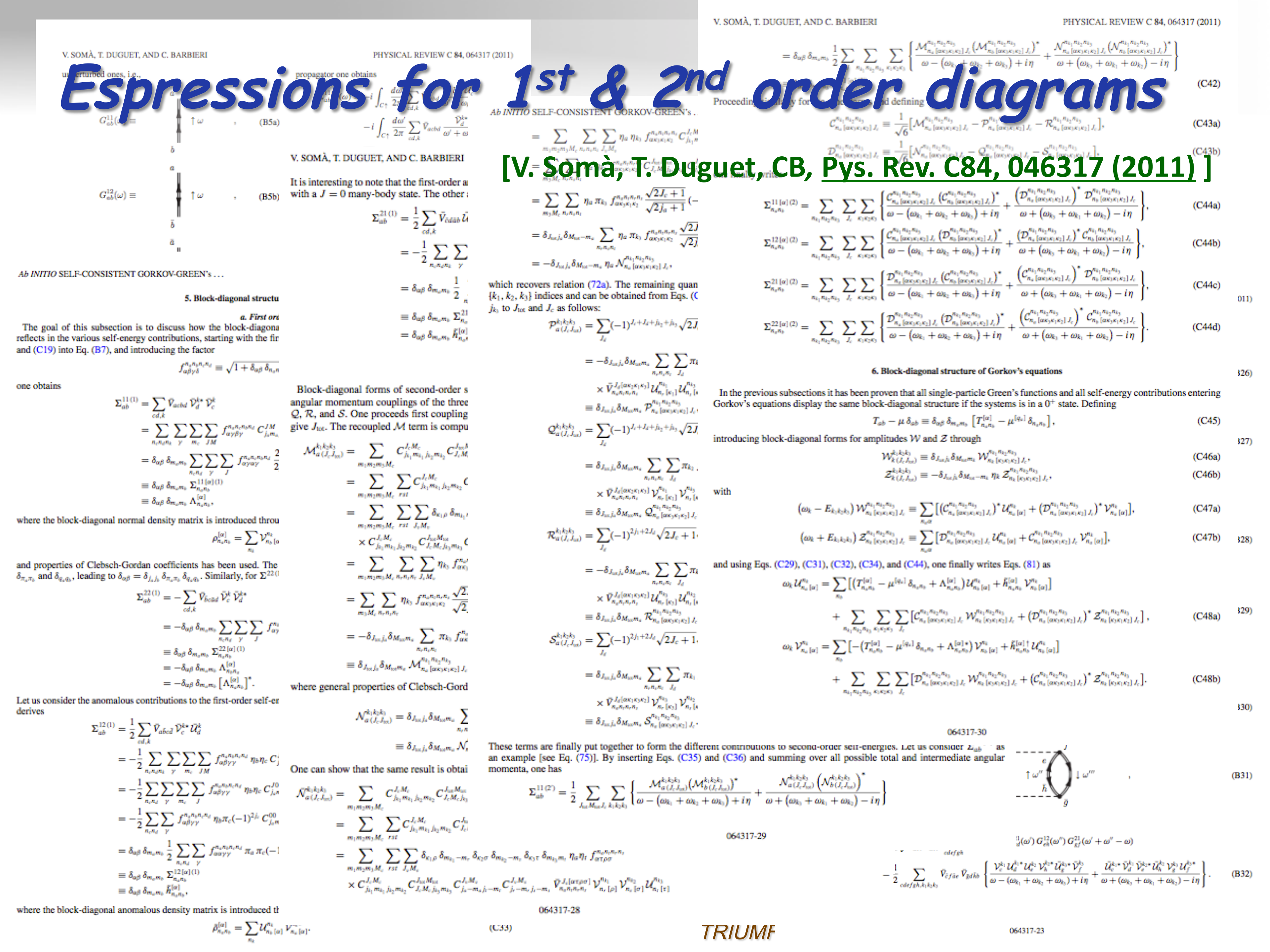
- Gorkov equations ⟶ eigenvalue problem

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

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

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)]

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

⇓

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

Energy *independent* eigenvalue problem

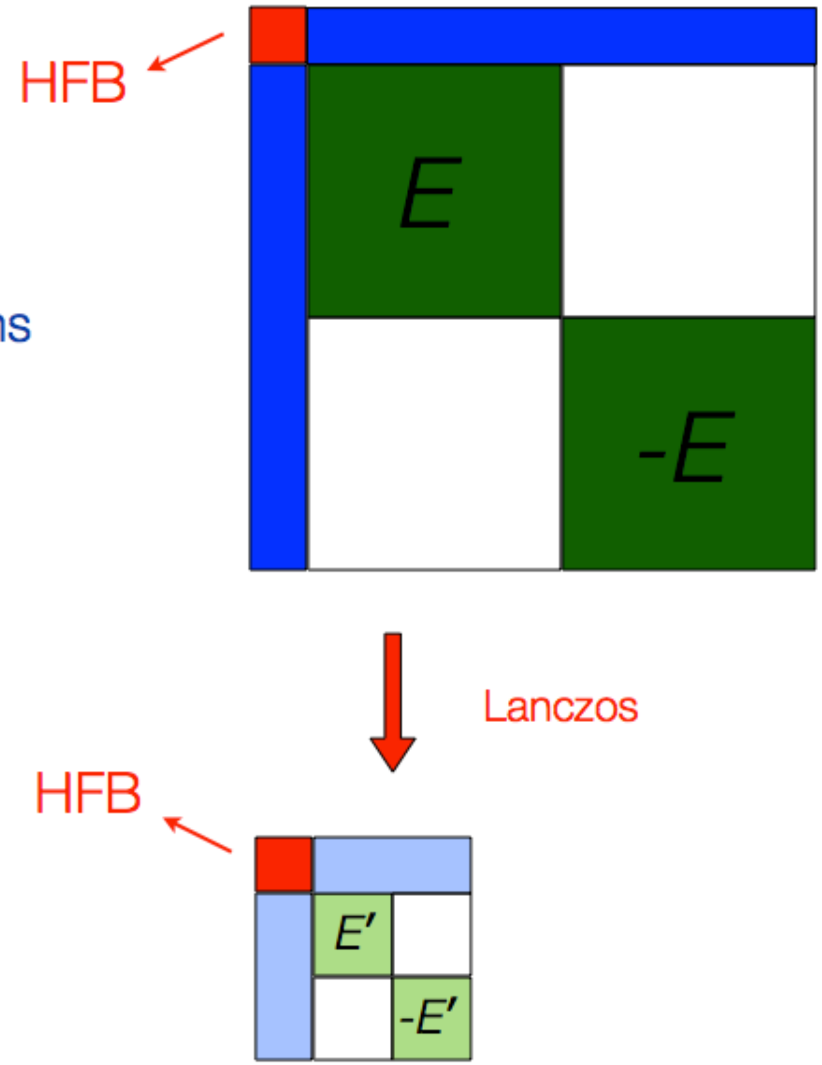
with the normalization condition $\sum_a \left[\left|\mathcal{U}^k_a\right|^2 + \left|\mathcal{V}^k_a\right|^2 \right] + \sum_{k_1 k_2 k_3} \left[\left|\mathcal{W}^{k_1 k_2 k_3}_k\right|^2 + \left|\mathcal{Z}^{k_1 k_2 k_3}_k\right|^2 \right] = 1$

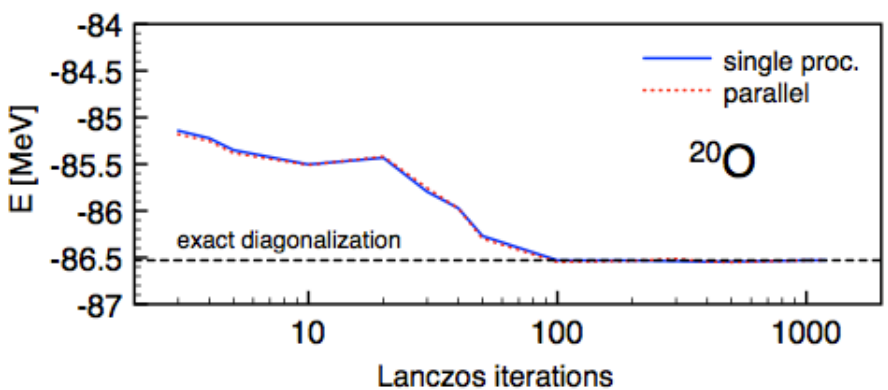
Lanczos reduction of self-energy

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

➟ Conserves moments of spectral functions

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

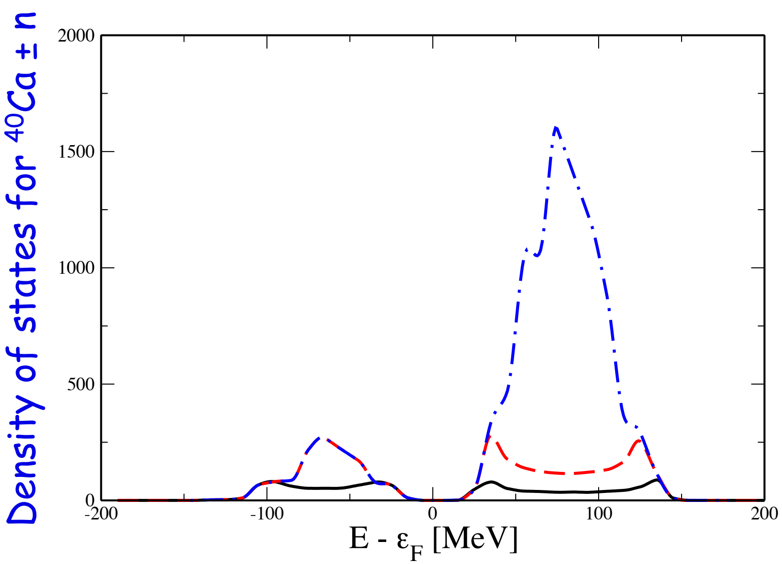


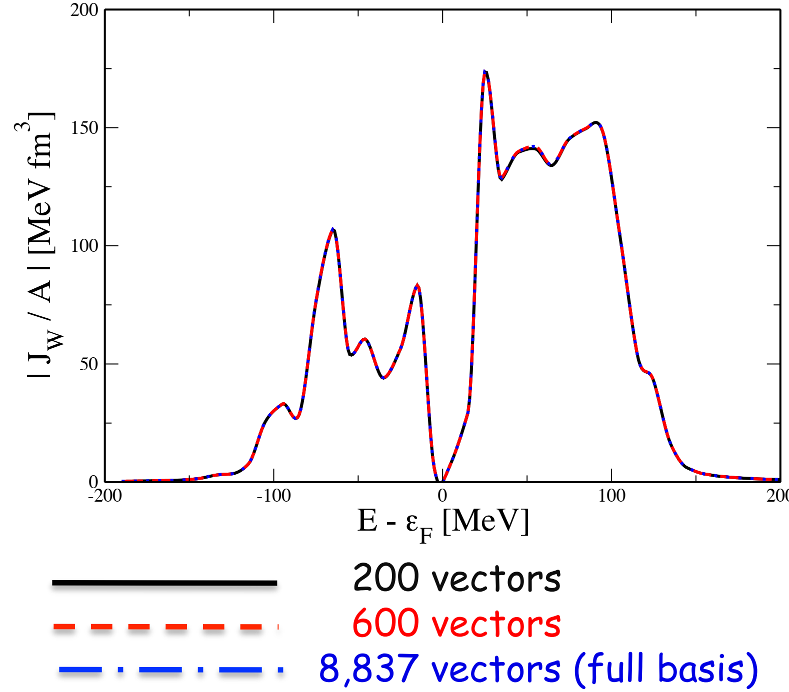


Application of Lanczos (example)

➔# 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





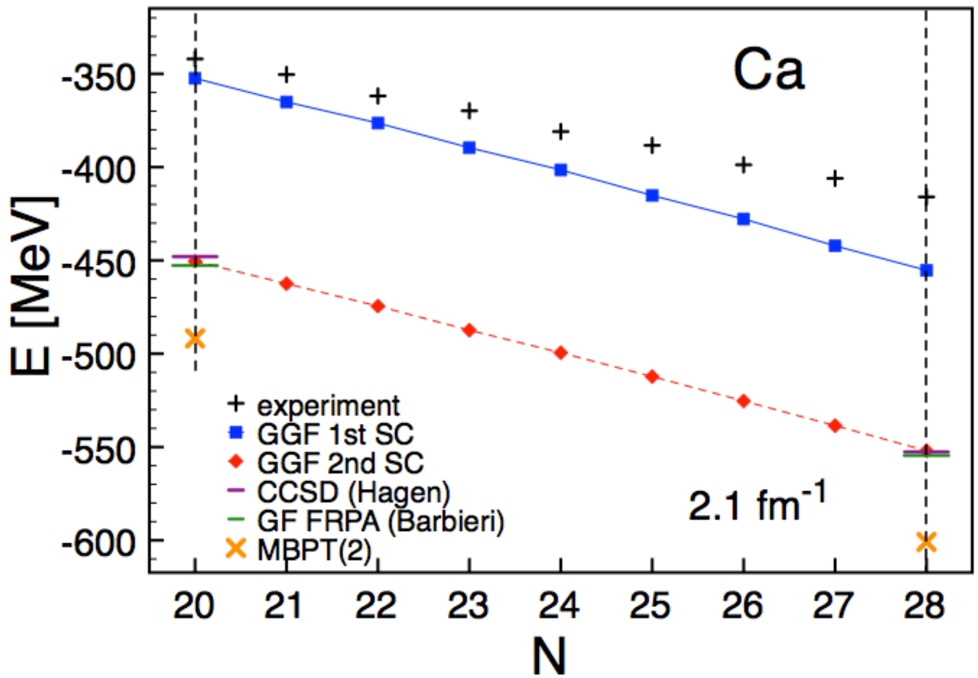
➔ Ground state energies converge with ≥ 200Lanczos vectors (10 osc. shells).

Preliminary Gorgov results

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

Binding energies

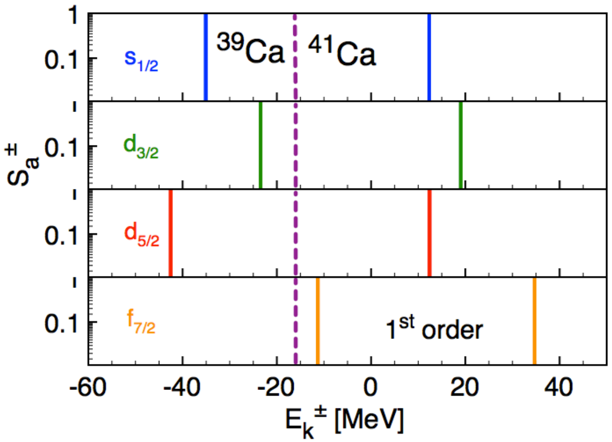
- Systematic along isotopic/isotonic chains has become available



- 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

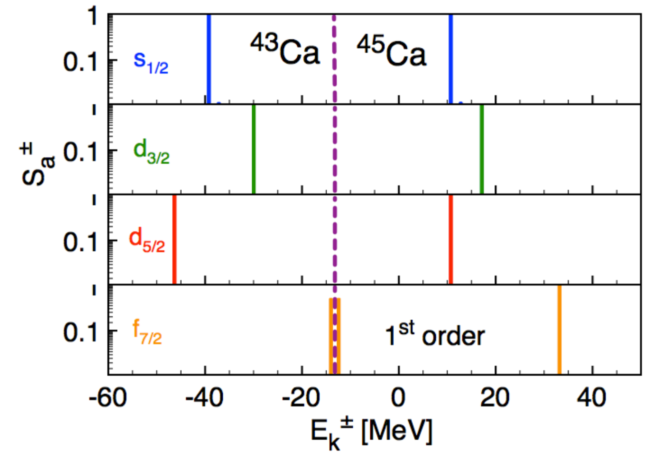
Spectral function

Dyson 1st order (HF)



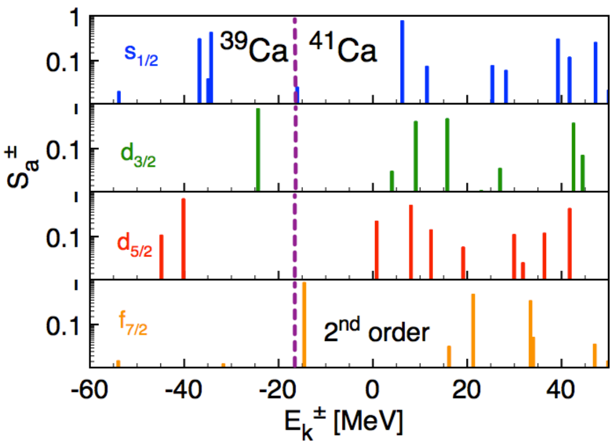
Fragmentation

Gorkov 1st order (HFB)



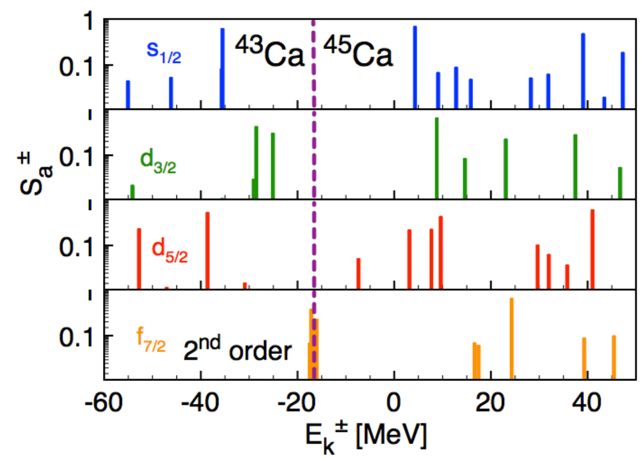
Static pairing

Dyson 2nd order



Dynamical fluctuations

Gorkov 2nd order

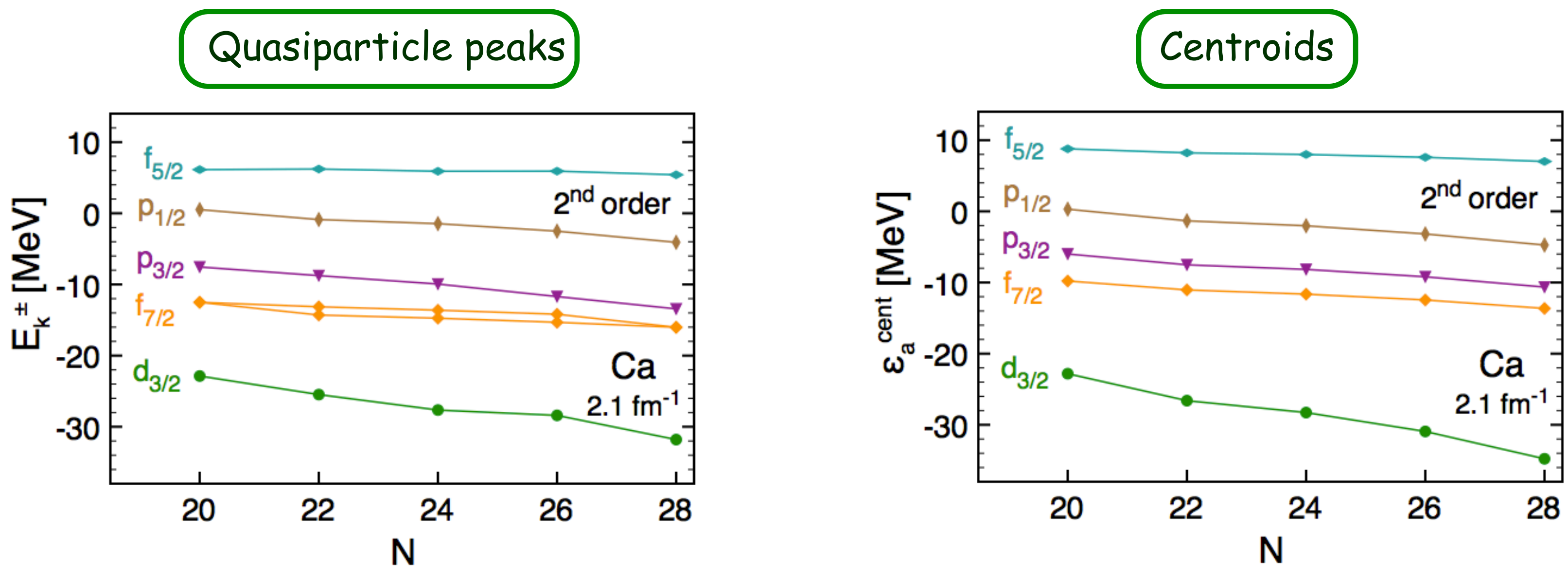


Shell structure evolution

- ESPE collect fragmentation of "single-particle" strengths from both N±1

$$\epsilon_a^{cent} \equiv h_{ab}^{cent}\,\delta_{ab} = t_{aa} + \sum_{cd} \bar{V}_{acad}^{NN}\,\rho_{dc}^{[1]} + \sum_{cdef} \bar{V}_{acdaef}^{NNN}\,\rho_{efcd}^{[2]} \equiv \sum_k S_k^{+a} E_k^{+} + \sum_k S_k^{-a} E_k^{-}$$

[Baranger 1970, Duguet, CB, *et al.* 2011]



➟ ESPE not to be confused with quasiparticle peak

➟ Particularly true for low-lying state in open-shell due to pairing

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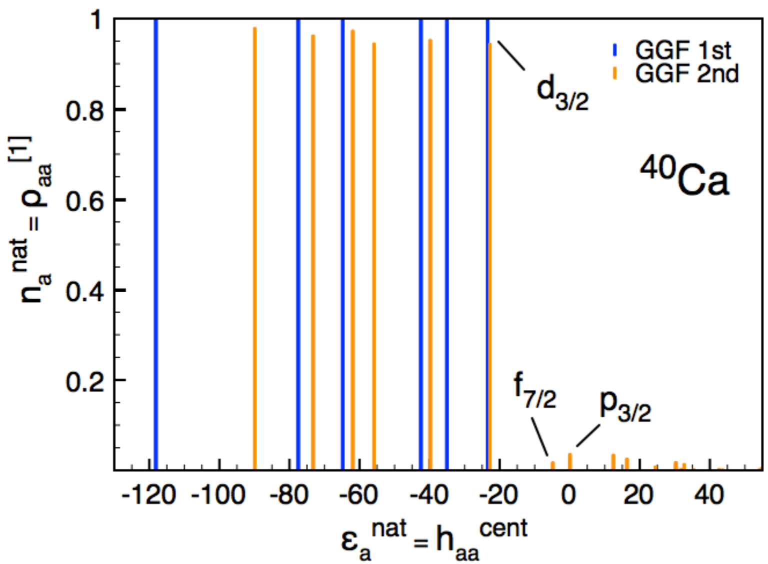
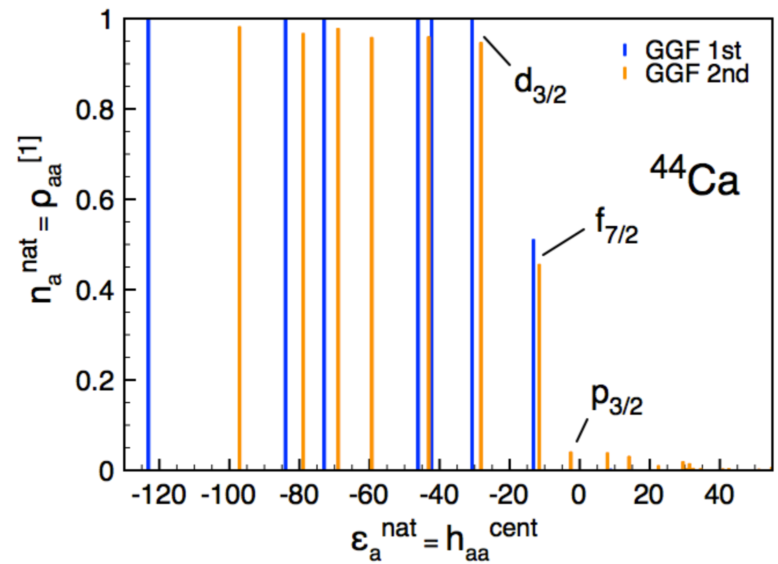
Natural single-particle occupation

- Natural orbit *a*: $\rho_{ab}^{[1]} = n_a^{nat}\, \delta_{ab}$
- Associated energy: $\varepsilon_a^{nat} = h_{aa}^{cent}$

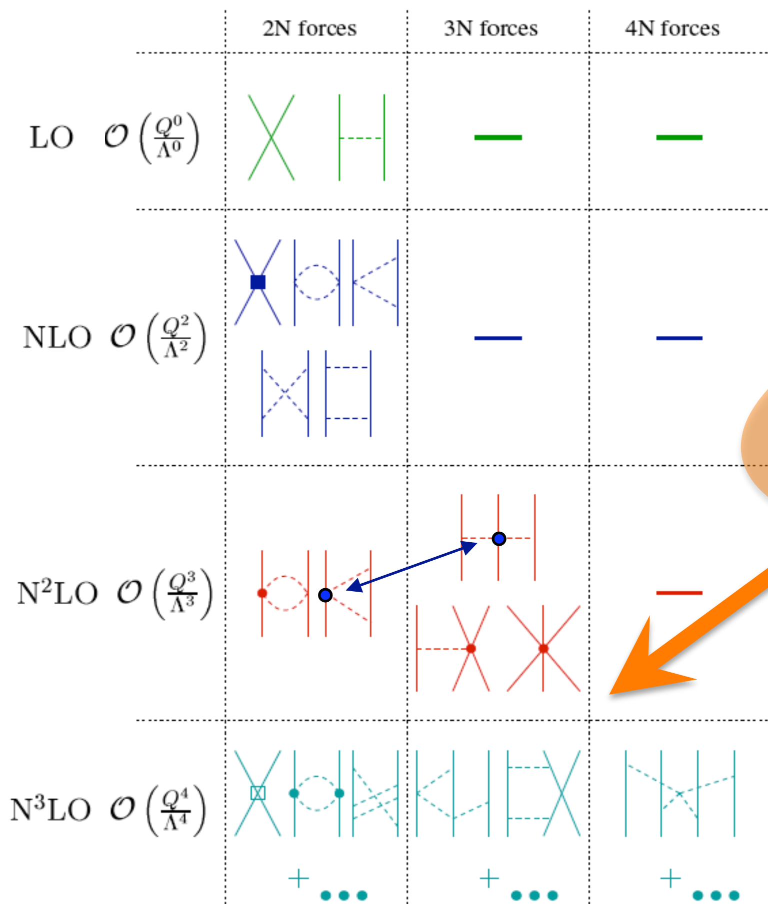




- Dynamical correlations similar for doubly-magic and semi-magic
- Static pairing essential to open-shells

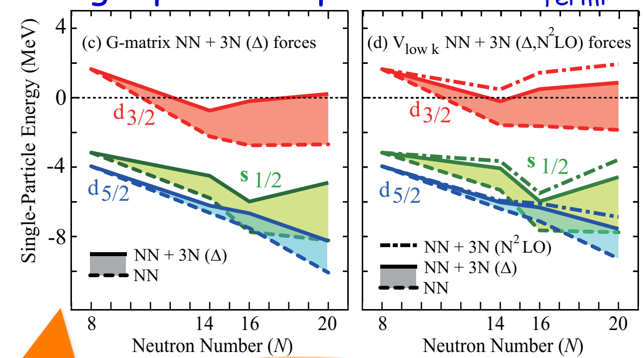
Modern realistic nuclear forces

Chiral EFT for nuclear forces:



(3NF arise naturally at N2LO)

Single particle spectrum at E_{fermi}:

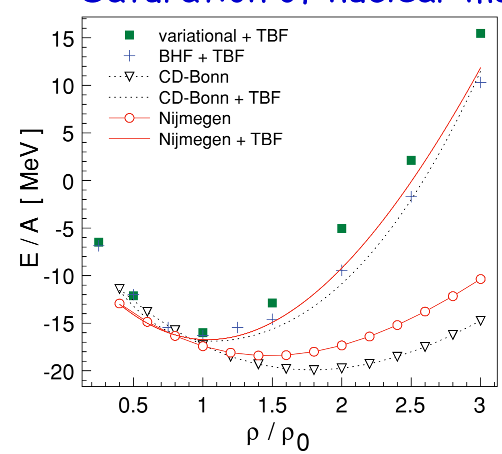


[T. Otsuka et al., Phys Rev. Lett **105**, 32501 (2010)]

Need at LEAST 3NF!!!

("cannot" do RNB physics without…)

Saturation of nuclear matter:

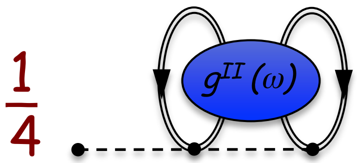


[V. Somà, Phys Rev. C **78**, 054003 (2008))]

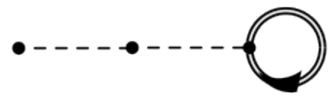
Inclusion of NNN forces

A. Cipollone, CB, P. Navratil

- NNN forces can enter diagrams in three different ways:



Correction to external
1-Body interaction



Correction to
non-contracted
2-Body interaction

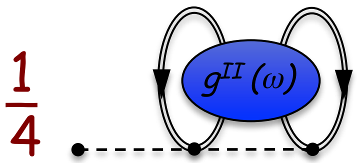
pure 3-Body
contribution

- Contractions are with *fully correlated density matices*
(NOT a normal ordering…)

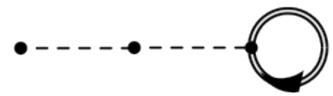
Inclusion of NNN forces

A. Cipollone, CB, P. Navratil

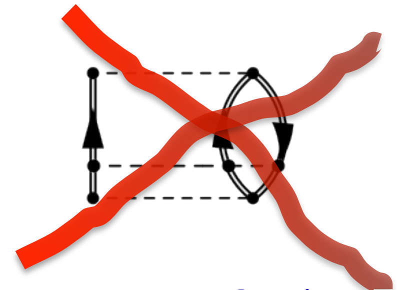
- NNN forces can enter diagrams in three different ways:



Correction to external 1-Body interaction



Correction to *non-contracted* 2-Body interaction



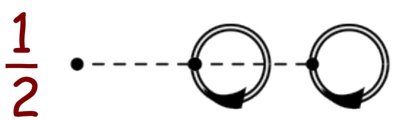
pure 3-Body contribution

- Contractions are with *fully correlated density matices* (NOT a normal ordering…)

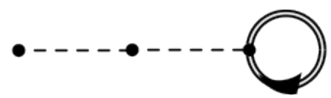
Inclusion of NNN forces

A. Cipollone, CB, P. Navratil

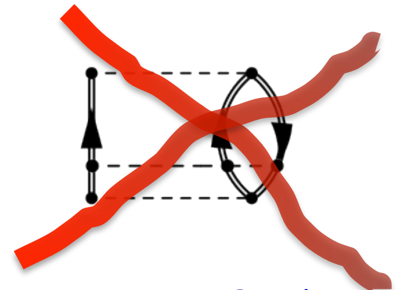
- NNN forces can enter diagrams in three different ways:



Correction to external 1-Body interaction



Correction to *non-contracted* 2-Body interaction



pure 3-Body contribution

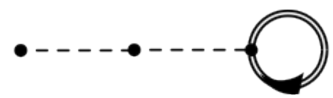
Inclusion of NNN forces

A. Cipollone, CB, P. Navratil

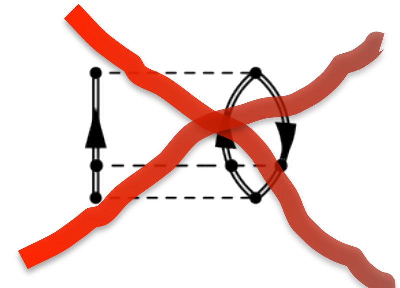
- NNN forces can enter diagrams in three different ways:

$\frac{1}{2}$ 

Correction to external 1-Body interaction

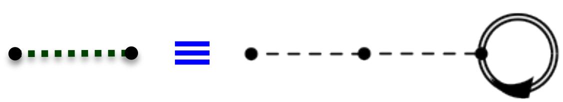


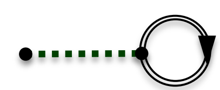
Correction to *non-contracted* 2-Body interaction



pure 3-Body contribution

BEWARE that defining:



and then: 

would *double count* the 1-body term.

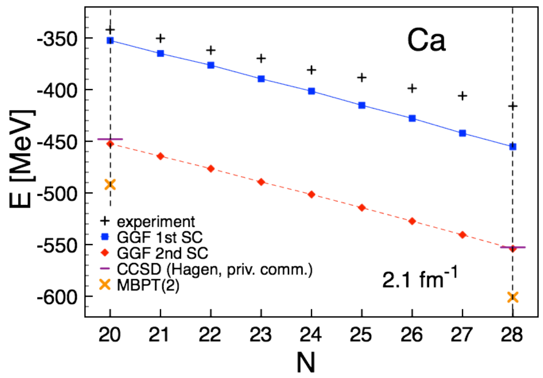
Summary

• Self-Consistent Green's Functions (SCGF), is a microscopic *ab-initio* method applicable to medium mass nuclei.

•The *greatest advantage* is the link to experimental information (→ spectroscopy)

• *The bigger challenges are:*
  • *Approach open-shells*
  • *Consistent description of structure and reactions*

• *SCGF* are the *optimal* choice
  • extension to Gorkov-formalism
    → Open-shell nuclei
    → Reactions at driplines
    → structure of next generation EDF



• *Proof of principle calculations Gorgov theory and* three nucleon forces (3NF) are underway.

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Thank you for your attention!!!