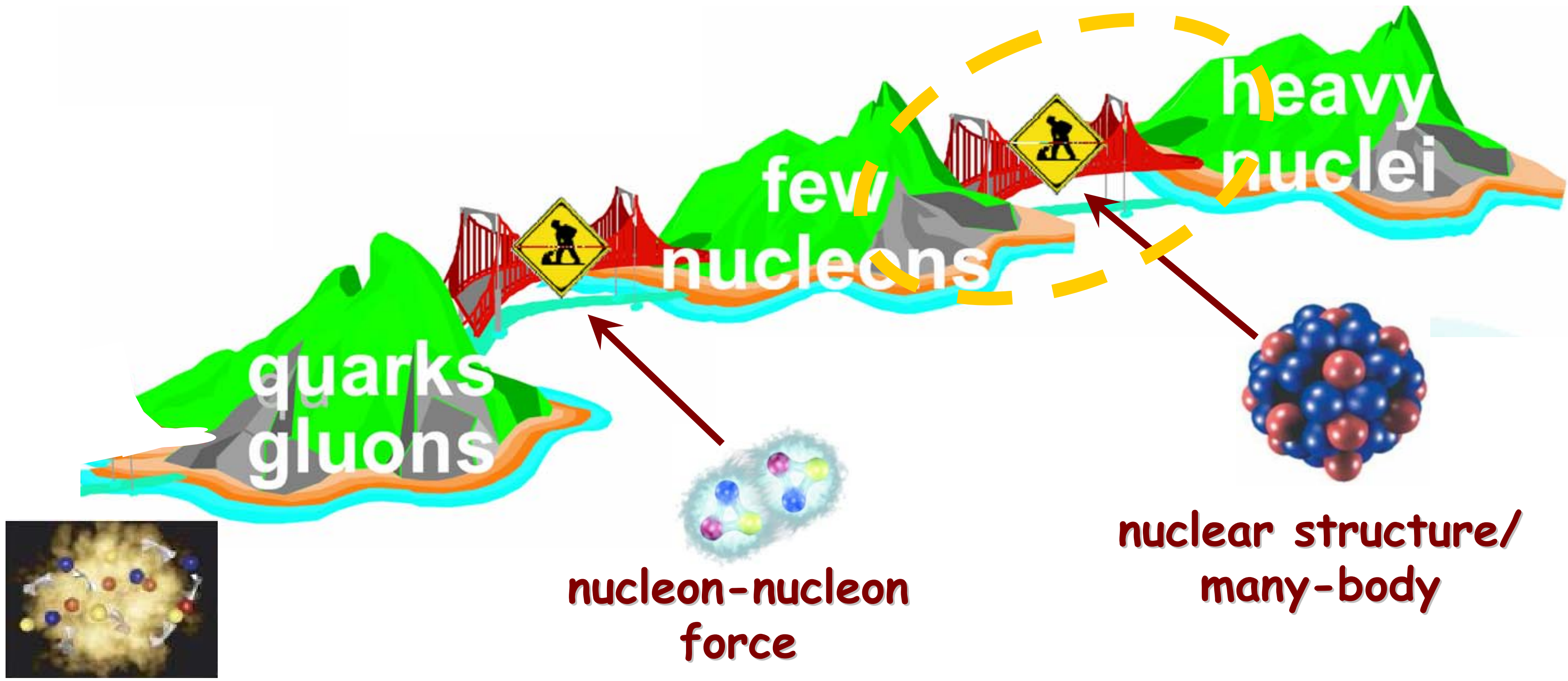
Applications of Green's Function Theory to Atoms and Nuclei

C. Barbieri

Collaborators: W. H. Dickhoff, D. Van Neck, K. Langanke,
G. Martinez-Pinedo , R. Roth , C. Giusti, F. D. Pacati

Nuclear Structure in the 21st Century



Microscopic nuclear structure theory

- Wish to predict properties of nuclei from the A-body Hamiltonian:

$$H = T + V = \sum_{i=1}^{A} \frac{p_i^2}{2\ m} + \sum_{i<j}^{A} V_{ij} + \ldots$$

- *ab-initio* approaches:
  - Monte Carlo methods (A ≤ 12)
  - no-core shell model, coupled cluster (^{16}O,^{40}Ca for now)
- *alternatives*:
  - Many-body Green's functions: "phonons" as degrees of freedom

→ strong link to spectroscopy
→ starts from the nucleon-nucleon force

→ optical potential (DOM) and QP-DFT

Green's functions in many-body theory

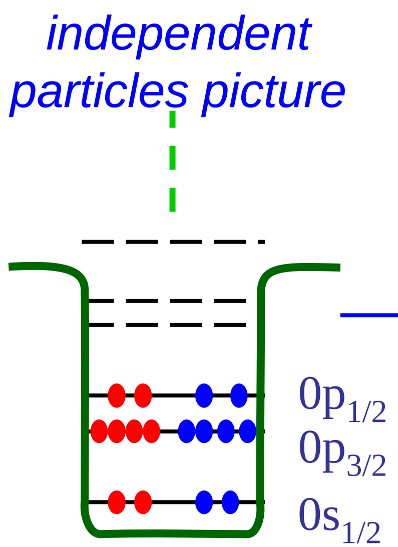
One-body Green's function (or propagator) describes the motion of quasi- **particles** and **holes**:

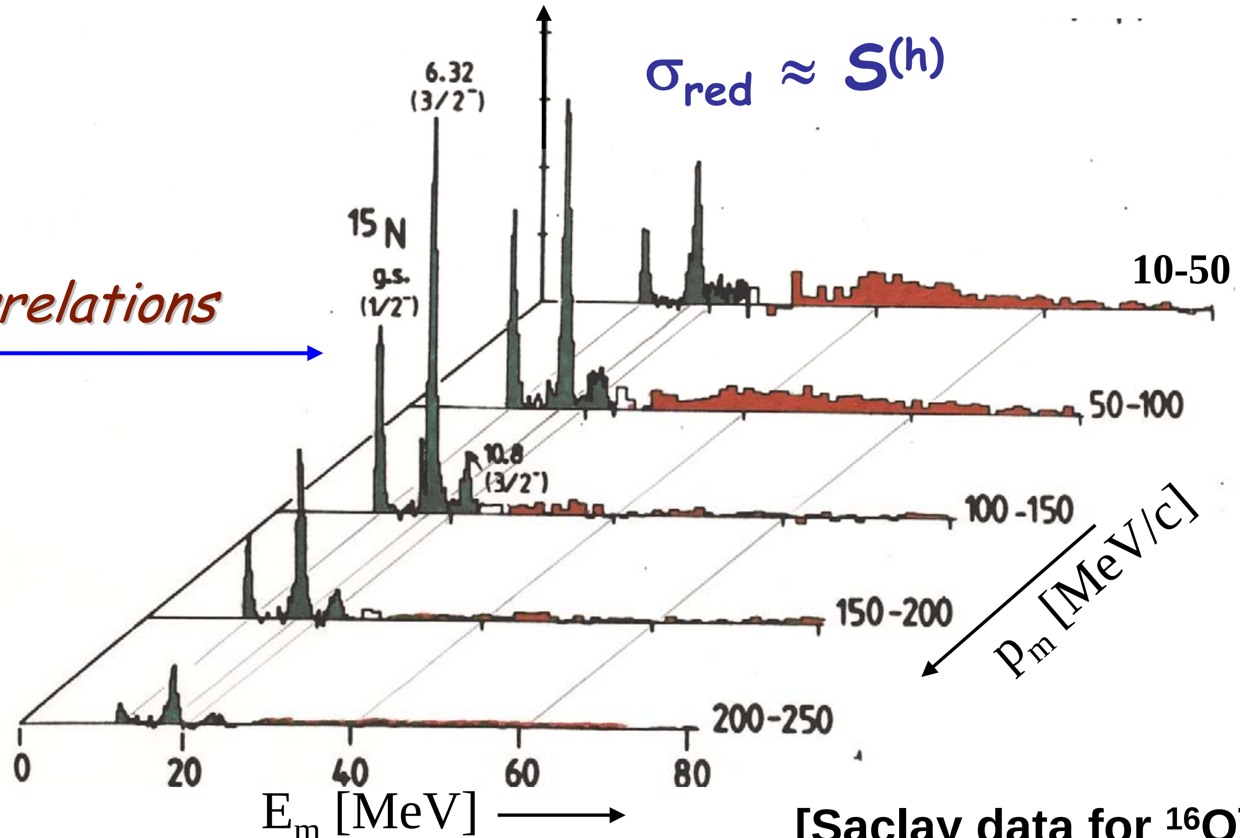
$$g_{\alpha\beta}(\omega) = \sum_n \frac{\langle\Psi_0^A|c_\alpha|\Psi_n^{A+1}\rangle\langle\Psi_n^{A+1}|c_\beta^+|\Psi_0^A\rangle}{\omega-(E_n^{A+1}-E_0^A)+i\eta} + \sum_k \frac{\langle\Psi_0^A|c_\beta^+|\Psi_k^{A-1}\rangle\langle\Psi_k^{A-1}|c_\alpha|\Psi_0^A\rangle}{\omega-(E_0^A-E_k^{A-1})-i\eta}$$

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

$$S_\alpha(\omega) = \frac{1}{\pi}\mathrm{Im}\, g_{\alpha\alpha}(\omega) = \sum_n \left|\langle\Psi_n^{A\pm1}|c_\alpha|\Psi_0^A\rangle\right|^2 \delta(\omega-(E_0^A-E_n^{A\pm1}))$$

One-hole spectral function -- example





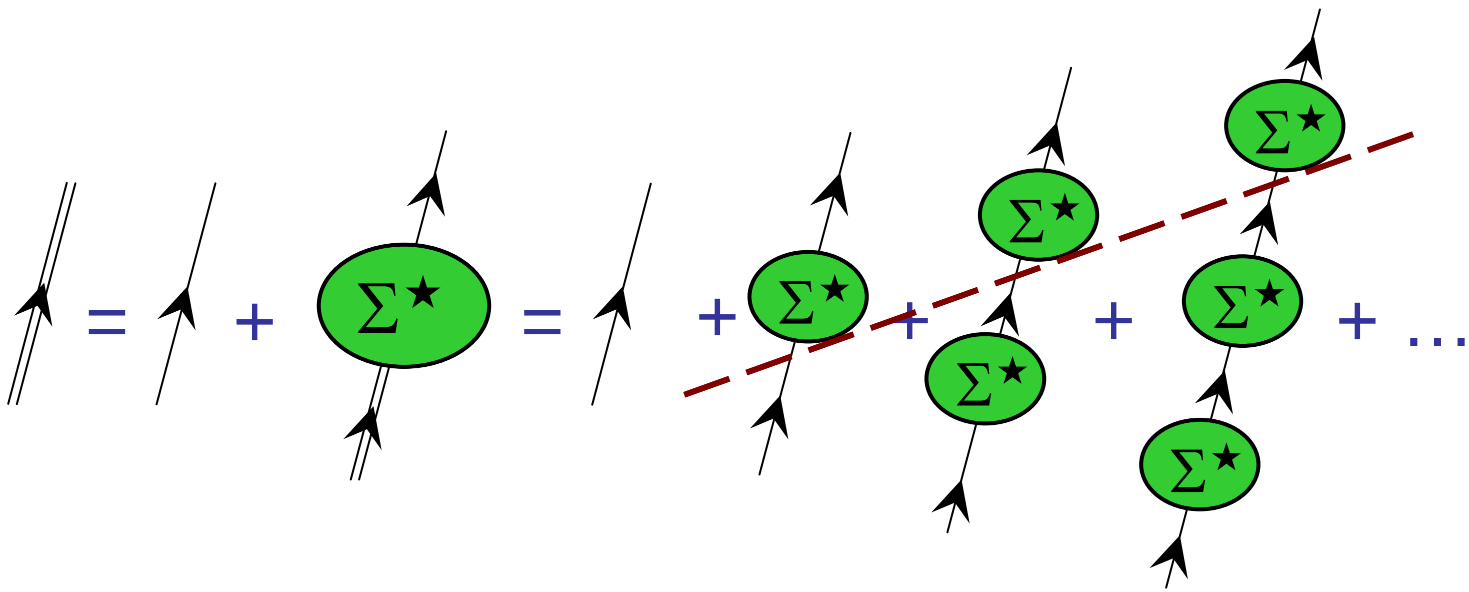
[Saclay data for ^{16}O]

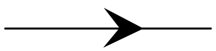
$$S^{(h)}(p_m, E_m) = \sum_n \left| \langle \Psi_n^{A-1} | c_{\vec{p}_m} | \Psi_0^A \rangle \right|^2 \delta(E_m - (E_0^A - E_n^{A-1}))$$

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

GSI theory

Dyson equation

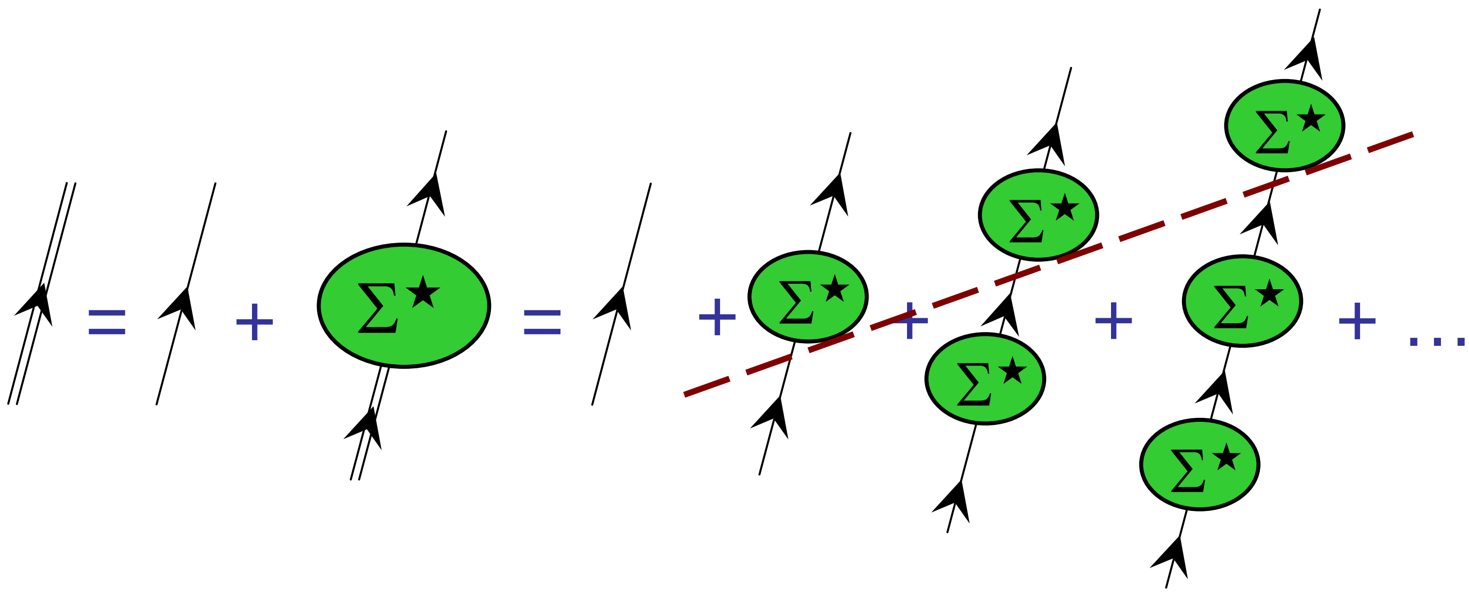


 , *free particle* propagator

 , *correlated particle* propagator

, *"irreducible"* self-energy

Coupling single particle to collective modes - I

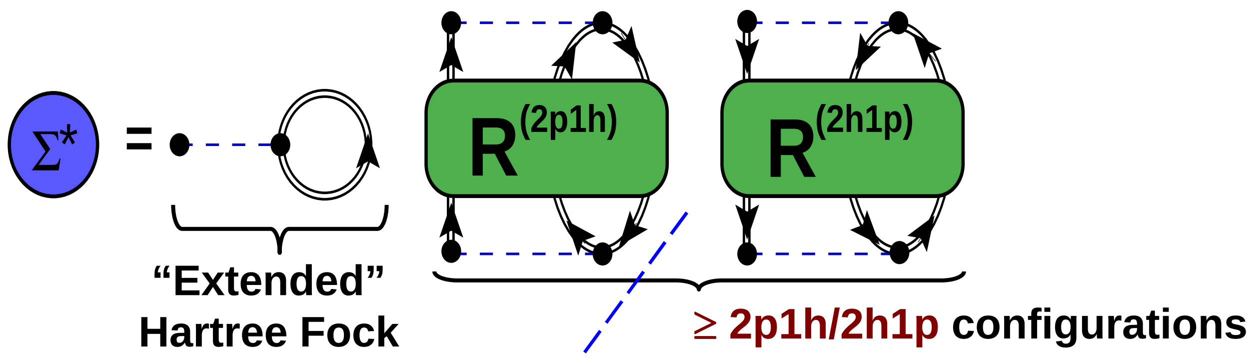


correlations are embedded in the *"irreducible"* self-energy: Σ*

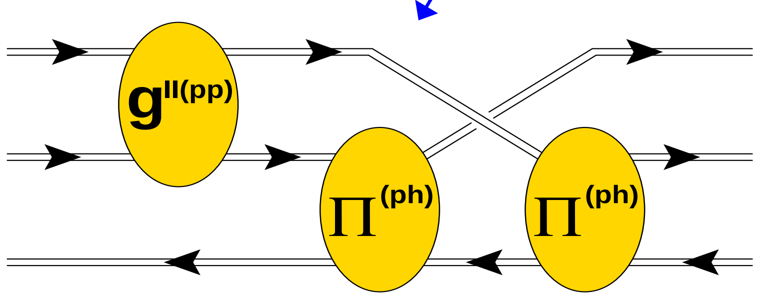
expand in terms of the dressed propagator: ⟹ all orders resummation

Coupling single particle to collective modes - II

- Non perturbative expansion of the self-energy:

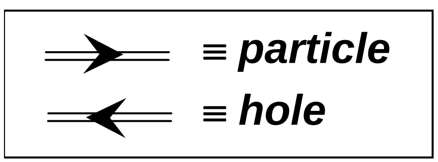


- Explicit correlations enter the “three-particle irreducible” propagators:



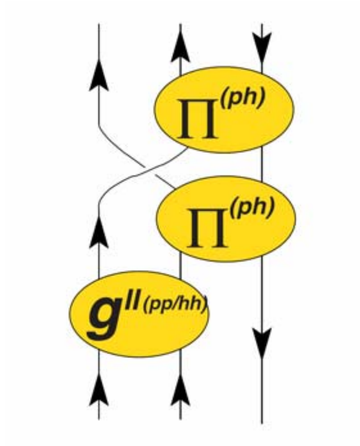
•Both pp (ladder) and ph (ring) modes included

•Pauli exchange at 2p1h/2h1p level

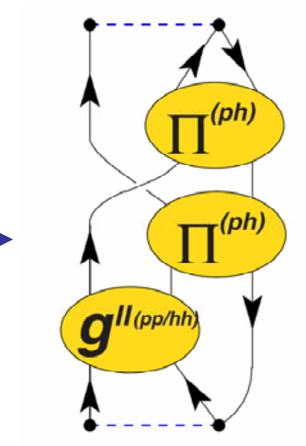


[CB, et al., PRC63, 034313 (2001)
PRC65, 064313 (2002)]

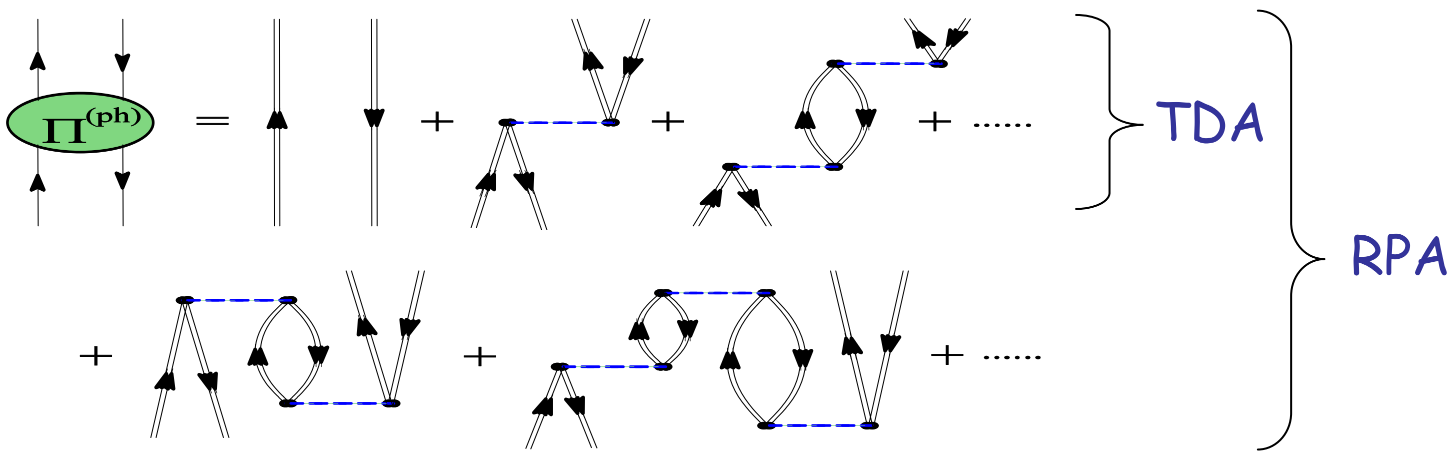
FRPA: Faddeev summation of RPA propagators



- Both pp (ladder) and ph (ring) modes included
- Pauli exchange at 2p1h/2h1p level
- All order summation through a set of Faddeev equations

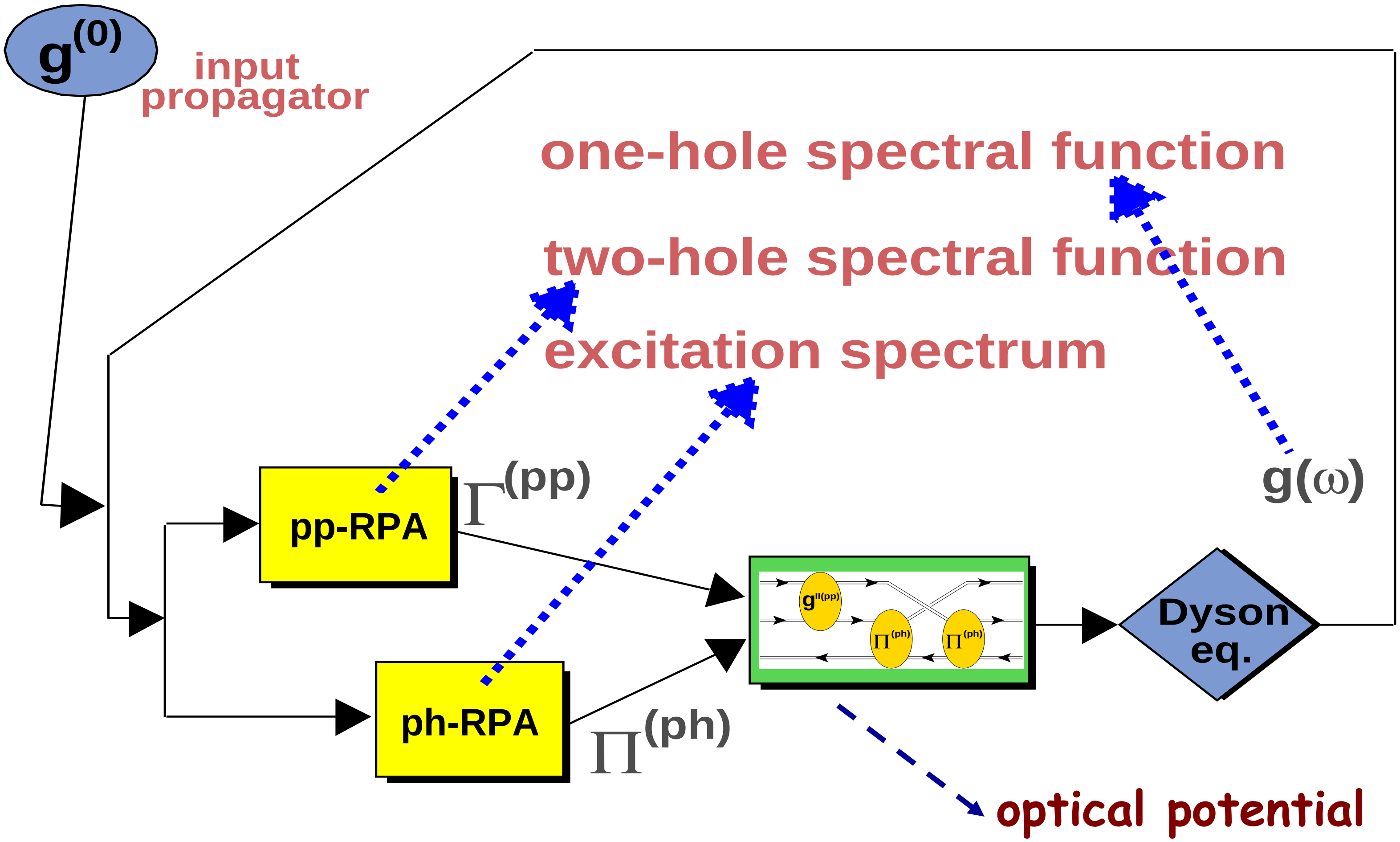


where:



References: CB, et al., Phys. Rev. C63, 034313 (2001); Phys. Rev. A76, 052503 (2007)

Self-consistent Green's function approach



…wide range of applications !!

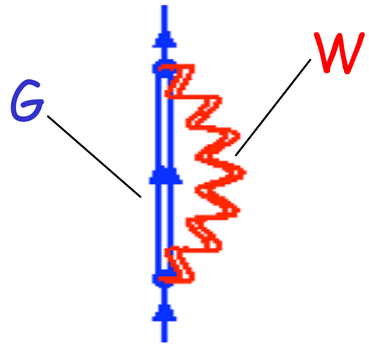
Why "self-consistent" propagators ?

- Dressed propagators account for (the observed) strength fragmentation

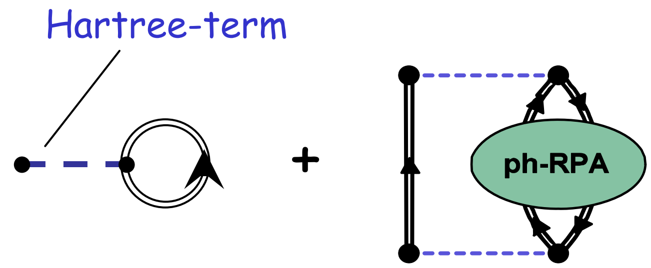
- Self-consistency guaranties:
  - fulfillment of basic conservation laws
    [but not trivial to reach beyond 1st order (HF)…]
  - consistency among different ways of evaluating the binding energy
  - independence from the reference state

Applications to Electron Systems

Self-consistent Green's function fot the Ground State Energy of the Electron Gas



or:



GW approximation:

$G \equiv$ self-consistent sp propagator

$W \equiv$ screened Coulomb interaction

➔RPA with dressed propagator

Electron gas : -XC energies (Hartrees)

Method	$r_s = 1$	$r_s=2$	$r_s=4$	$r_s=5$	$r_s=10$	$r_s=20$	Reference
QMC	0.5180	0.2742	0.1464	0.1197	0.0644	0.0344	CA80
	0.5144	0.2729	0.1474	0.1199	0.0641	0.0344	OB94;OHB99
GW	0.5160	0.2727	0.1450	0.1185	0.0620	0.032	GG01
		0.2741	0.1465				HB98

Accurate self-energies are needed for extending DFT to include quasiparticles explicitly (QP-DFT):

- Quasiparticles and ionization energies:
  need 3rd order PT minimum
  → ADC(3), Heidelberg group ≡ F-TDA
- Extended systems: need RPA → plasmon structure

F-RPA !!

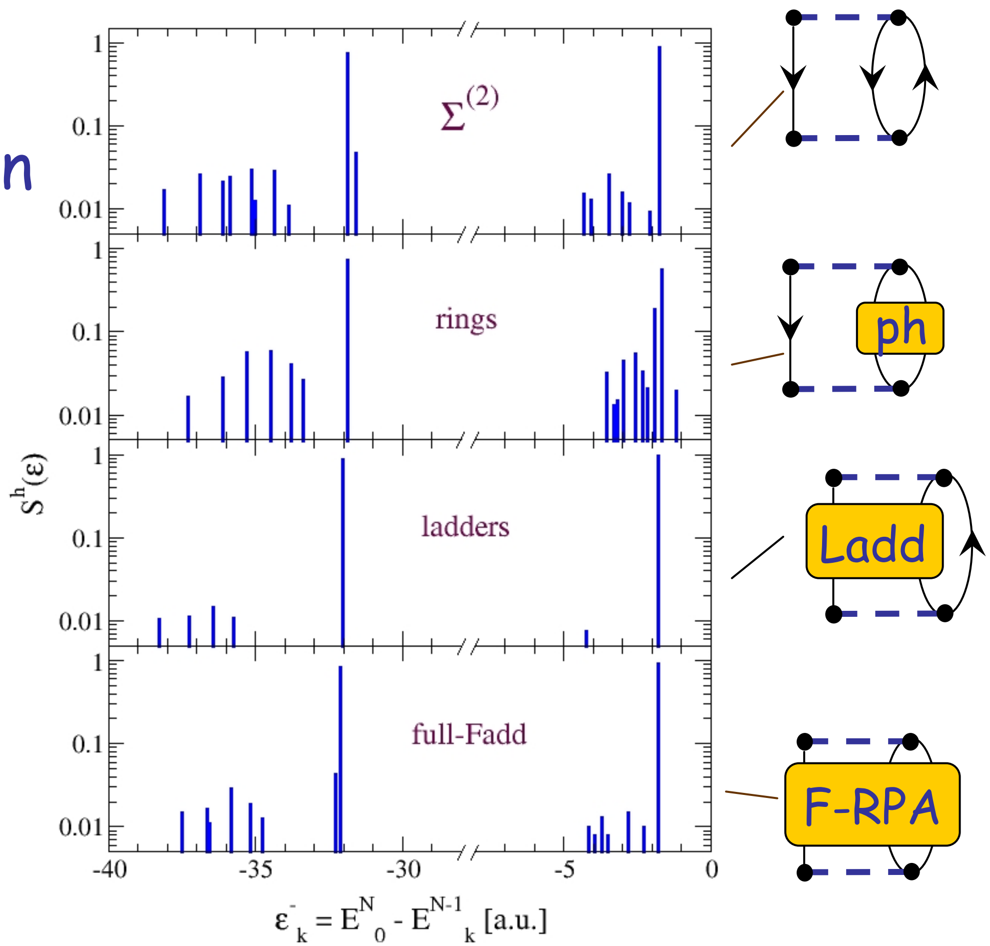
CB, D. Van Neck, W.H.Dickhoff, Phys. Rev. A76, 052503 (2007)
—Published yesterday! ☺

FRPA for the Neon atom

1s and 2s strength in Neon

quasiparticles easily identified

inteference!



CB, D. Van Neck, W.H.Dickhoff, Phys. Rev. A76, 052503 (2007).

Binding energies for Atoms

	HF	FTDA	FRPA	Exp.
He:	+44	+1	+1	-2.904
Be:	+94	+24	+24	-14.667
Ne:	281	+15	+11	-128.928
Mg:	426	+358	+356	-200.043
Ar:	723	+377	+373	-527.549

Energies in Hartree /

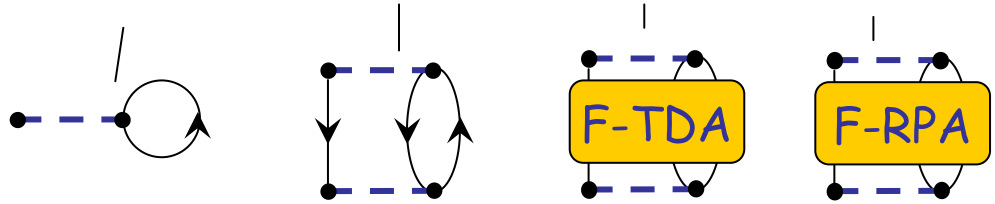
Relative to the experiment in mH

cc-pV(TQ)Z bases, extrapolated as $E_X = E_\infty + AX^{-3}$

Phys. Rev. A76, 052503 (2007).
+ work in progress

Valence Ionization Energies

	HF	2^{nd}	FTDA	FRPA	Exp.
He: 1s	-14	-2	+2	+4	-0.904
Be: 2s	+34	+23	+20	+21	-0.343
1s	-200	-87	-11	-7	-4.533
Ne: 2p	-57	+30	-15	-10	-0.793
2s	-149	+32	-21	-15	-1.782
Mg: 3s	+28	+7	+11	+4	-0.281
2p	-161	-26	-10	-10	-2.12
Ar: 3p	-11	-6	-1	+1	-0.579
3s	201	-84	-13	+10	-1.075
2p	-410	-359	-53	-39	-9.160

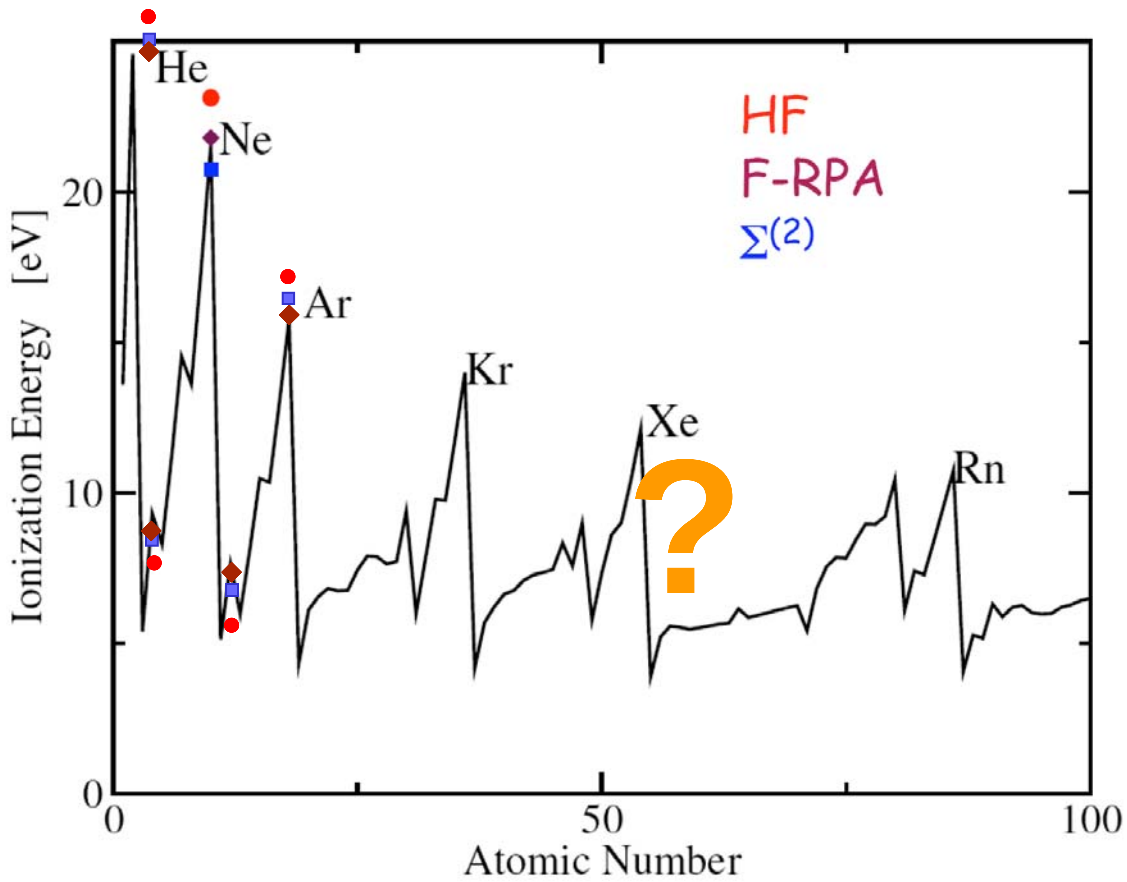


Systematic improvement of ionization energies when including RPA propagators: about 4mH for valence orbits

Energies in Hartree/
Difference w.r.t. the experiment in mH

cc-pV(TQ)Z basis, extrapolated

Periodic Table



Conclusions on Atoms

- FRPA is of at least the same quality (or even a bit better) than FTDA/ADC(3), *but:*
  - it holds promise for a coherent description of both small and large systems
  - and satisfies the requirements for of developemts of quasiparticle-DFT

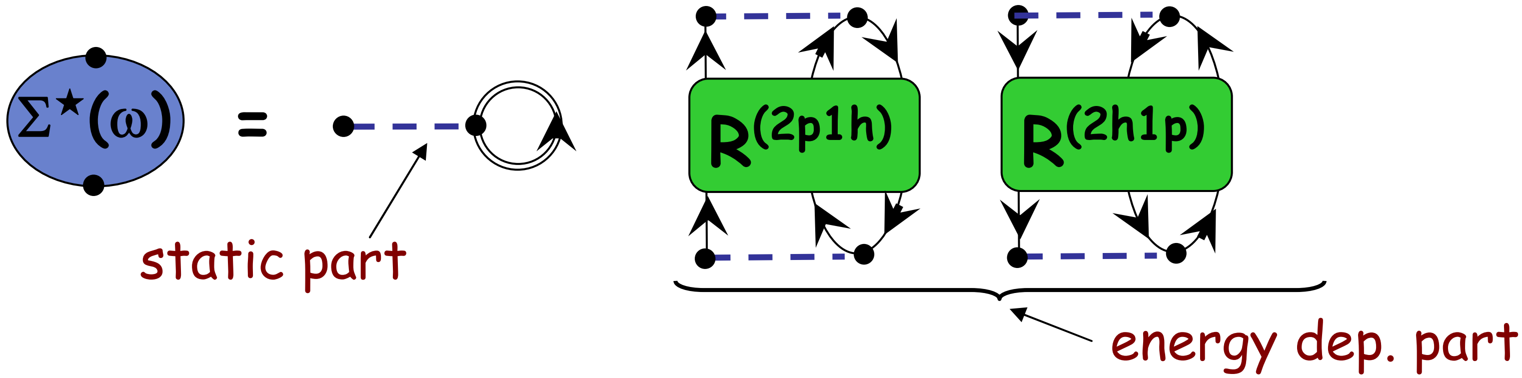
- More needs to be done…
  - Investigations for larger atoms are under way
  - Self-consistency
  - Relativistic effects can be added

Applications to Nuclei

- Strong short-range cores require “renormalizing” the interaction:
  - G-matrix, V_{UCOM}, Lee Suzuki, Bloch-Horowitz, $V_{low\text{-}k}$, …
- Long-range correlations → FRPA !!

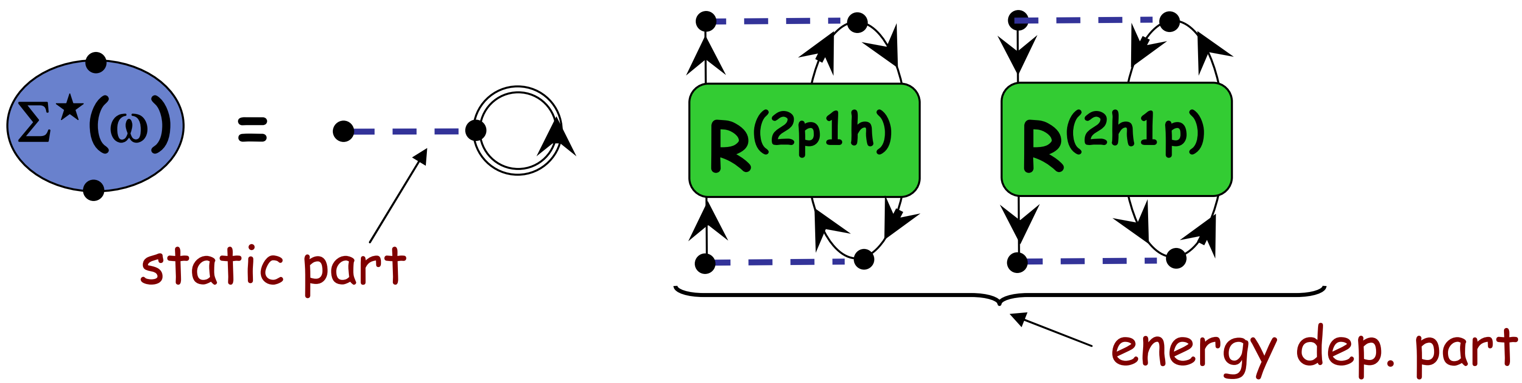
Treating short-range correlations directly…

- Non perturbative expansion of the self-energy:



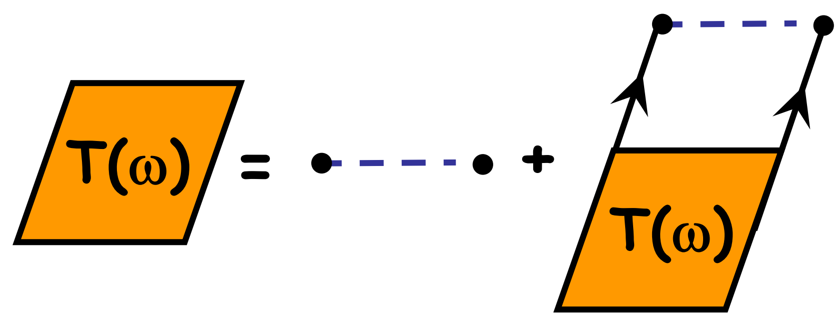
Treating short-range correlations directly…

- Non perturbative expansion of the self-energy:



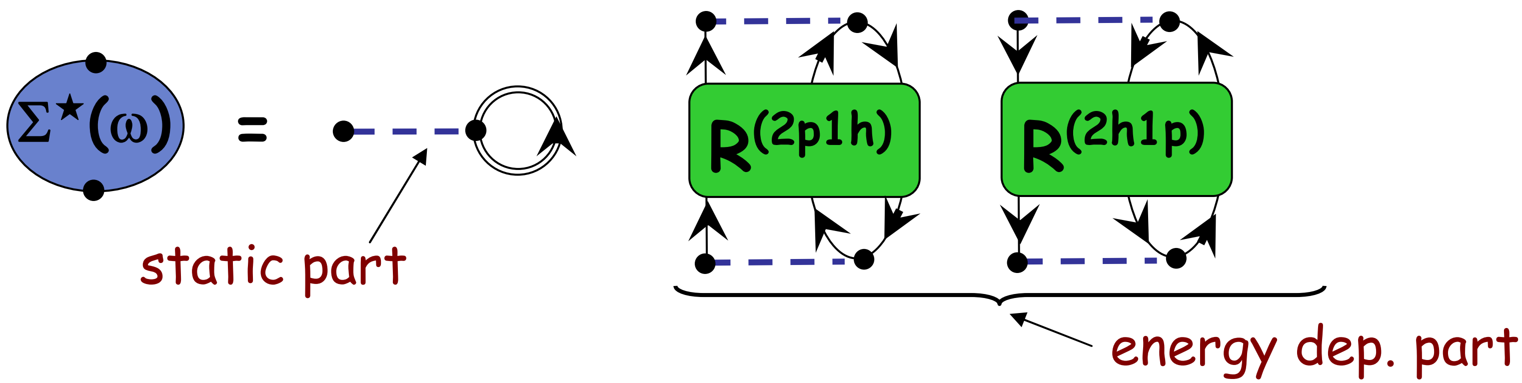
- 2 nucleons in free space: → solve for the scatt. matrix…

$$T(\omega) = V + V \frac{1}{\omega - (k_a^2 + k_b^2)/2m + i\eta} T(\omega)$$



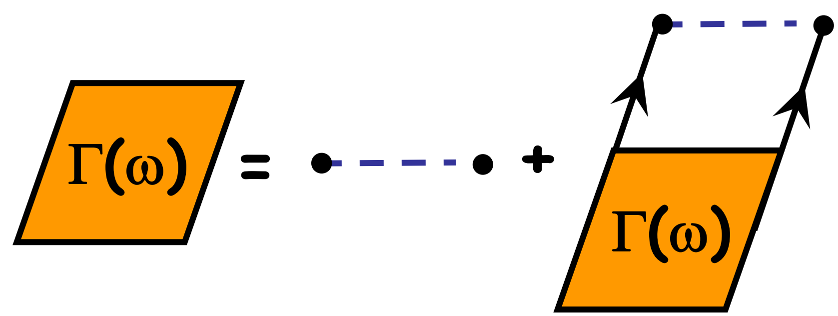
Treating short-range correlations directly…

- Non perturbative expansion of the self-energy:



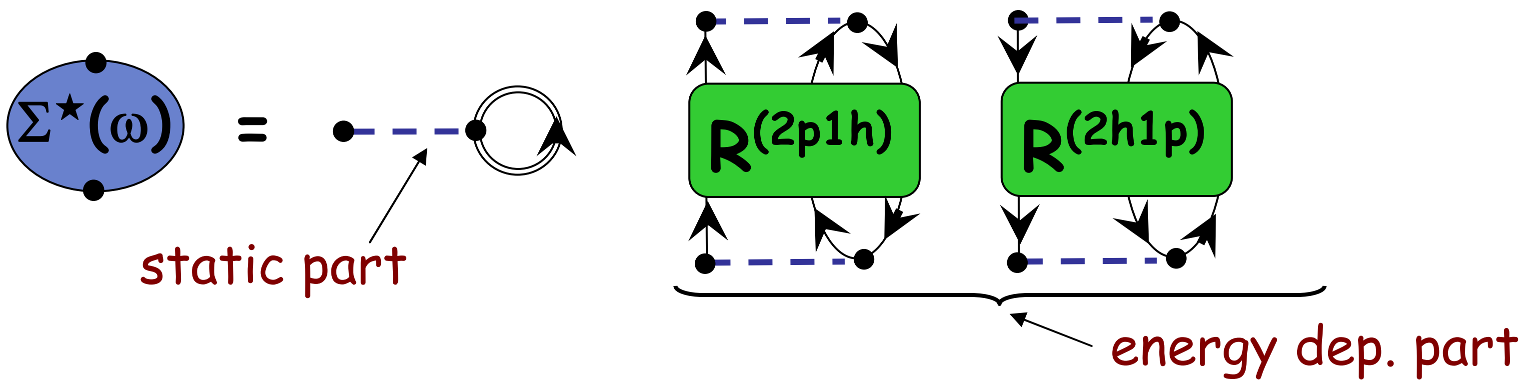
- 2 nucleons in medium: → resum pp ladders…

$$\Gamma(\omega) \approx V + V \frac{n(k_a)\,n(k_b)}{\omega - (k_a^2 + k_b^2)/2m + i\eta} \Gamma(\omega)$$

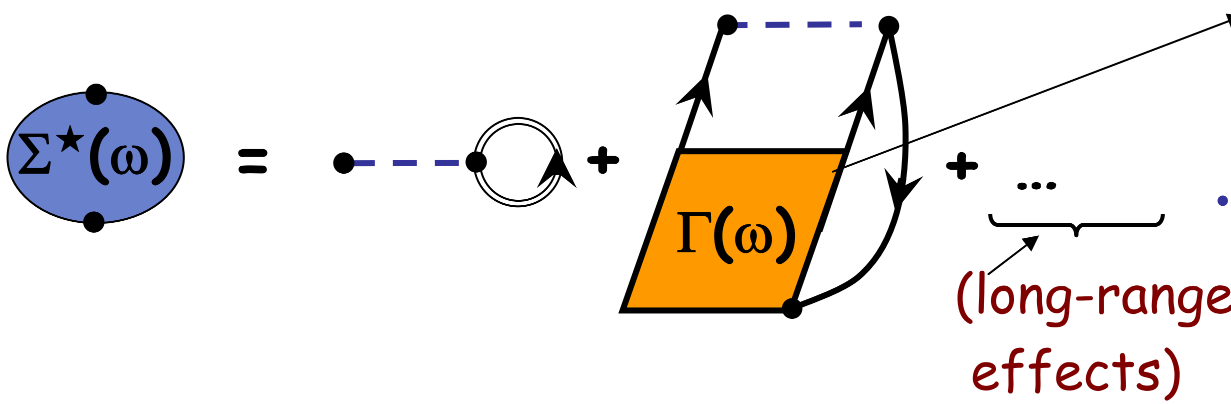


Treating short-range correlations directly…

- Non perturbative expansion of the self-energy:



- Identify the pp resummations (which account for short range correlations) in the expansion of R(ω):



•Inside the MS:

→ladders already accouted by FRPA

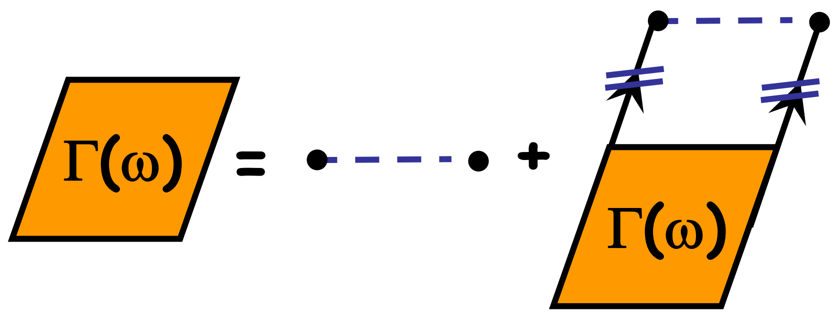
•Outside the MS:

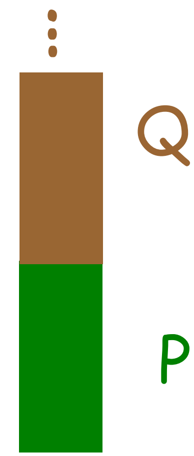
→ one still NEEDS to resum ladders

Treating short-range corr. with a G-matrix

- The short-range core can be treated by resumming ladders outside the model space:

$$\Gamma(\omega) = V + V \frac{\hat{Q}}{\omega - (k_a^2 + k_b^2)/2m + i\eta} \Gamma(\omega)$$

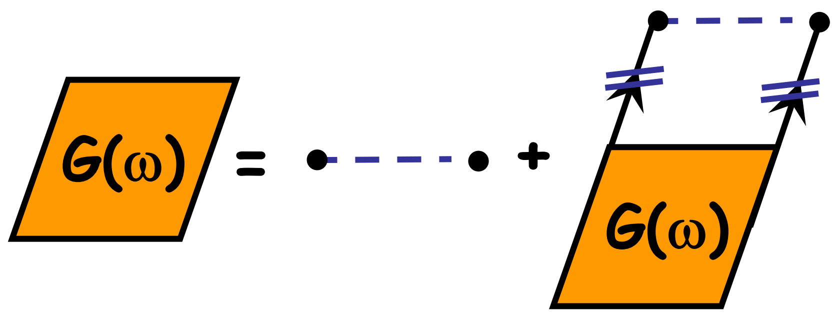


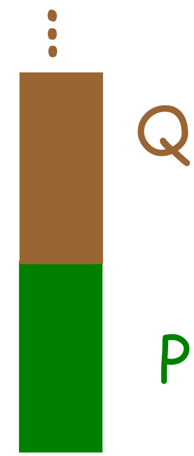


Treating short-range corr. with a G-matrix

- The short-range core can be treated by resumming ladders outside the model space:

$$G(\omega) = V + V \frac{\hat{Q}}{\omega - (k_a^2 + k_b^2)/2m + i\eta} G(\omega)$$

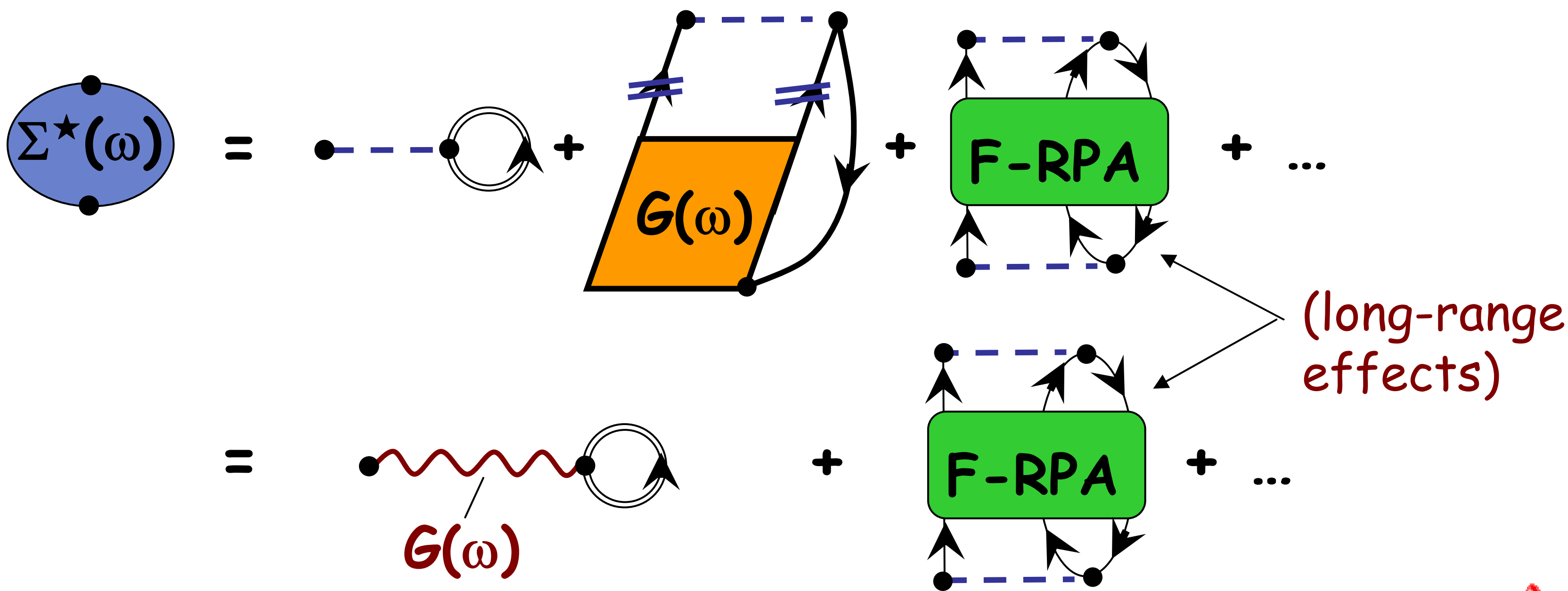




Treating short-range corr. with a G-matrix

- The short-range core can be treated by resumming ladders outside the model space:

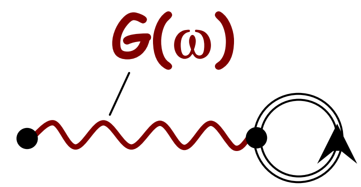
$$G(\omega) = V + V \frac{\hat{Q}}{\omega - (k_a^2 + k_b^2)/2m + i\eta} G(\omega)$$

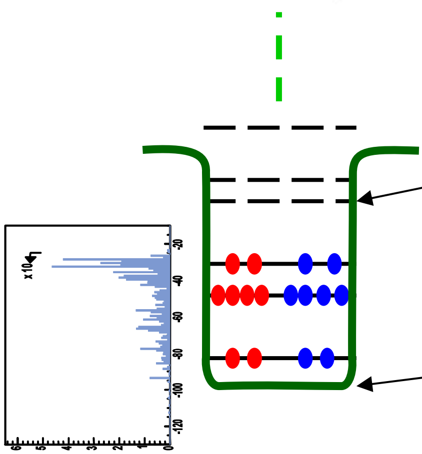


Treating short-range corr. with a G-matrix

- The short-range core can be treated by resumming ladders outside the model space:

$$\Sigma^{\mathrm{BHF}}_{\alpha\beta}(\omega) = i \sum_{\gamma\delta} \int \frac{d\omega'}{2\pi} G_{\alpha\gamma,\delta\beta}(\omega+\omega') g_{\delta\gamma}(\omega') \quad =$$





Near E_F: long-range / SM-like physics
→ stronger eff. interaction

Deeply bound "orbits": binding!
the HF mean-field is weaker

➔ *It is NOT a good idea to fix the starting energy in G(ω) at the HF/mean field level !!*

Unitary correlator operator method (UCOM)

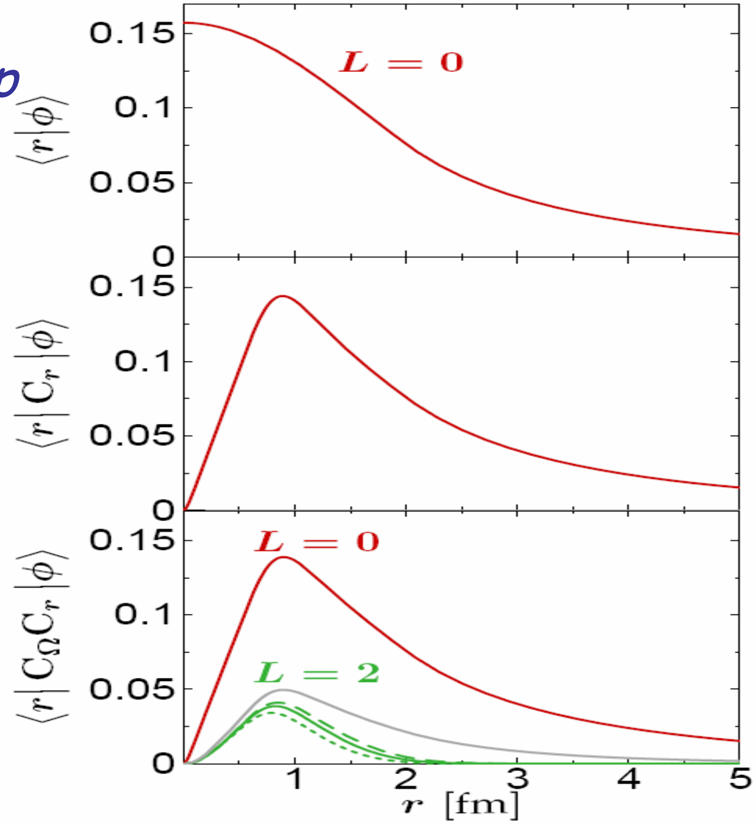
Use a unitary operator $e^{ig(x,p)}$ to correct the short-range behavior of the wave function

Equivalent to the renormalization group

$$|\Psi\rangle = \hat{U}|\phi\rangle = e^{i\hat{g}(x,p)}|\phi\rangle$$

Since $e^{ig(x,p)}$ is unitary:

$$\langle\Psi|H|\Psi\rangle = \langle\phi|\,\hat{U}^{-1}H\hat{U}\,|\phi\rangle \equiv \langle\phi|V_{UCOM}|\phi\rangle$$



[R.Roth, et al., PRC72, 034002 (2005)]

"Unitary Correlator Operator Method" potential (V_{UCOM})

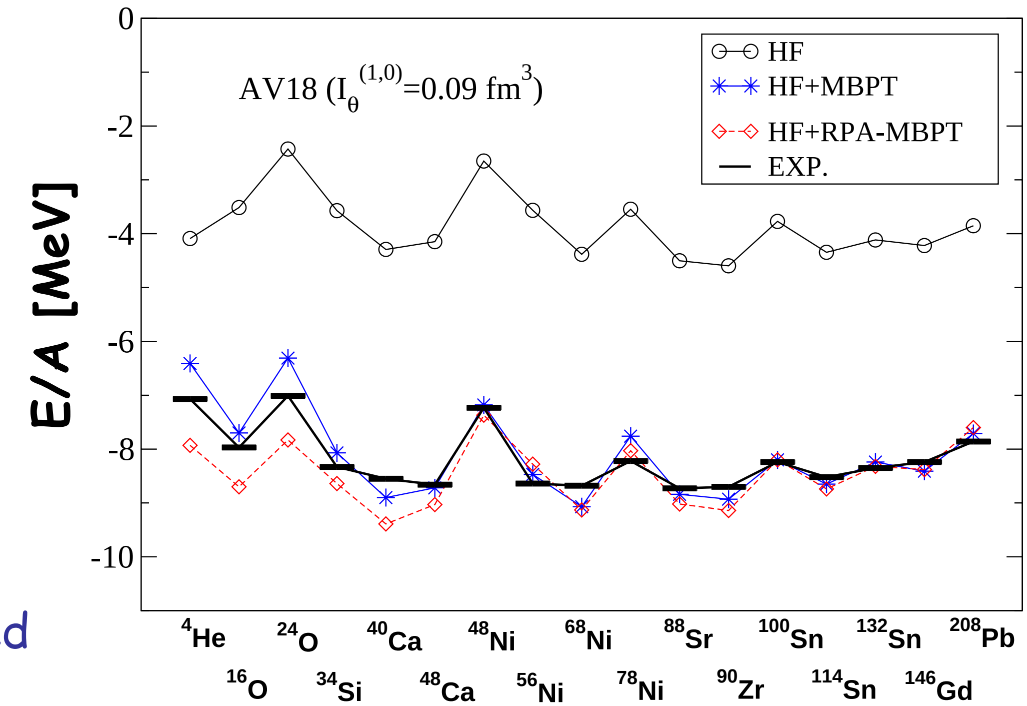
V_{UCOM} is a truncation of the UCOM expansion at the 2-body level:

-phase shift equivalent (low energies)

-amenable of perturbative calculations

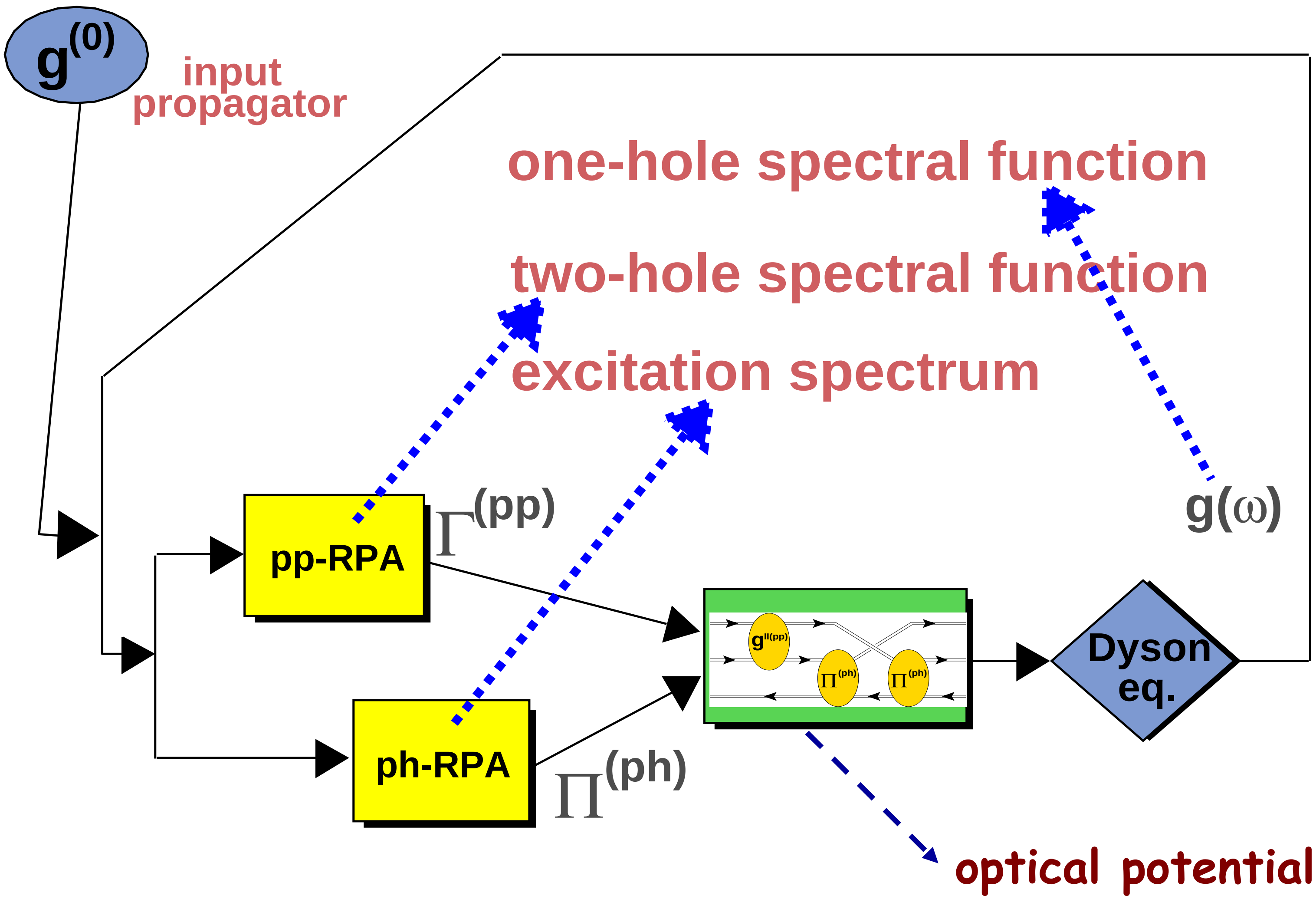
-reproduces well energies throughout the nuclear chart

(24.1 MeV rms error, for 17 closed shell nuclei, using RPA theory).



[CB, N.Paar, R.Roth, P.Papakostantinou, nucl-th/0608011]

Self-consistent Green's function approach



Ab-initio calculations with the F-RPA method

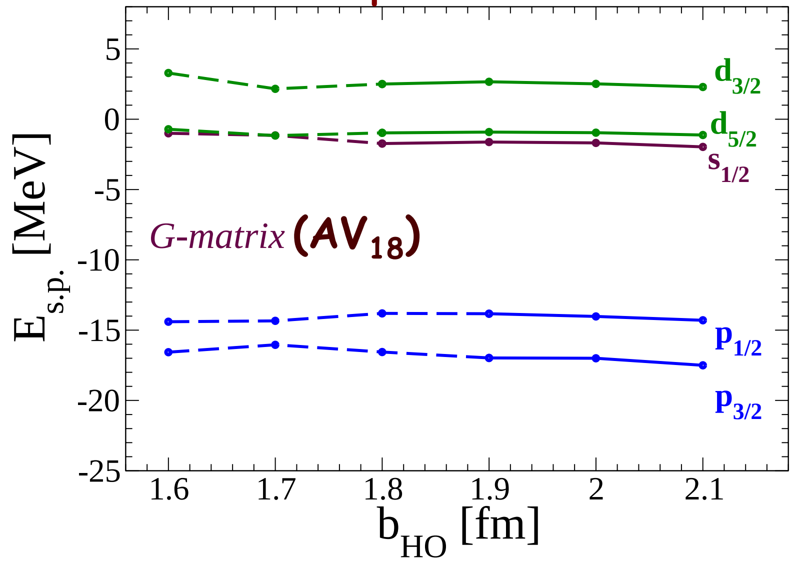
- Self-consistency loop in bases of up to 8 oscillator shells (~10^4 2p1h/2h1p confgurations)

- V_{UCOM} (AV_{18} based)
- G-matrix (AV_{18} based)

- Little dependence on the oscillator parameter (b_{HO}) for the G-matrix → convergence !!

[CB, Phys. Lett. **B643**, 268 (2006)]

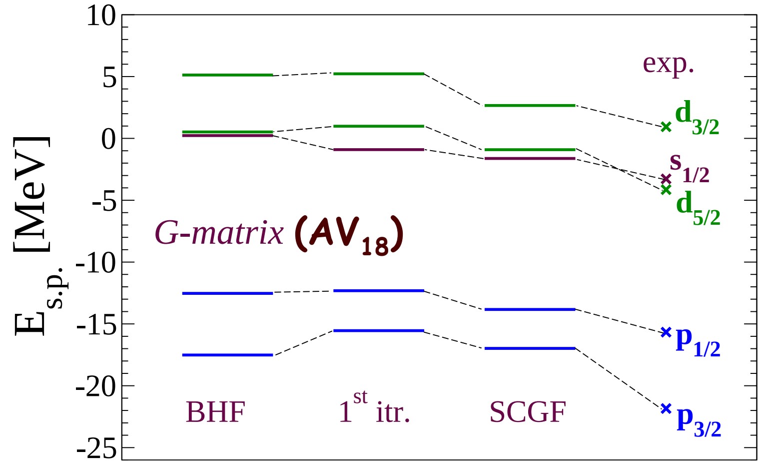
neutron s.p. states $^{17}O/^{15}O$

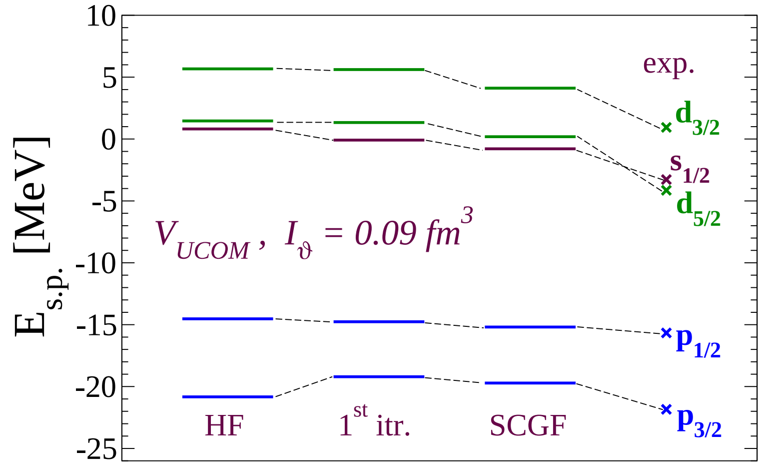


→ Recent technical improvements: larger bases/isotopes possible, up to ~10^7 Dyson states. Work is in progress…

GSI theory

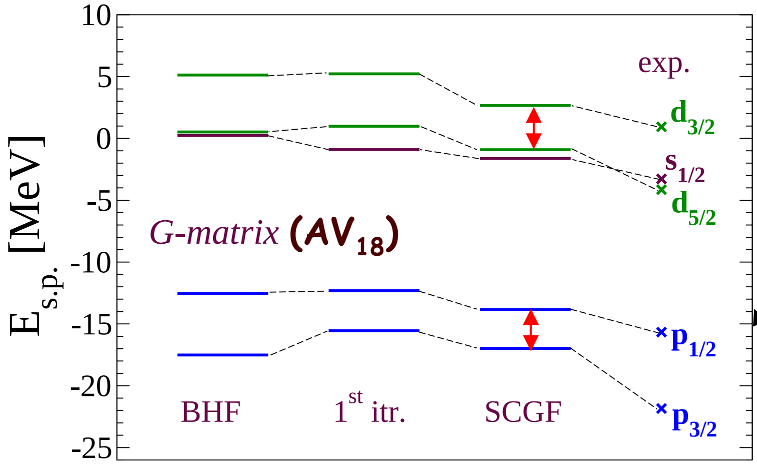
Single neutron levels around ^{16}O (G-mtx & V_{UCOM})

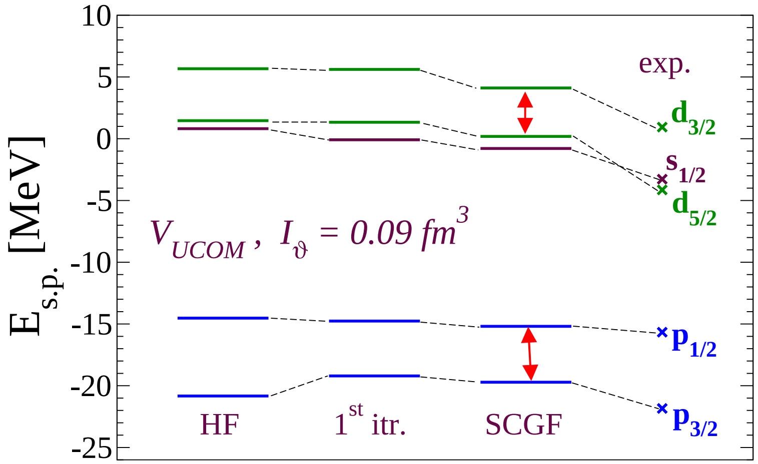




[CB, Phys. Lett. **B643**, 268 (2006)]

Single neutron levels around ^{16}O (G-mtx & V_{UCOM})





$p_{3/2}$-$p_{1/2}$ spin-orbit splitting for av18:

- 3.4 MeV, VMC [PRL'93]
- 4.5 MeV, CCSD, fixed ω G-mtx [PRC'06]
- 3.1 MeV, FRPA, G(ω) ['06]

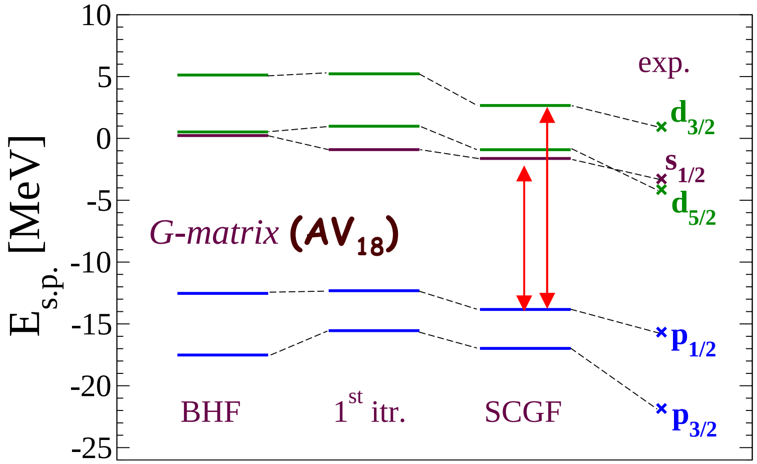
For V_{UCOM} (not av18!): 4.4 MeV

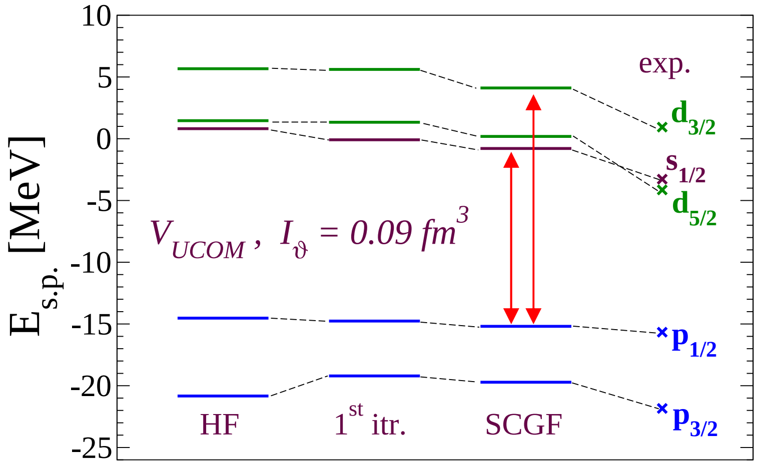
3NF are (still) missing!

	Theory:	Exp.:
$G-matrix$:		
$\Delta E_{p_{1/2}-p_{3/2}}$	3.1	6.176
$\Delta E_{d_{3/2}-d_{5/2}}$	3.5	5.084
V_{UCOM}:		
$\Delta E_{p_{1/2}-p_{3/2}}$	4.4	6.176
$\Delta E_{d_{3/2}-d_{5/2}}$	3.6	5.084

[CB, Phys. Lett. **B643**, 268 (2006)]

Single neutron levels around ^{16}O (G-mtx & V_{UCOM})



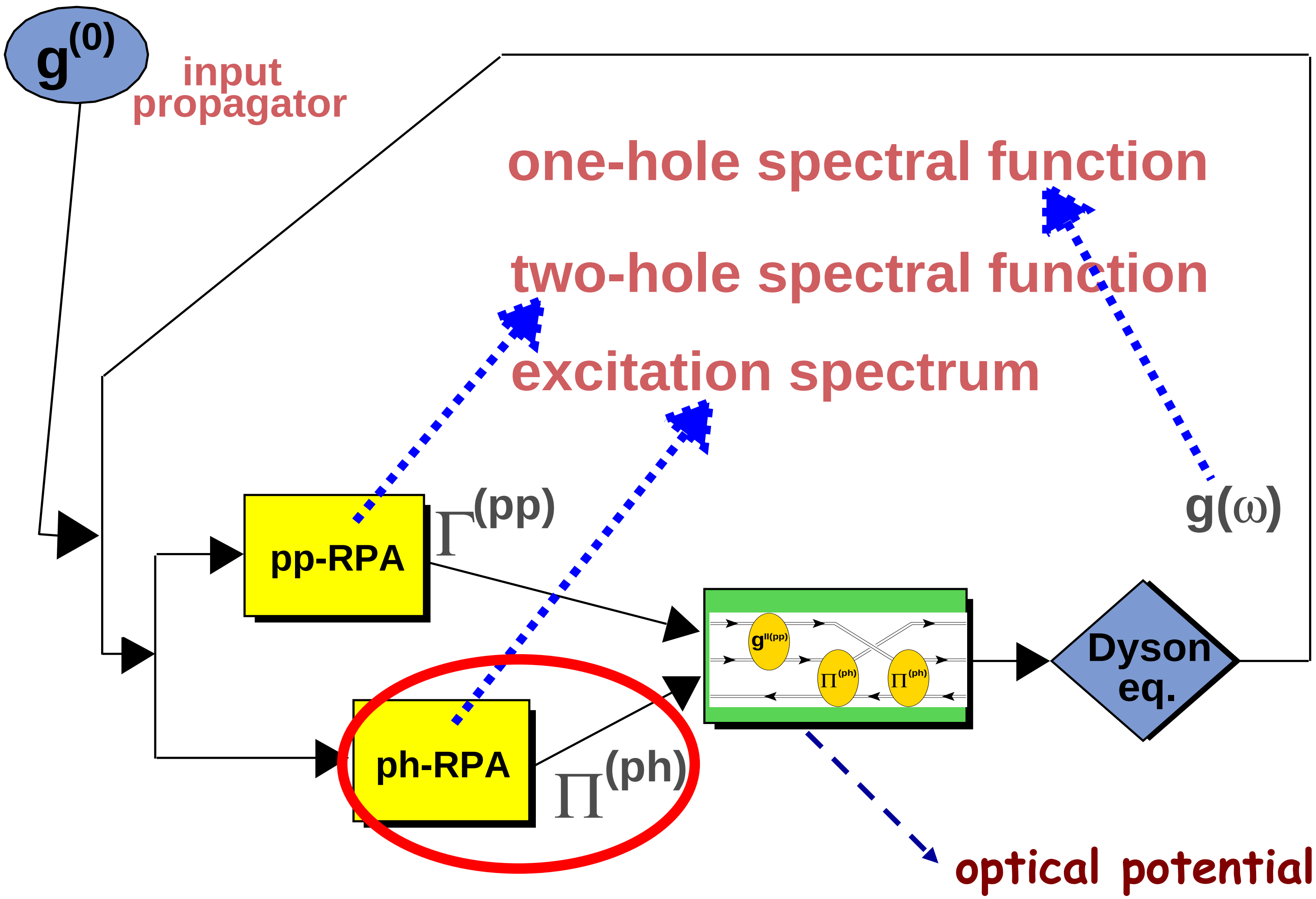


- Particle-hole gap, better described by the 2-body G-matrix interaction

	Theory:	Exp.:
G-matrix:		
$E_{d3/2}-E_{p1/2}$	16.5	16.6
$E_{s1/2}-E_{p1/2}$	12.2	12.4
V_{UCOM}:		
$E_{d3/2}-E_{p1/2}$	19.3	16.6
$E_{s1/2}-E_{p1/2}$	14.6	12.4

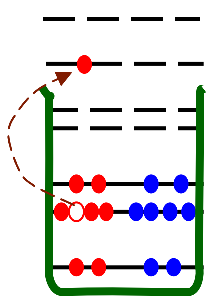
[CB, Phys. Lett. **B643**, 268 (2006)]

Self-consistent Green's function approach



Two-phonons in (D)RPA – (explicit 2p2h)

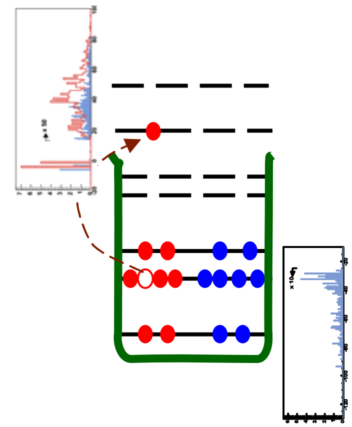
RPA



• ph states described in terms of MF orbits

• includes correlations in the g.s.

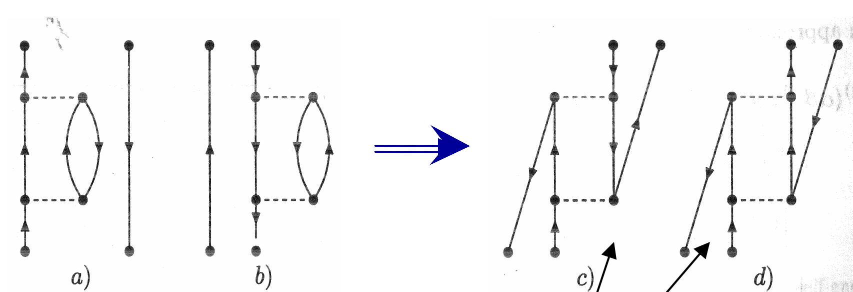
Dressed RPA



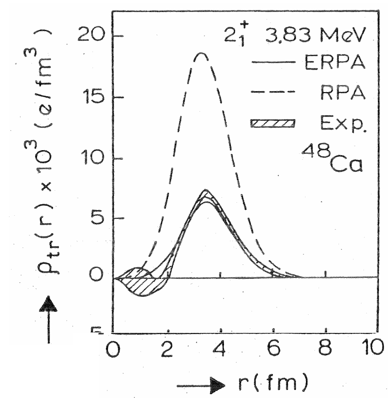
• account for spectral distribution of qp and qh

Contributions from 2p2h

• conservation laws and dressing, together, require additional 2p2h diagrams (Baym-Kadanoff theorem)



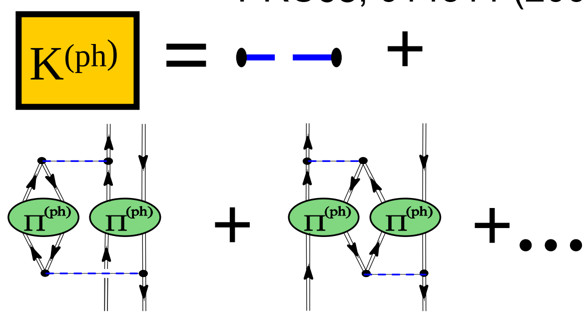
screening diagrams

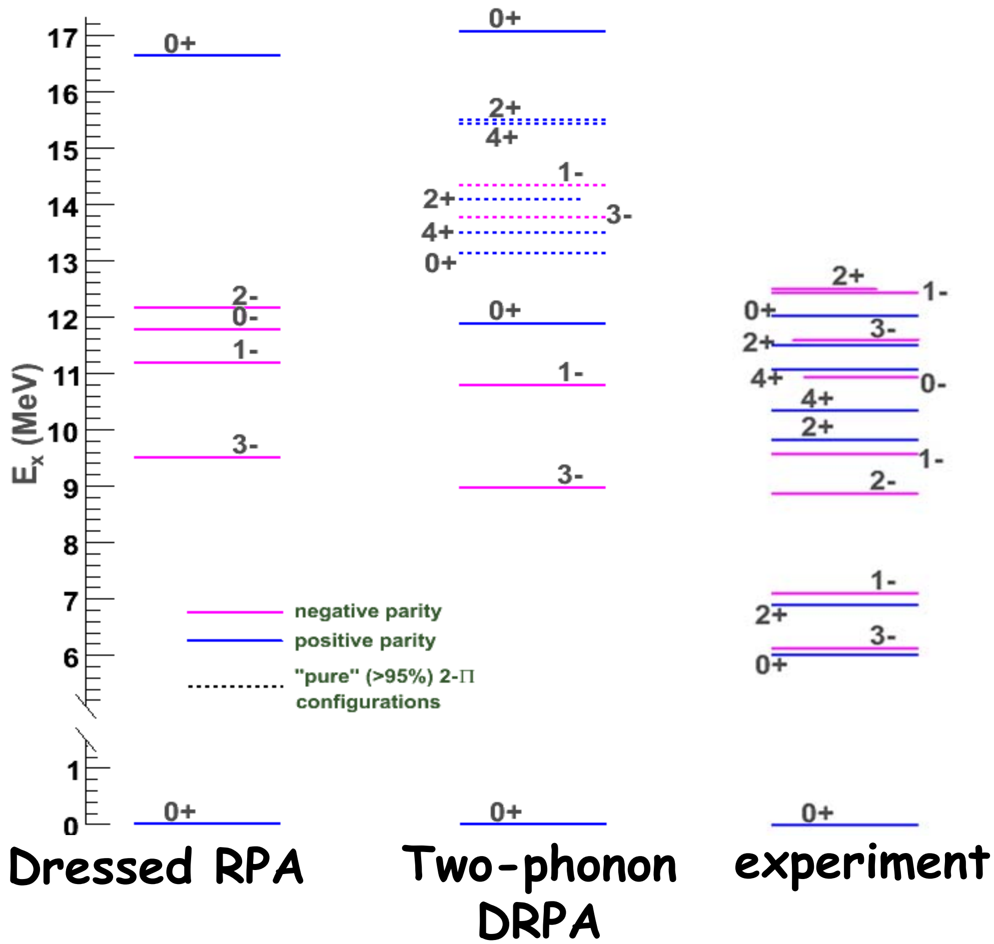


[Brand et al. Nucl. Phys. **A509**, 1 (1990)]

One- and two-phonons in ^{16}O

C.B., W.H.Dickhoff, PRC**68**, 014311 (2003).





States with a strong p-h character are only slightly modified by 2-phonon configurations

→ 3 body forces? clustering?

Several new levels arise as two-phonon states

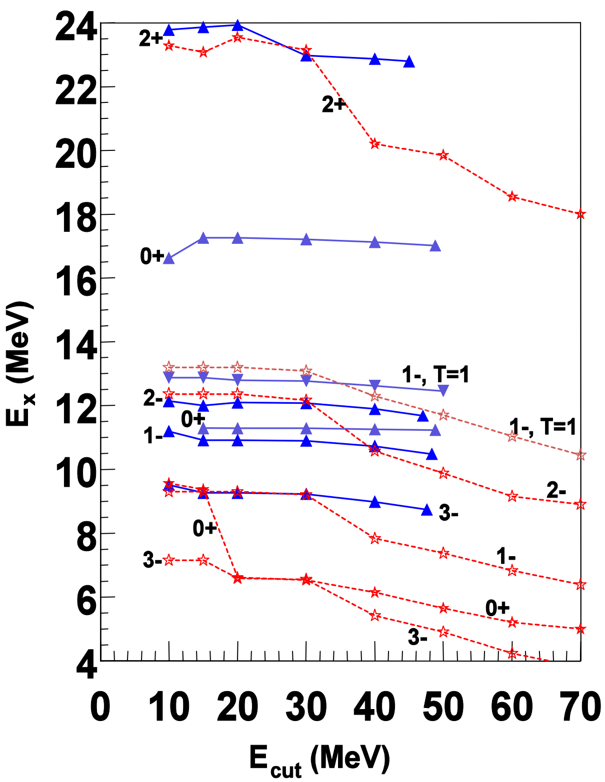
Anharmonicity effects are not strong for this nucleus… but still present (splitting of multiplets)

- 6 major oscillator shells
- G-matrix based on Bonn-C

GSI theory

Stability with dressed propagators

Two-phonon (D)RPA (^{16}O)

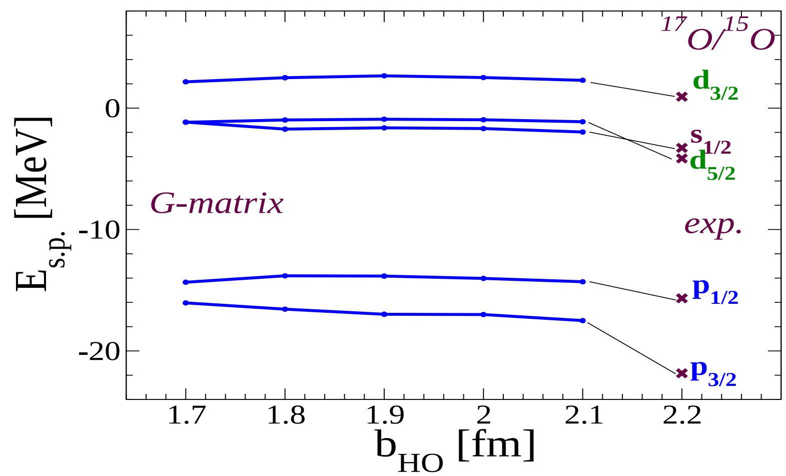


Undressed input (h.o. wave functions)

Dressed

E_{cut} = max energy of two-phonon configurations

Neutron s.p. spectra for 1b GF, vs h.o. length b_{HO}



The results for the low energy excitations become more stable when dressing (self-consistency) is included.

→ dressing improves convergence by including selected contributions from higher np-nh excitations

Conclusions and Outlook

- Self-Consistent Green's Functions (SCGF), in the Faddeev RPA (FRPA) approximation are well suited to describe the coupling between particle and collective modes of a many-body system.

- *Ab-initio* applications:
    - accurate ionization energies for atoms
    - coherent description of atoms/ e^- gas, possible?
    - convergent calculations in nuclei

  } work in progress…

- Possible applications to nuclear structure and nuclear astrophysics are many (but not covered in this talk):
    - spectral strength/correlations
    - one- and two- nucleon knock out
    - nuclear response (giant resonances, neutrino scattering)

- Theoretical background for developing dispersive optical model (DOM) and quasiparticle-DFT (QP-DFT).

Thanks to my group and my collaborators:

W. H. Dickhoff

(Washington University, St.Louis)

D. Van Neck

(University of Gent)

G. Martinez-Pinedo, K. Langanke

(GSI, Darmstadt)

R. Roth

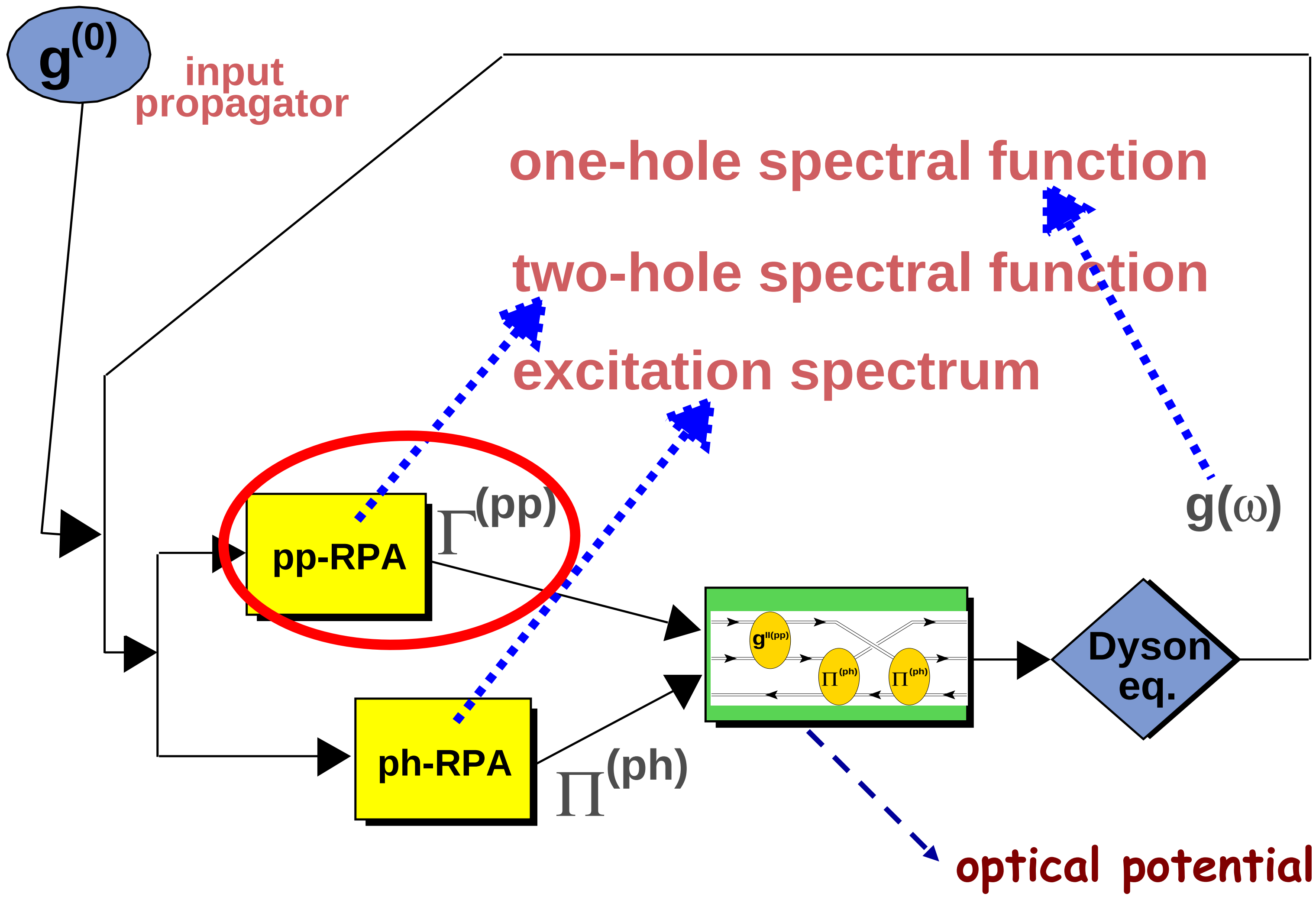
(TU, Darmstadt)

C. Giusti, F. D. Pacati

(University of Pavia)

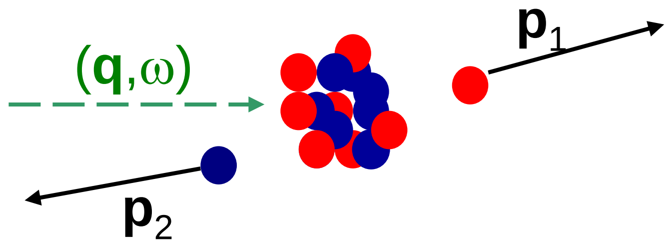
…and THANKS for your attention!

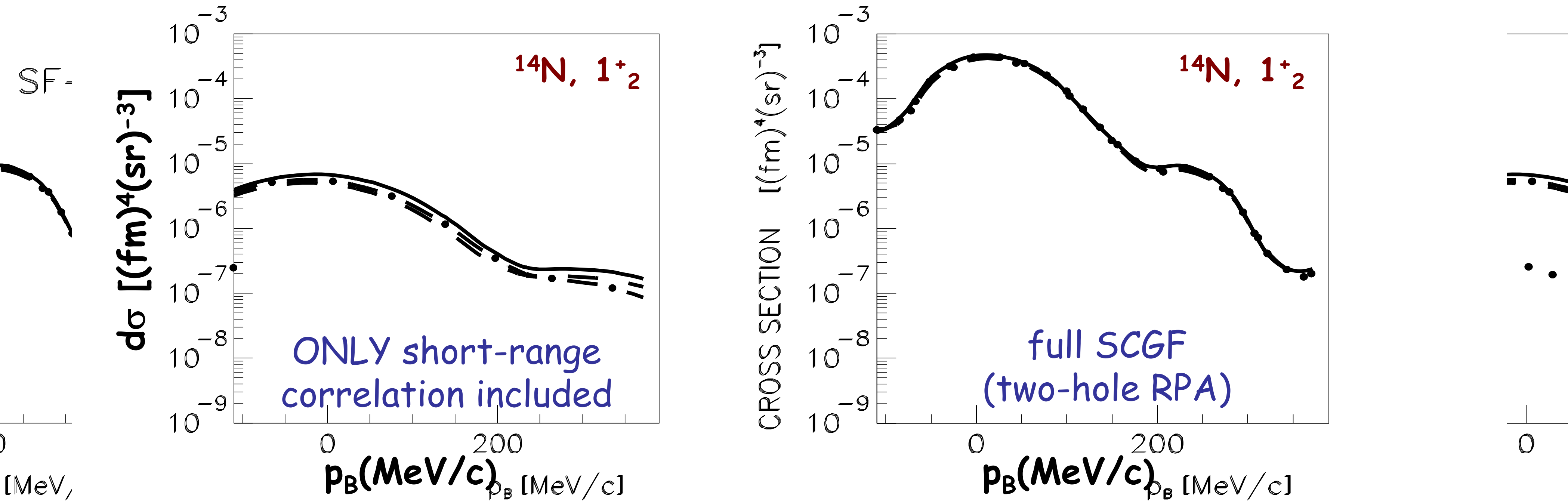
Self-consistent Green's function approach



Correlations form two-nucleon knock out

- $^{16}O(e,e'pn)^{14}N$
- initial wave function from SCGF
- Pavia model for final state interactions
- $\mathbf{p}_B \equiv \mathbf{q} - \mathbf{p}_1 - \mathbf{p}_2$

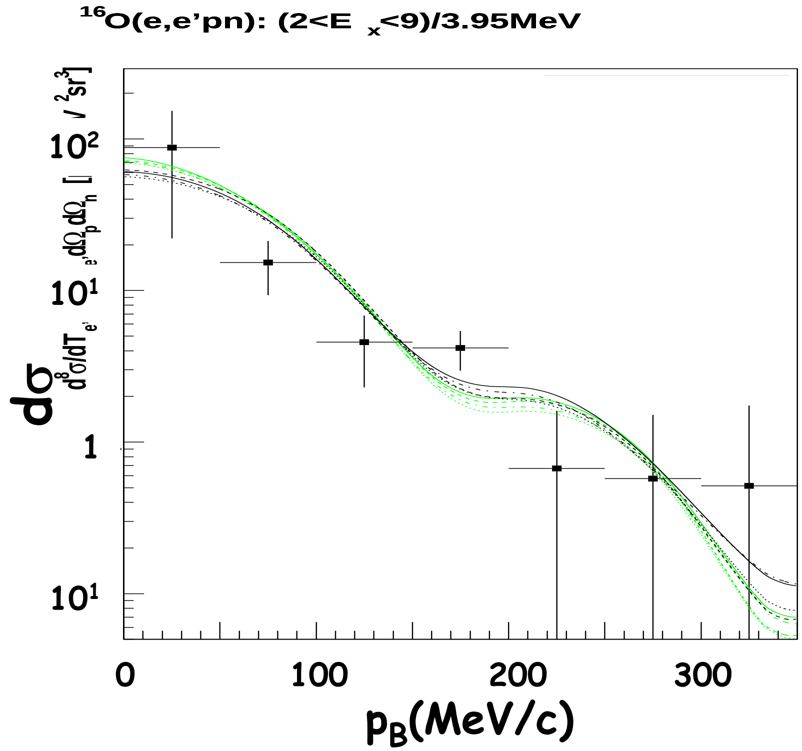




- two orders of magnitude from long range correlations !!

Proton-neutron knockout: $^{16}O(e,e'pn)^{14}N$

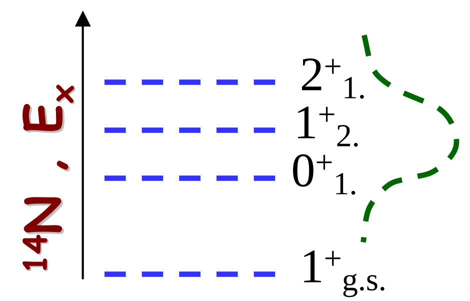
[D. Middleton, et al. Eur. J. Phys. A**29**, 261 (2006)]



Experiment: MAMI

Theory: SCGF/Pavia scattering model

- Test run, low energy resolution:



- The 1^+_2 final state dominates – tensor correlations!
- *long-range* correlations in the two-hole wave function are critical