Applications of propagator theory to nuclei (and atoms)

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RIKEN

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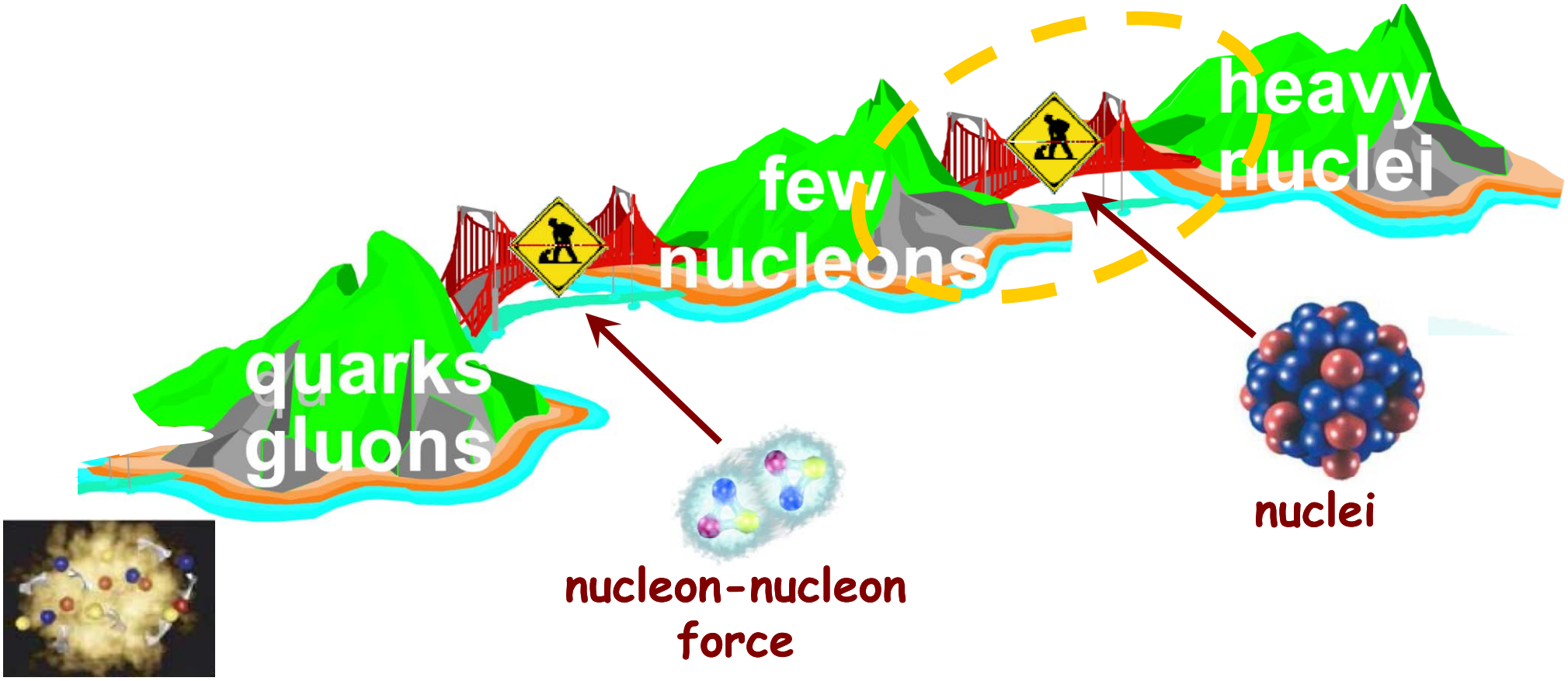
First EMMI-EFES Workshop on Neutron-Rich Nuclei

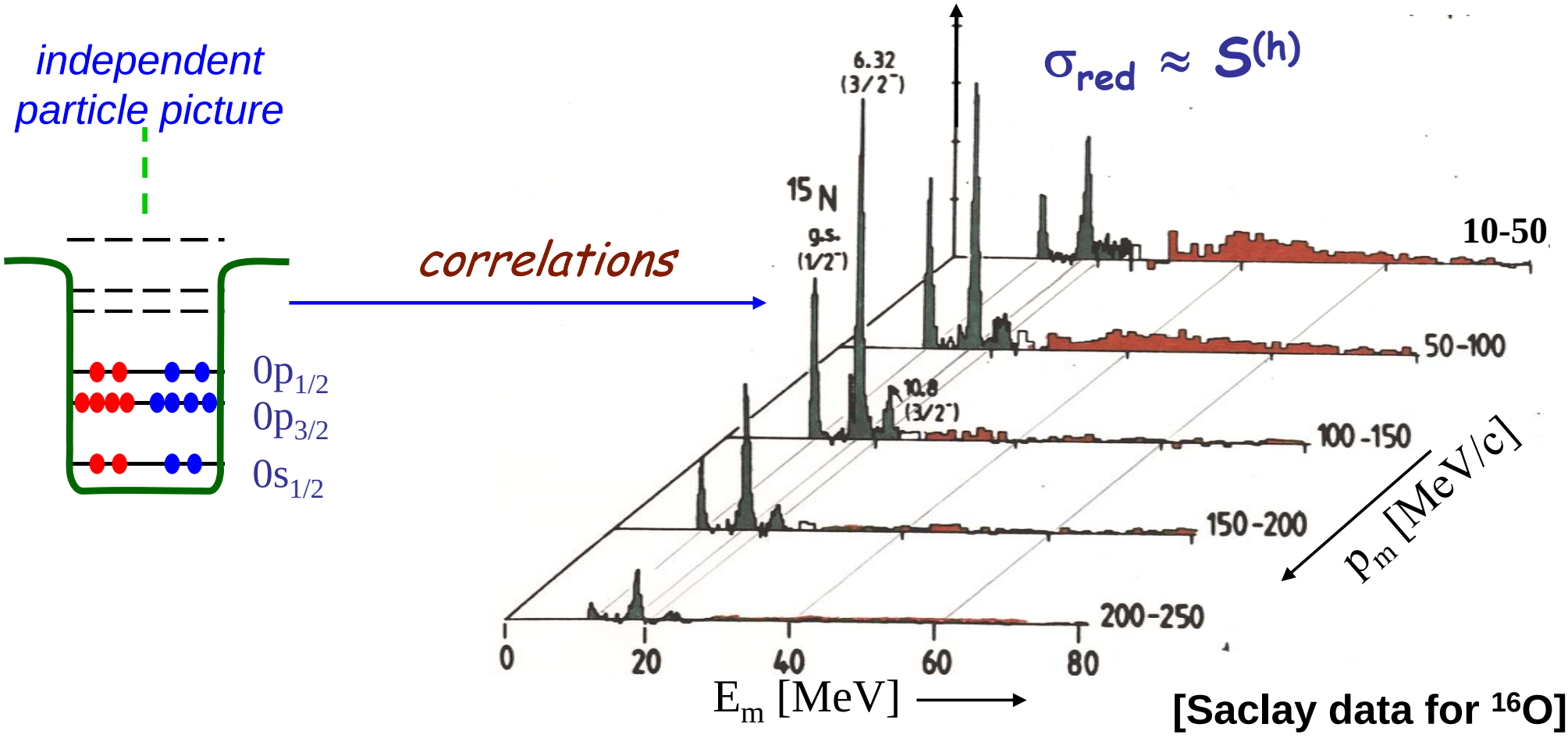
Nuclear structure in the 21st century



Outline

- nuclear spectral function
- Self-consistent Green's function (SCGF) method and Faddeev-RPA expansion
- Results for spectroscopic factors
- (time permitting: applications to atoms)

One-hole spectral function -- example



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

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

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

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

Why many-body Green's functions??

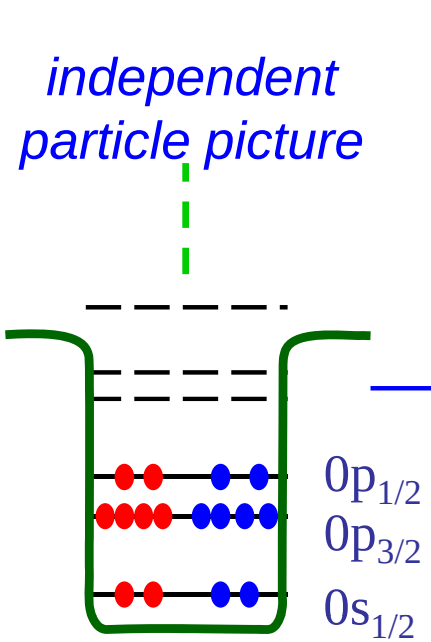
- "ab-initio" approach
- hierarchy of equations—can improve systematically
- Linked diags → **extensivity**
- Self-consistency: "no" reference

- Closely related to spectroscopy ←→ experiments
- "phonons" as degrees of freedom←→ phenomenology

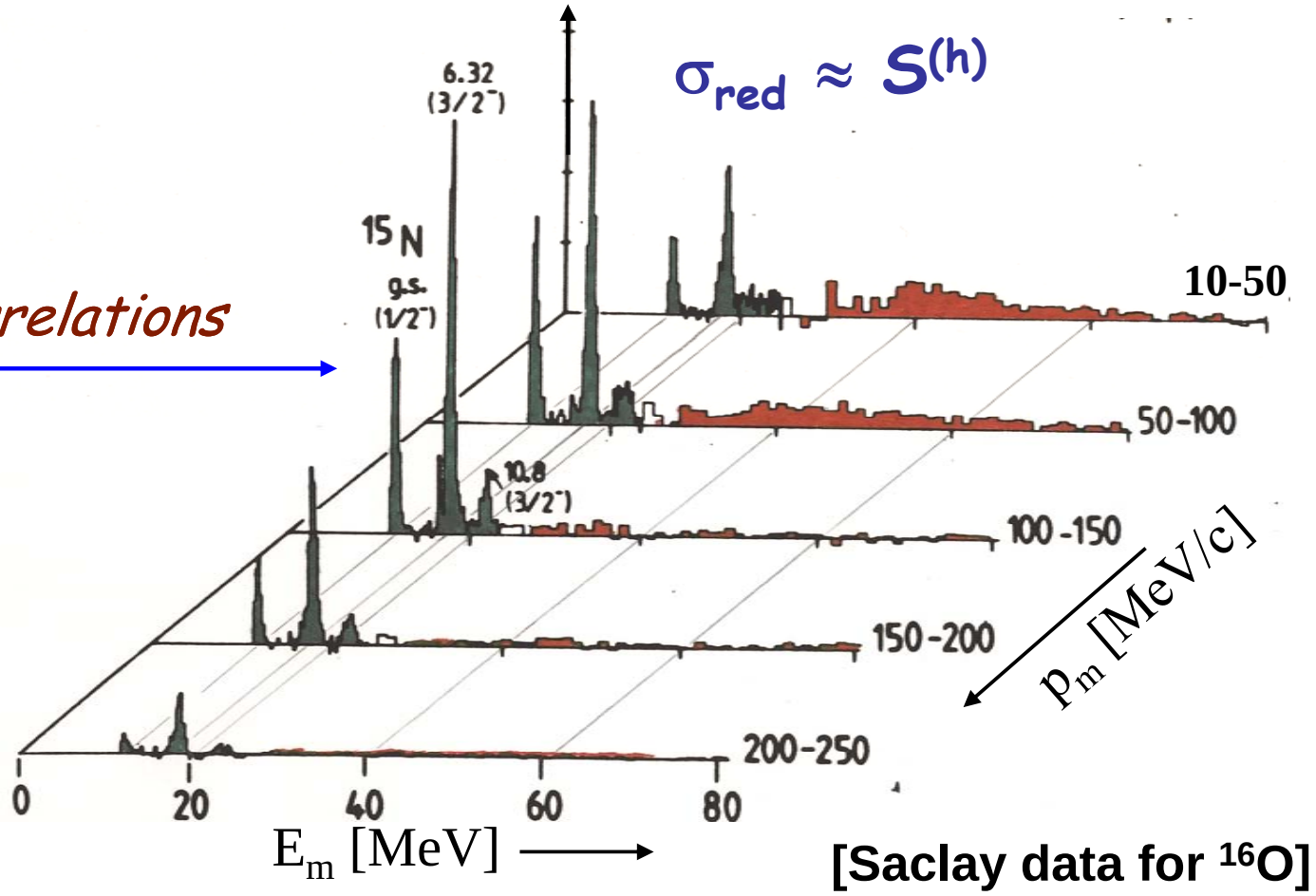
APPLICATIONS:

- Faddeev RPA
- optical potential (disp. opt. mod. ≡DOM)
- quasiparticle-DFT (QP-DFT)

One-hole spectral function -- example



correlations



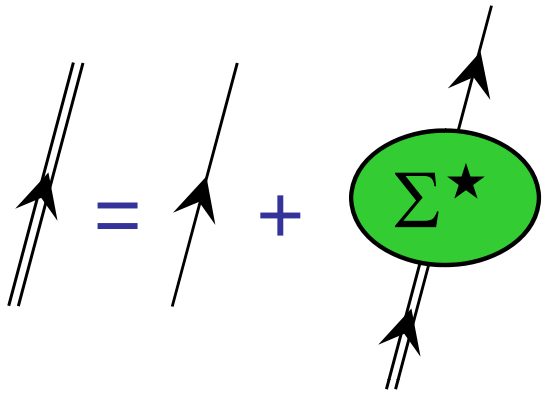
[Saclay data for ^{16}O]

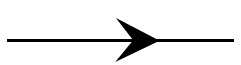
$$S^{(h)}(p_m, E_m) = \sum_n \left| \langle \Psi_n^{A-1} | c_{\vec{p}_m} | \Psi_0^A \rangle \right|^2 \delta(E_m - (E_0^A - E_n^{A-1}))$$

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

Dyson-Schwinger equation

In diagrammatic form:




, *free particle* propagator


, *correlated* propagator

, *"irreducible"* self-energy

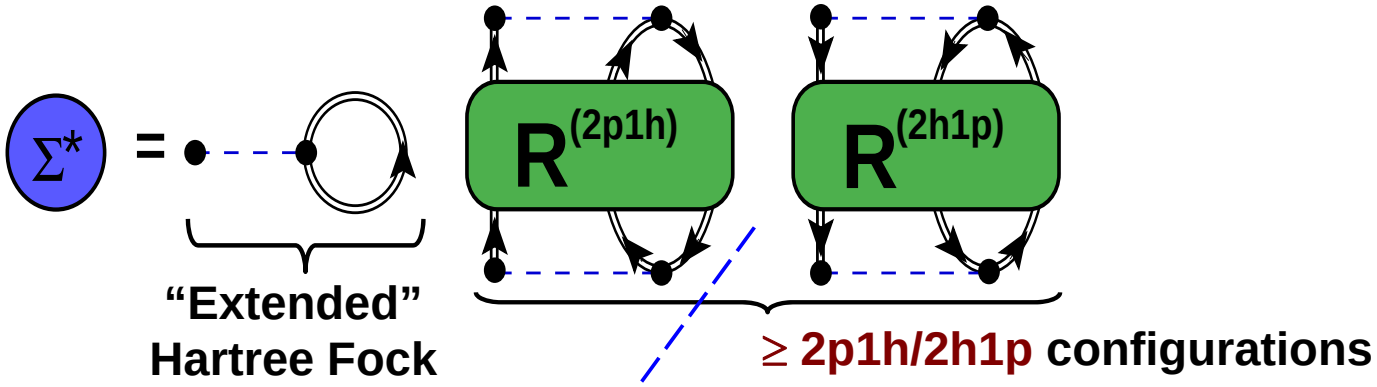
→ it leads to a 1-body equation:

$$\frac{\hat{p}^2}{2m}\psi^{(qp/qh)}(\vec{r}) + \int d\vec{r}\,\Sigma^*(\vec{r},\vec{r}';\omega)\;\psi^{(qp/qh)}(\vec{r}') = \;\omega\,\psi^{(qp/qh)}(\vec{r})$$

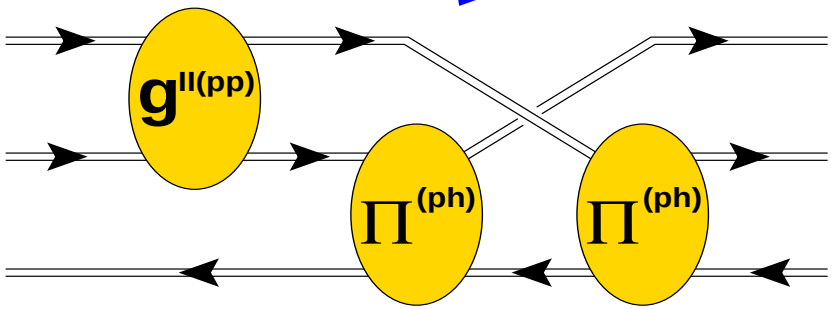
$$\psi^n(\vec{r}) \equiv \langle \Psi_n^{A\pm1} \mid c_{\vec{r}}^{(+)} \mid \Psi_0^A \rangle$$

Coupling single particle to collective modes

- Non perturbative expansion of the self-energy:



- Explicit correlations enter the "three-particle irreducible" propagators:

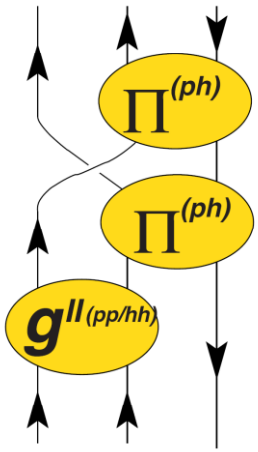


- Both pp/hh (ladder) and ph (ring) response included
- Pauli exchange at 2p1h/2h1p level

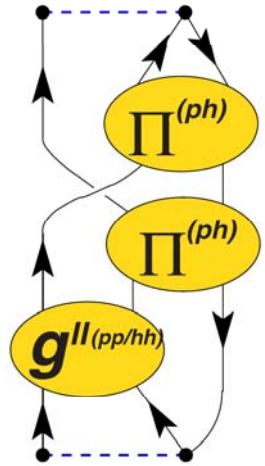
PRC63, 034313 (2001)
PRC65, 064313 (2002)
PRA76, 052503 (2007)

≡ particle
≡ hole

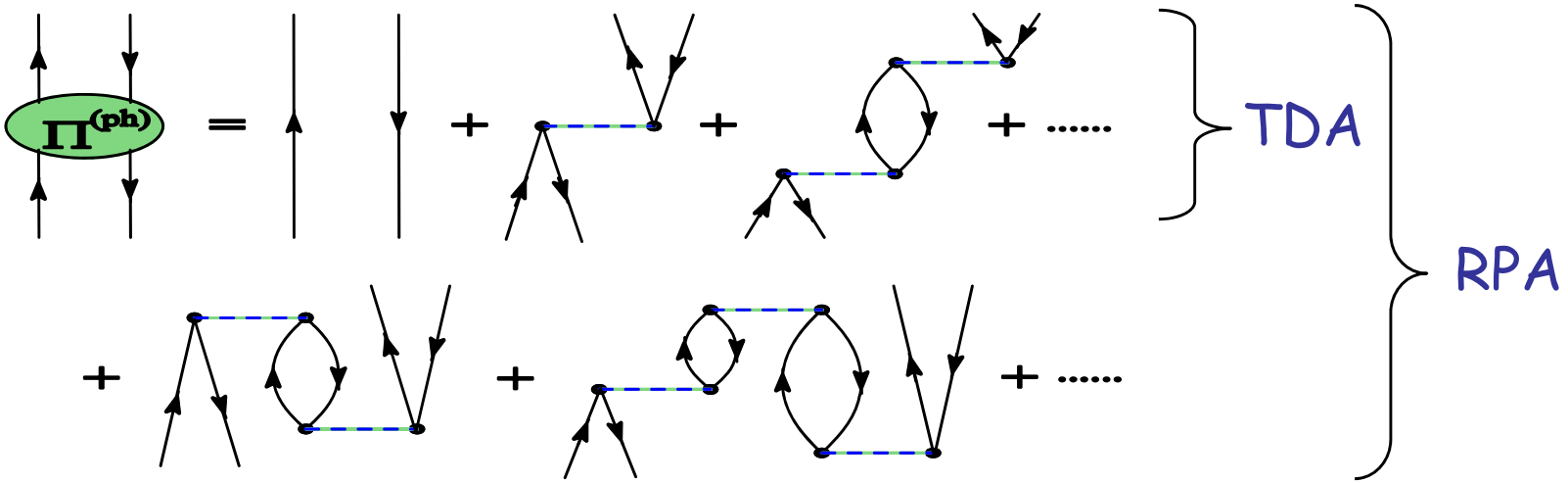
FRPA: Faddeev summation of RPA propagators



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

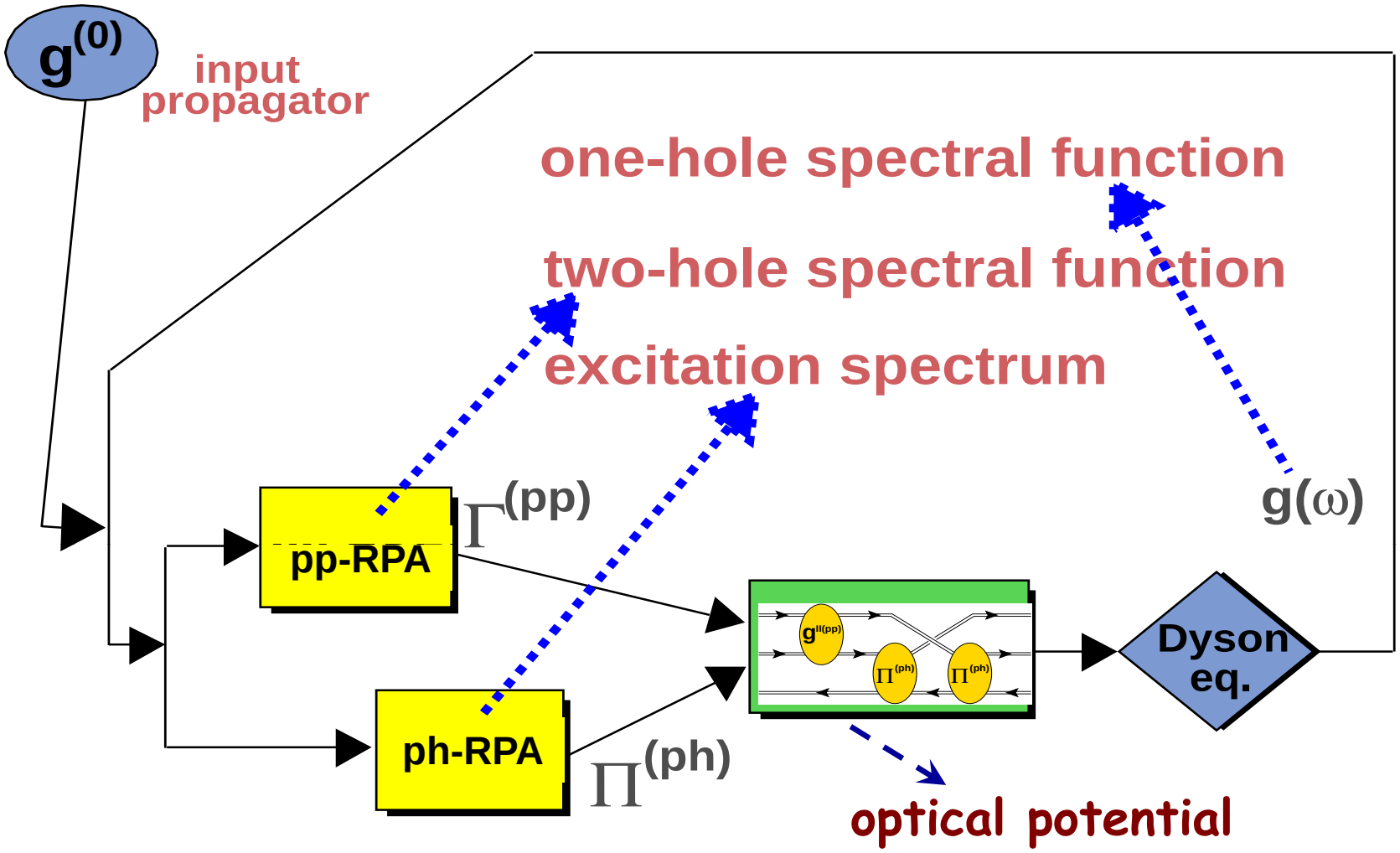


where:



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

Self-consistent Green's function approach



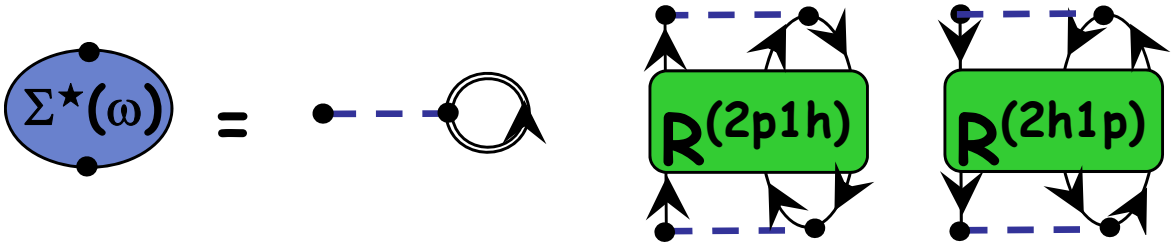
FULL self consistency in mid size bases in now POSSIBLE:
^{16}O , 8 shells ~ *CB, Phys. Lett. B643, 268 (2006)*

Applications to Nuclei

- Strong short-range cores require "renormalizing" the interaction:
  - G-matrix, V_{UCOM}, Lee Suzuki, Bloch-Horowitz, V_{low-k}, ...
- Long-range correlations → FRPA !!

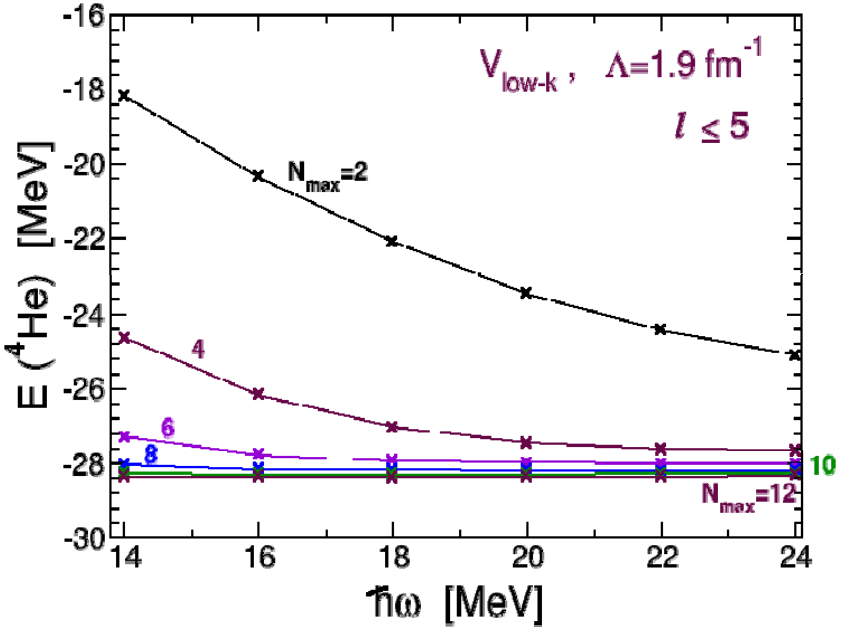
Binding energy - ^{4}He case

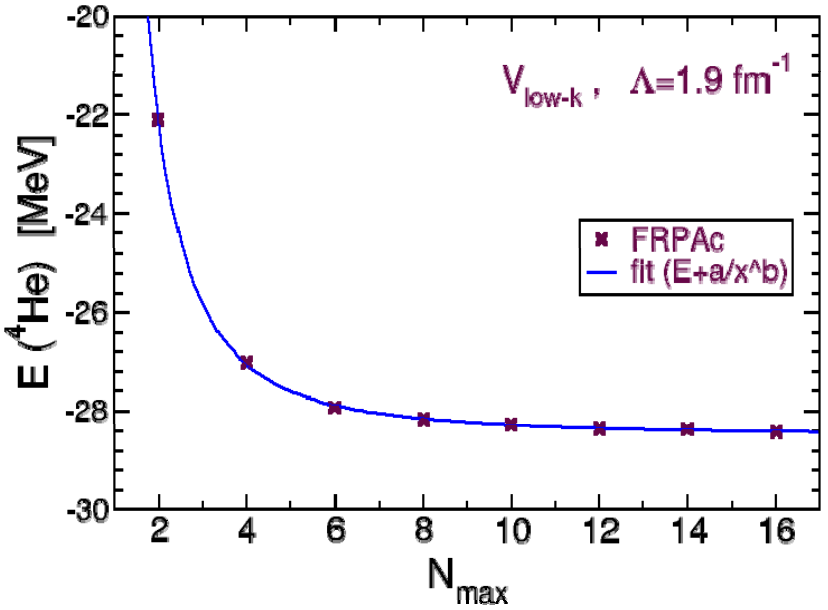
[C. B., to be published]



$$E_0^A = \frac{1}{2}\int_{-\infty}^{\varepsilon_F^-} d\omega \sum_{\alpha\beta} \left[\frac{(k^2)_{\alpha\beta}}{2m} + \omega\delta_{\alpha\beta}\right] S^{(h)}_{\beta\alpha}(\omega)$$

binding energy
(Migdal-Galitski-Koltun)





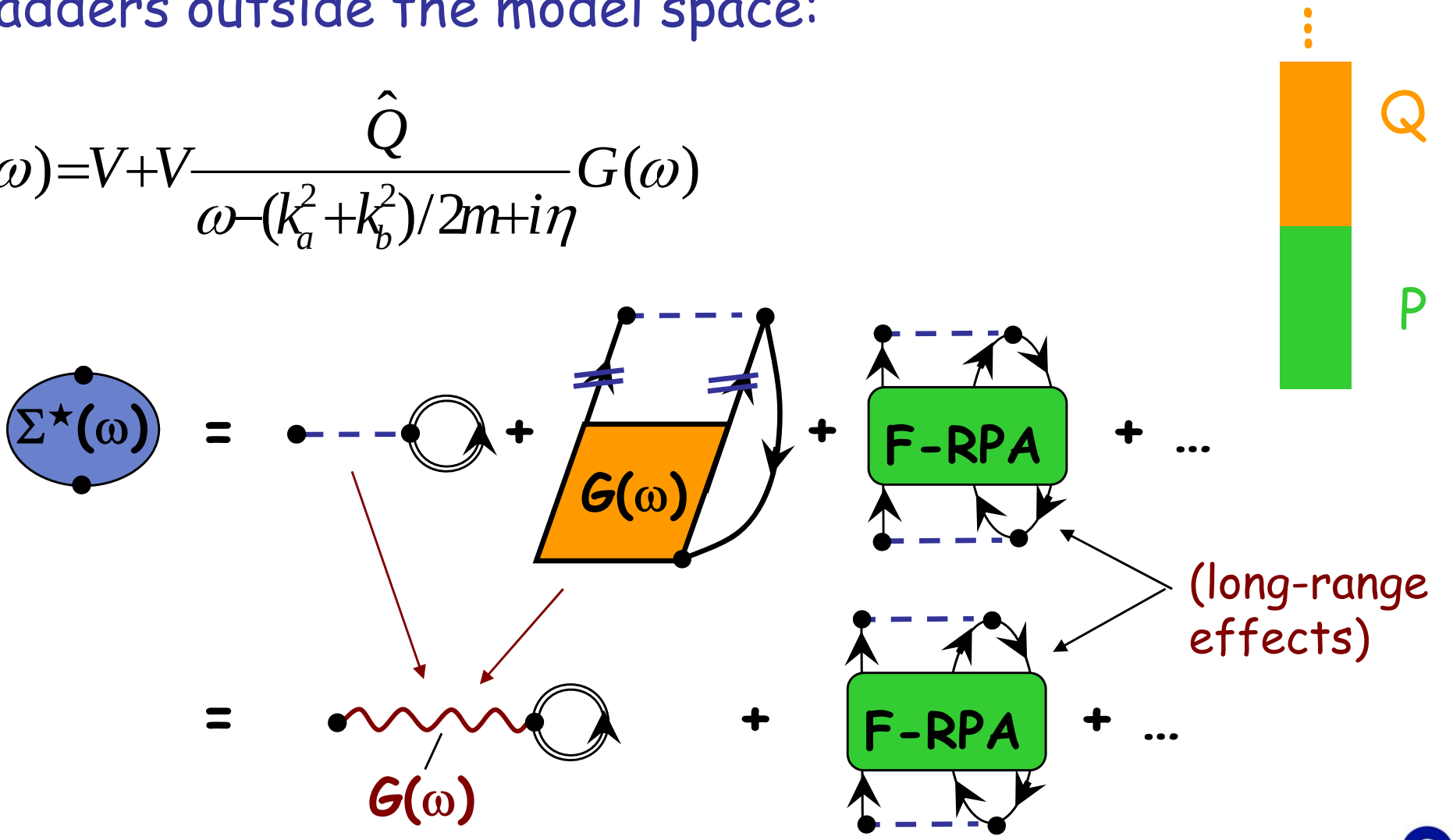
Based on the intrinsic Hamiltonian:

$H_{int} = T + V - T_{int}$

Treating short-range corr. with a G-matrix

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

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

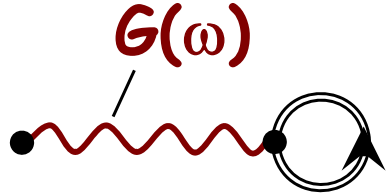


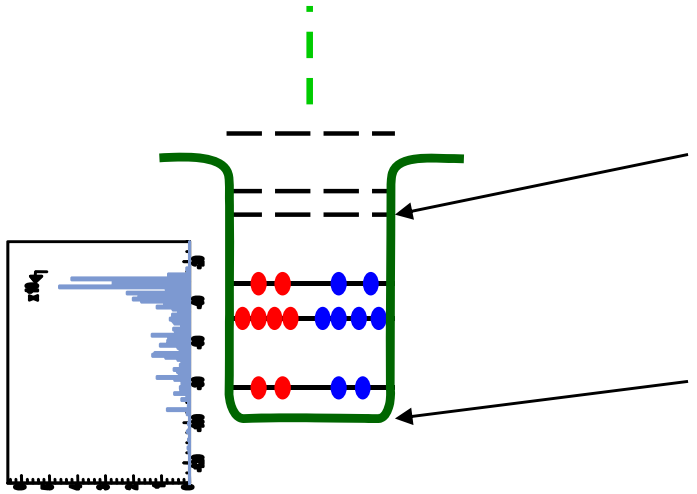
Treating short-range corr. with a G-matrix

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

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

=





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

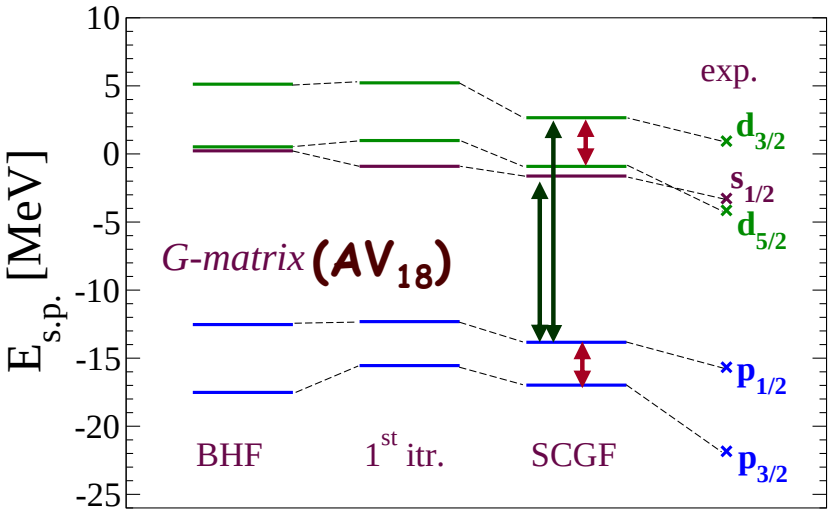
Deeply bound "orbits": binding!
the HF mean-field is weaker

Details of calculations

^{16}O →
- 8 major oscillator shells
- G-matrix derived from Argonne v18
- Full self-consistency

^{48}Ca, ^{56}Ni, etc... →
- Up to 10 major oscillator shells
- G-matrix derived from N3LO + Coulomb
- Monopole correction to mock 3NF
- Partial self-consistency only for the mean-field

Single neutron levels around ^{16}O with FRPA



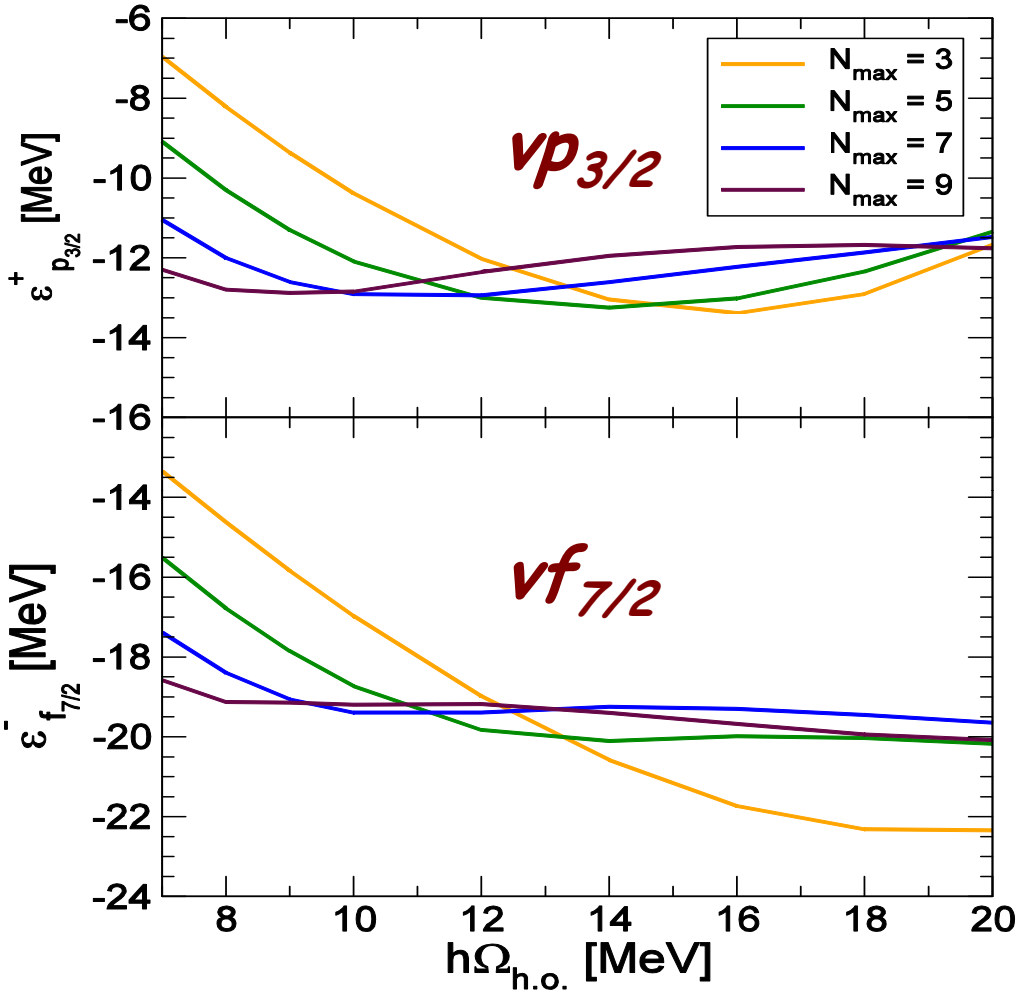
[CB, Phys. Lett. B643, 268 (2006)]

	Theory(MeV)	Exp.[MeV]
p-h gap:		
$E_{d3/2}$-$E_{d5/2}$	3.5	5.08
$E_{p1/2}$-$E_{p3/2}$	3.1	6.12
p-h gap:		
$E_{d3/2}$-$E_{p1/2}$	16.5	16.6
$E_{s1/2}$-$E_{p1/2}$	12.2	12.4

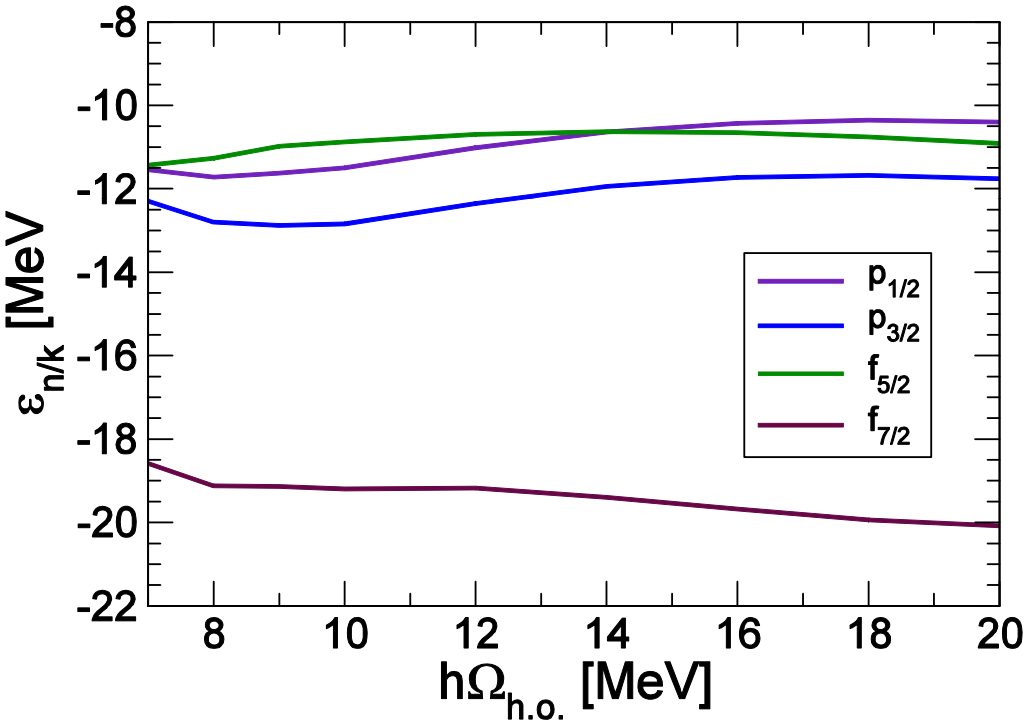
- particle-hole gap accurate with a G-matrix with ω-dependence

- $p_{3/2}$-$p_{1/2}$ spin-orbit splitting close to the VMC estimates ≈3.4MeV
  [S. Pieper et al. PRL70 ('93) 2541, using AV_{14}]

Convergence of valence orbits in ^{56}Ni

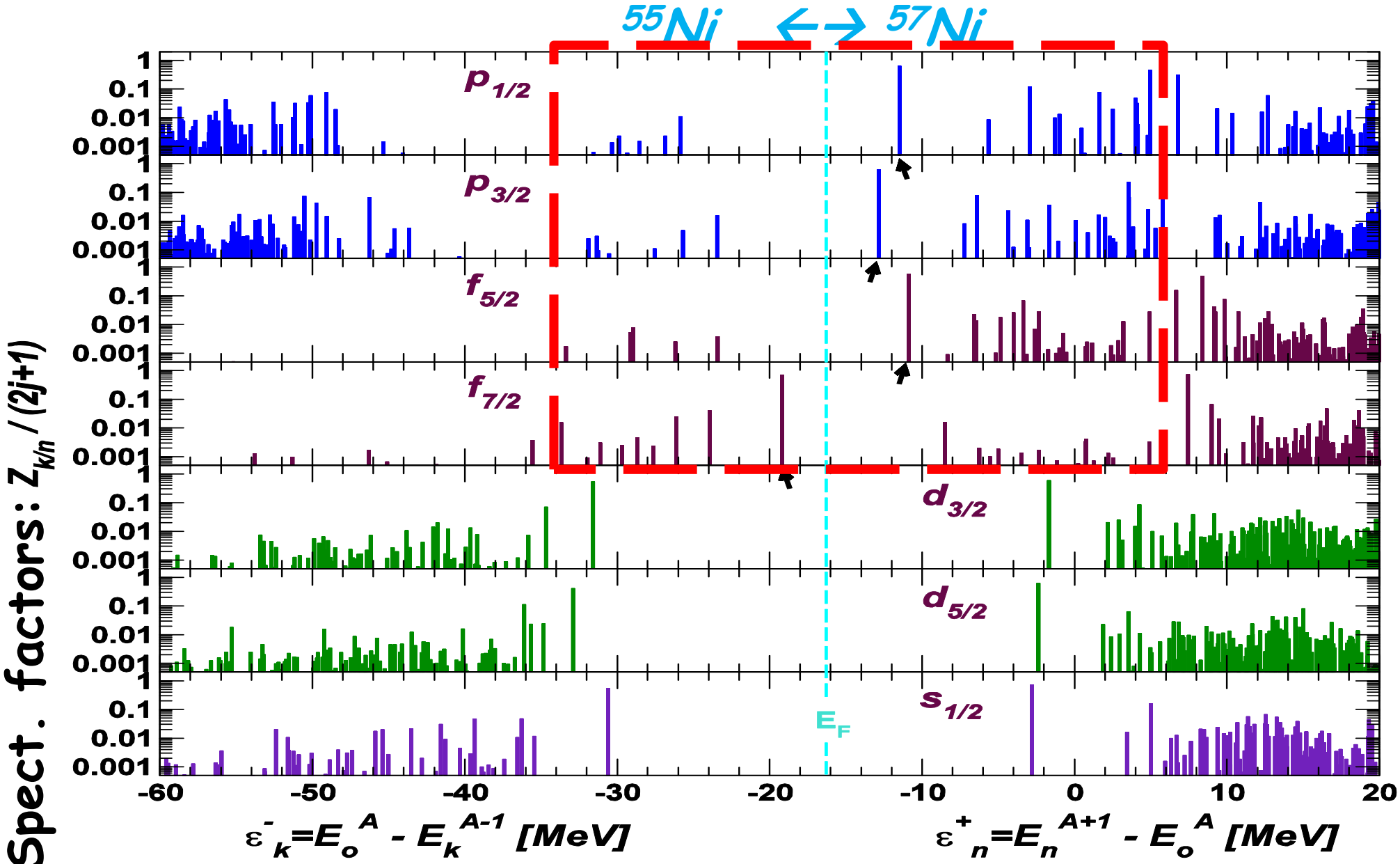


- single-particle energies almost converged (within ~1MeV) for 10 oscillator shells
- Little dep. on the oscillator parameter



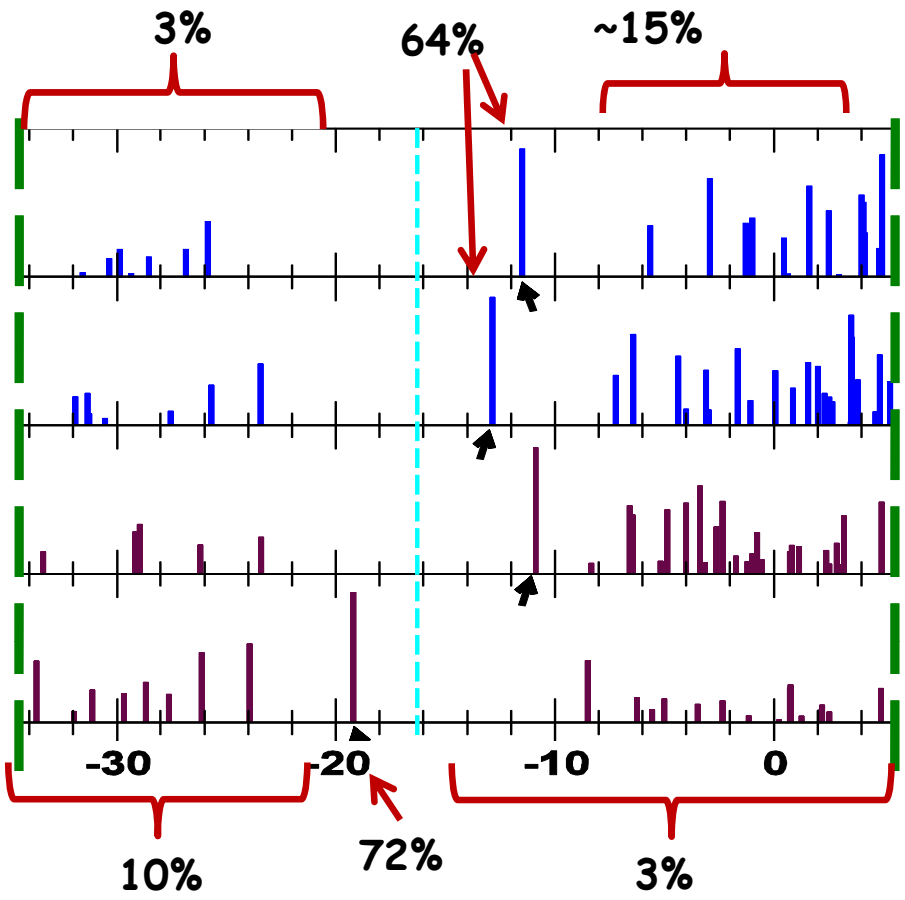
N3LO interaction + monopole corr. [CB, M.Hjorth-Jensen, arXiv [nucl-th] Feb. 2009]

Particle and hole spectral distribution of ^{56}Ni



N3LO interaction + monopole corr. [CB, M.Hjorth-Jensen, arXiv [nucl-th] Feb. 2009]

Fragmentation of valence orbits around ^{56}Ni



Spectroscopic factor of valence orbits:

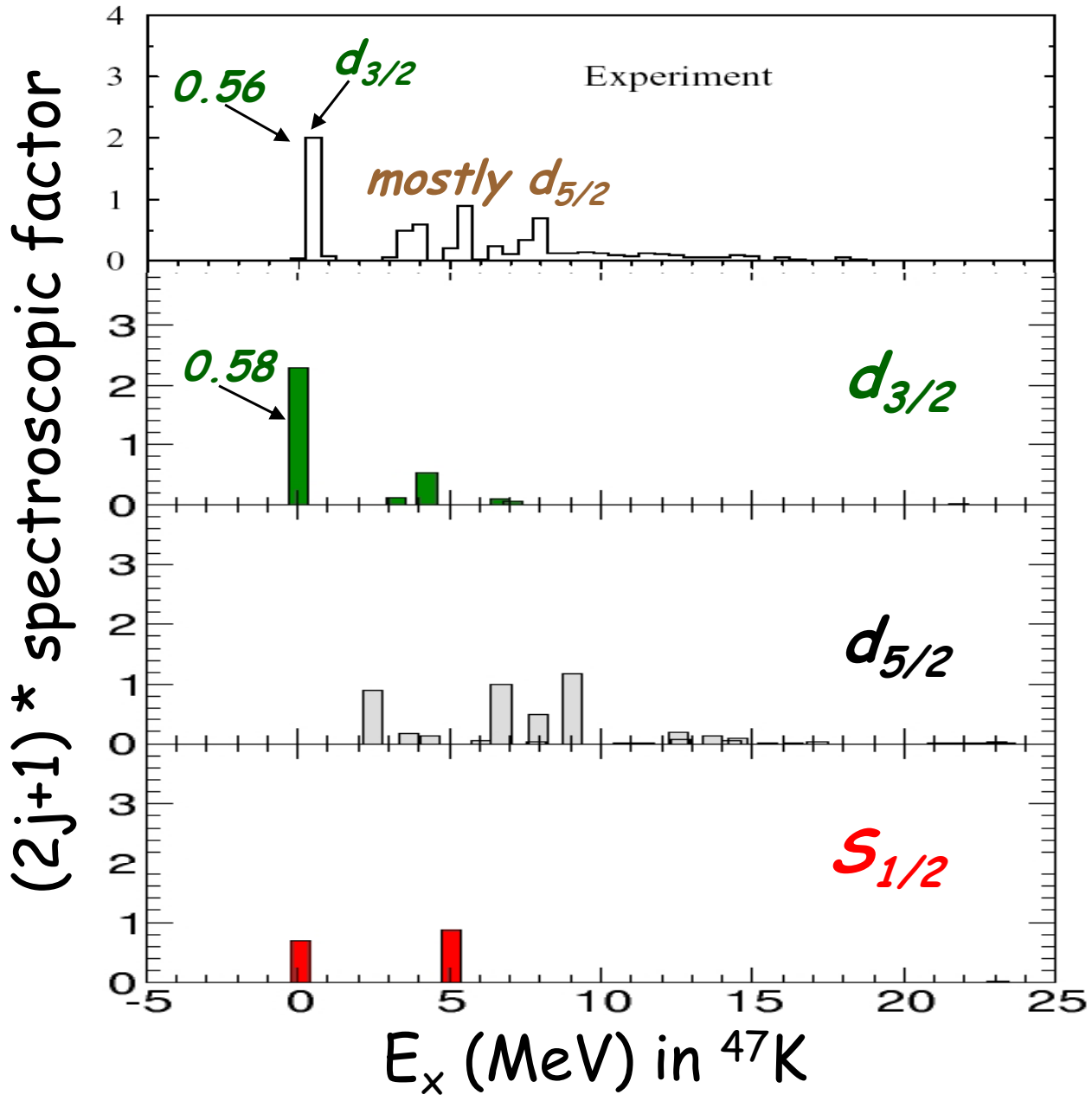
	$\varepsilon_n^+, \varepsilon_k^-$		$Z_n/(2j+1), Z_k/(2j+1)$	
	FRPA	Exp.	FRPA	Exp.
^{57}Ni:				
$\nu p_{1/2}$	-11.50	-9.134	0.627	
$\nu f_{5/2}$	-10.87	-9.478	0.578	
$\nu p_{3/2}$	-12.84	-10 247	0.644	0.58(11)
^{55}Ni:				
$\nu f_{7/2}$	-19.20	-16.641	0.716	
^{57}Cu:				
$\pi p_{1/2}$	-1.35	+0.417	0.651	
$\pi f_{5/2}$	-0.64		0.595	
$\pi p_{3/2}$	-2.60	-0.695	0.664	
^{55}Co:				
$\pi f_{7/2}$	-9.06	-7.165	0.724	

PRC74 (06), 024304

- results are consistent with the spectral distribution expected for good closed shell nuclei !!

N3LO interaction + monopole corr. [CB, M.Hjorth-Jensen, arXiv [nucl-th] Feb. 2009]

Spectral function ^{48}Ca (e,e´p) ^{47}K



NIKHEF
G. Kramer, Thesis

Includes :
low-energy mixing in the Fadd-RPA scheme
☑ long-range correlations

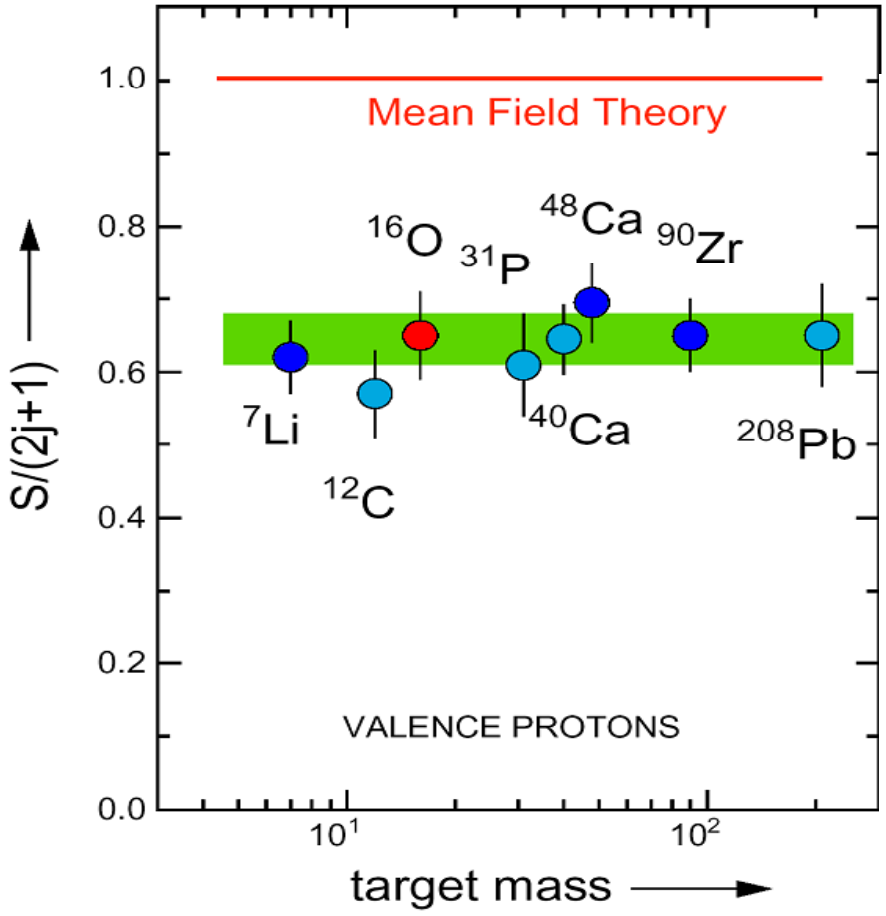
high-energy mixing
☑ short-range correlations

(N3LO based G-matrix)

CB, to be published

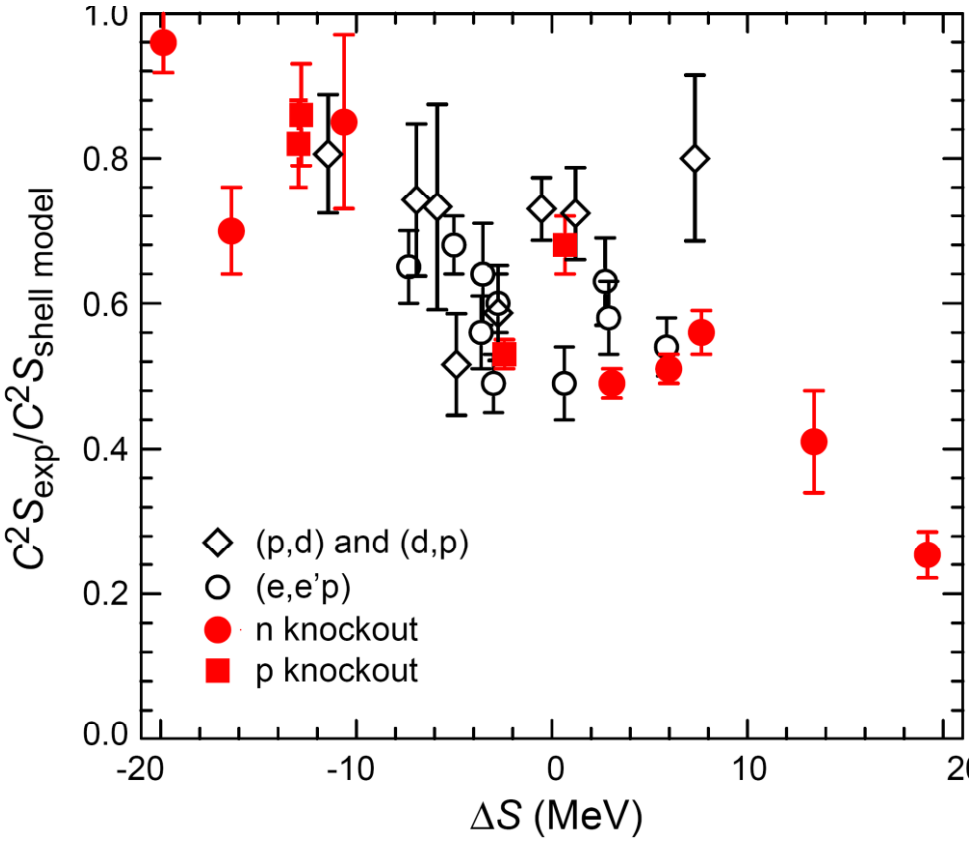
Experimental spectroscopic factors

NIKHEF



Nucl. Phys. A553 (1993) 297c

MSU/NSCL



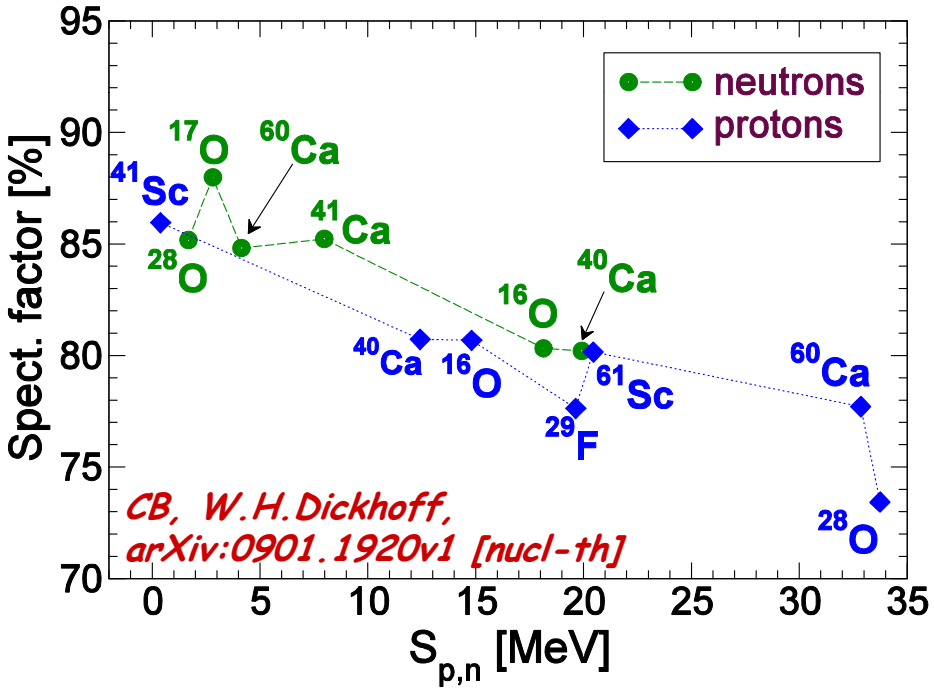
PRL93, 042501 (2004)

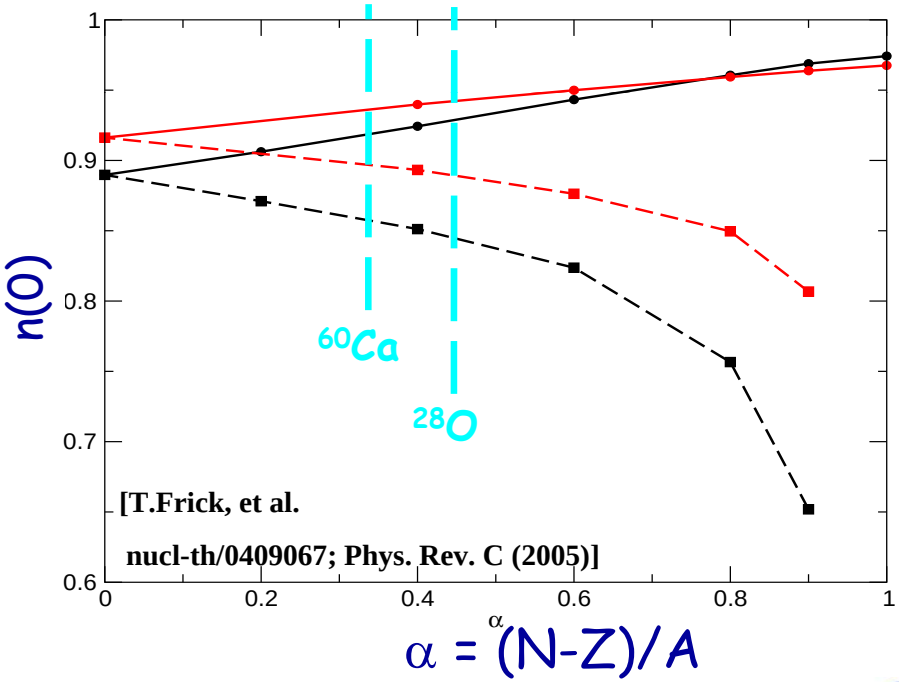
Asymmetry dependence: F-RPA estimate…

Explorative, FRPA calculations show only a slight dependence of spect. factors on separation energies (asymmetry):

- in rough agreement with nuclear matter calculations…
- collective modes may not be fully realistic…

Occupation number at the Fermi surface (for nucleonic matter):





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.

- Large scale *"ab-initio"* applications:
  - accurate correlations and ionization energies for atoms
  - convergent calculations in nuclei are becoming a reality*!!!*
  - not limited to g.s. energies

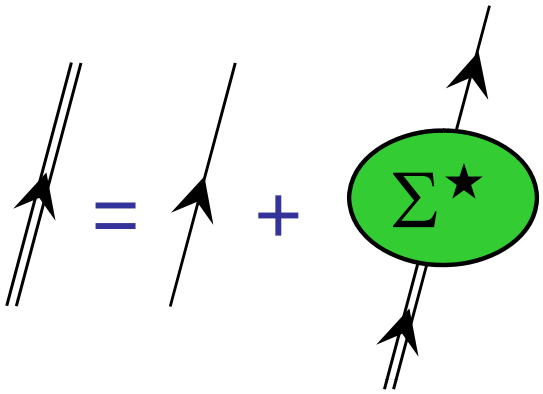
- ^{56}Ni spectral function:
  - $^{57}Ni_{g.s.} \rightarrow {}^{56}Ni_{g.s.}$ spect. Factor aggree with experimental data
  - ^{56}Ni is predicted to be a good shell closure

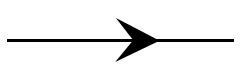
- Physics @ driplines: the observed asymmetry dependence of spectroscopic factros is still unexplained by theory(ies).

...THANKS for your attention!

Dyson-Schwinger equation

In diagrammatic form:




, *free particle* propagator


, *correlated* propagator

, *"irreducible"* self-energy

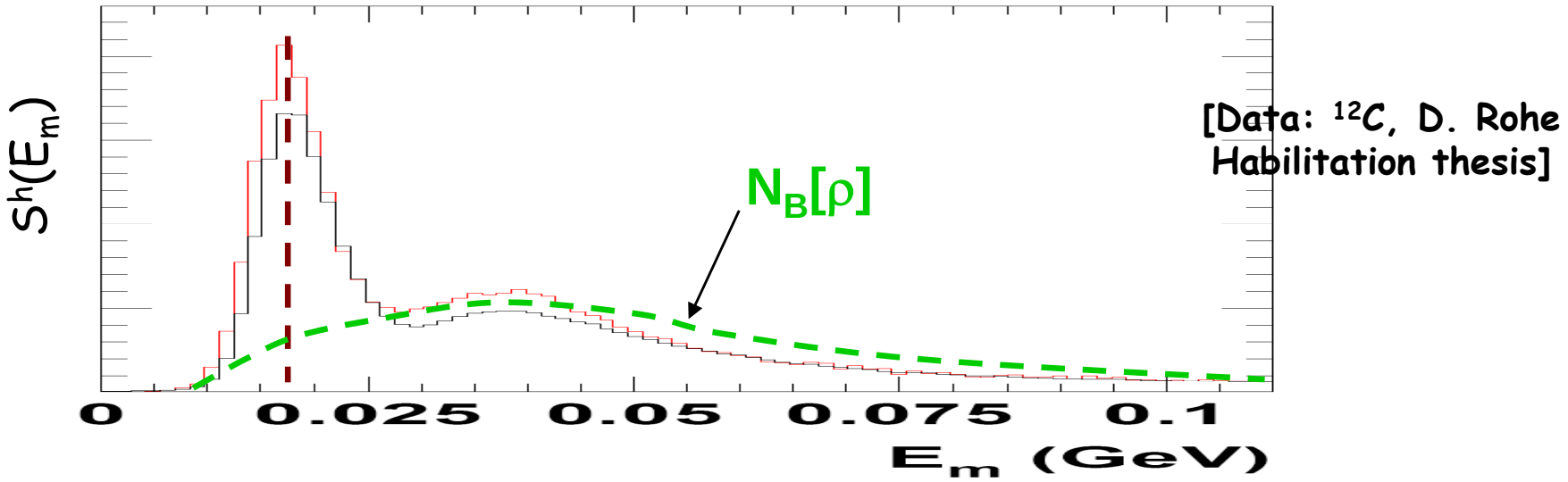
→ it leads to a 1-body equation:

$$\frac{\hat{p}^2}{2m}\psi^{(qp/qh)}(\vec{r}) + \int d\vec{r}\,\Sigma^*(\vec{r},\vec{r}';\omega)\;\psi^{(qp/qh)}(\vec{r}') = \omega\,\psi^{(qp/qh)}(\vec{r})$$

Quasiparticle (QP-)DFT in two words…

Basic idea:

- separate the quasiparticle peak from spectral function
- model background as a functional of density



DETAILS? → Van Neck et al., and Phys. Rev. A74, 042501 (2006).

Quasiparticle (QP-)DFT in two words…

QP-DFT equation (generalized eigenvalue problem):

$$\left([H_0]+\left[\tilde{V}_{HF}\left\{N^{(-)}\right\}\right]-\left[M_B\left\{N^{(-)}\right\}\right]\right)u_j=\varepsilon_{Qj}\left([I]-\left[N_B\left\{N^{(-)}\right\}\right]\right)u_j$$

density matrix: $[N]=[N_Q]+[N_B]$

removal energy matrix: $[M]=[M_Q]+[M_B]$

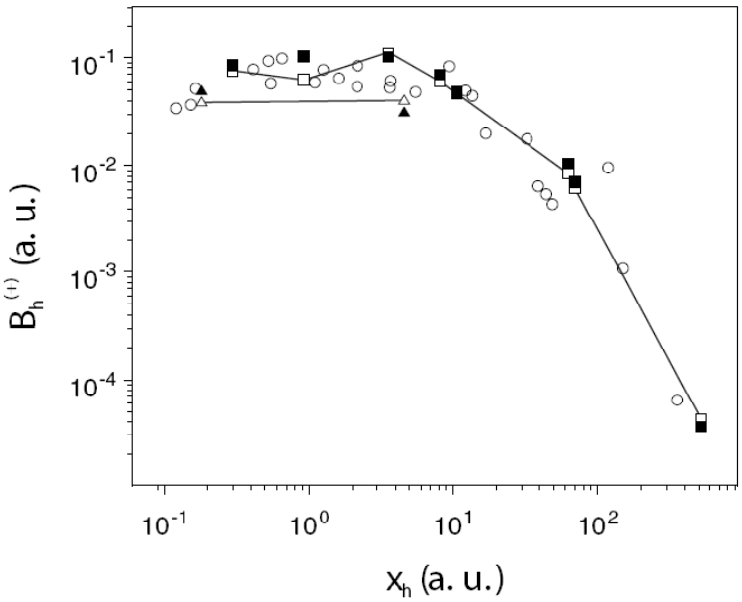
} background contributions (B) are functionals of density!

- one still solves a one-body (HF-like) equation
- generalizes Kohn-Sham (KS) eq. to two functionals (KS for $[M_B]=0$ and $[M_B]=[V_F]-[V_{xc}]$)
- energy, density, and QP properties (sp. energies and spect. factors!)

DETAILS? → Van Neck et al., and Phys. Rev. A74, 042501 (2006).

Extracting the QP-DFT background functionals...

first attempt to extract the background:



← *GW* calculations on small atoms

[Phys. Rev. ***A74***, 062503 (2006)]

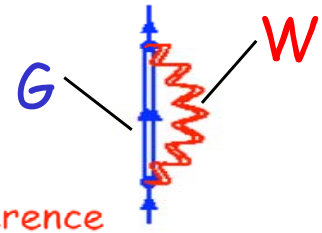
→ *need* accurate "ab-initio" calculations of QP properties, *from small atoms/molecules to the electron gas!!*

Why a Faddeev (F-)RPA?

- Electron gas → screening of Coulomb → need RPA
  Correlation energies (GW):

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



- Finite systems → QP and ionization energies
  GW does NOT work → need 3rd order PT minimum
  ADC(3), Heidelberg (chem.) group ≈ F-TDA

F-RPA!!

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

Characteristics of FRPA and CC

TABLE I. Characteristics of nD-ADC and CC methods (explicit configuration space, perturbation-theoretical consistency for ionization energies (Ω), and ground-state (E_0) energies scaling).

Method	Configuration space	Ω		E_0	Scaling[a]
		$1h$	$2h$-$1p$		
ADC(2)	$1h$, $2h$-$1p$	2	0	2	n^4
ADC(2)-E	$1h$, $2h$-$1p$	2	1	2	n^5
CCSD	$1h$, $2h$-$1p$	2	1	3	n^6
F-RPA, F-TDA ≈ ADC(3)	$1h$, $2h$-$1p$	3	1	3	n^5
CCSDT	$1h$, $2h$-$1p$, $3h$-$2p$	3	2	4	n^8

A.B.Trofimov, J. Schirmer, J. Chem. Phys. **123**, 144115 (2005).

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	-12	-15	-200.043

(preliminary)

Phys. Rev. A76, 052503 (2007).

+ CB and van Neck, arXiv:0901.1735v1 [physics.chem-ph]

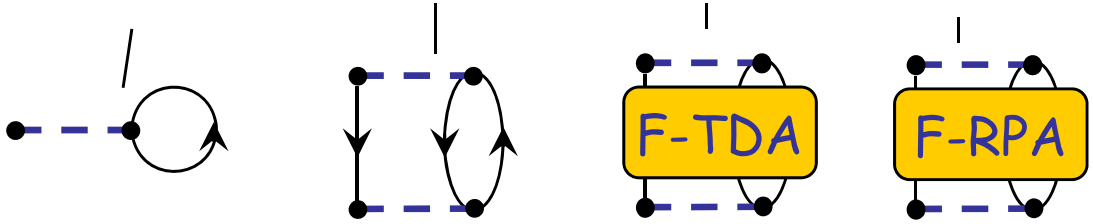
Energies in Hartree /
Relative to the experiment in mH

cc-pV(TQ)Z bases, extrapolated as $E_X = E_\infty + AX^{-3}$ (≈ 5mH accuracy)

Valence Ionization Energies

CB, D. Van Neck, arXiv:0901.1735v1 [physics.chem-ph]

	HF	2nd	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	-13	-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

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.

- Large scale *"ab-initio"* applications:
  - accurate correlations and ionization energies for atoms
  - convergent calculations in nuclei are becoming a reality*!!!*
  - *not limited to g.s. energies*

- ^{56}Ni spectral function:
  - $^{57}Ni_{g.s.} \rightarrow {}^{56}Ni_{g.s.}$ spect. Factor aggree with experimental data
  - ^{56}Ni is predicted to be a good shell closure

- Physics @ driplines: the observed asymmetry dependence of spectroscopic factros is still unexplained by theory(ies).

...THANKS for your attention!