Spectral function (and spectroscopic factors) of finite nuclei

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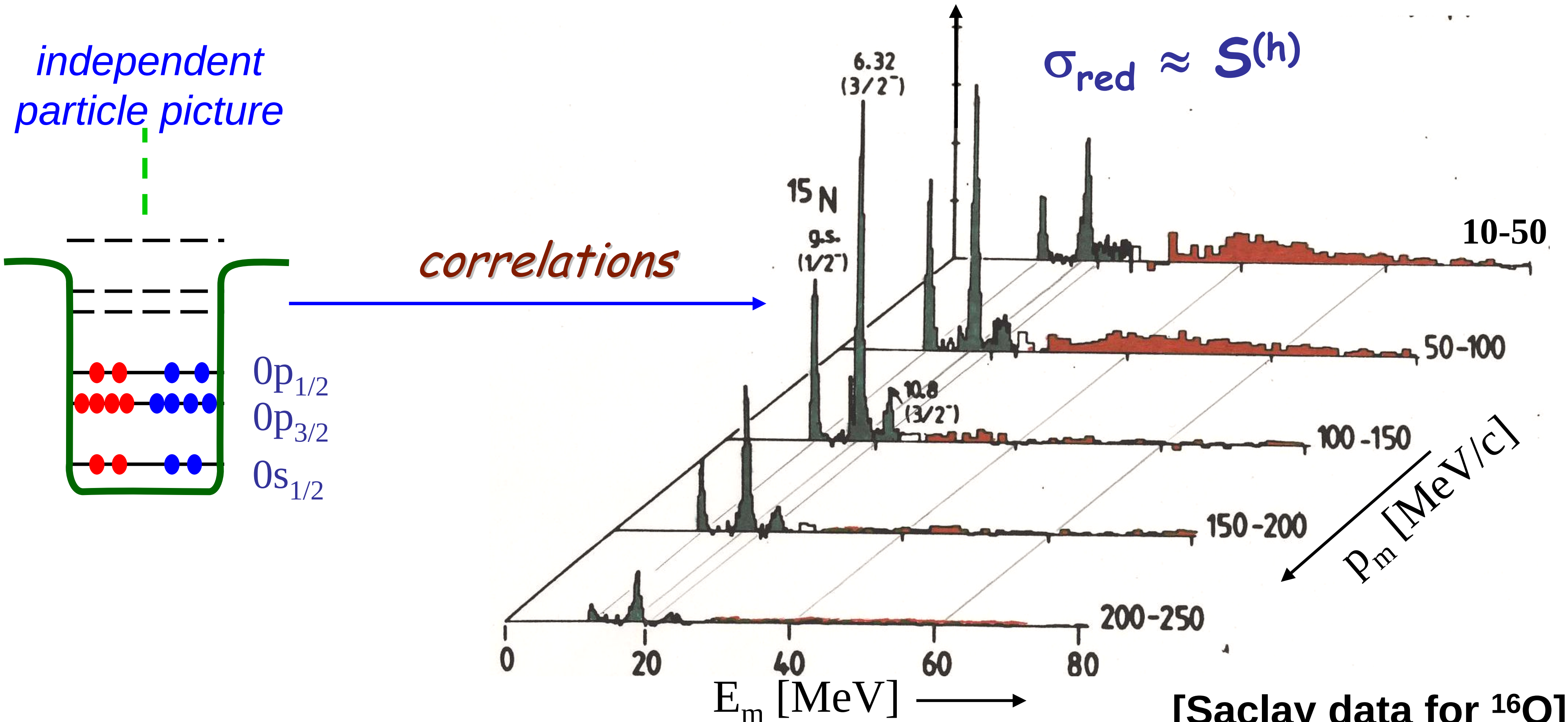
Collaborators: W. H. Dickhoff, D. Van Neck, D. Rohe, L. Lapikás, I. Sick, M. Hjorth-Jensen, C. Giusti, F. D. Pacati, G. Martínez-Pinedo, K. Langanke

Quasi-free Scattering with Radioactive Ion Beams, ECT*, Trento, 7-11 April 2008

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

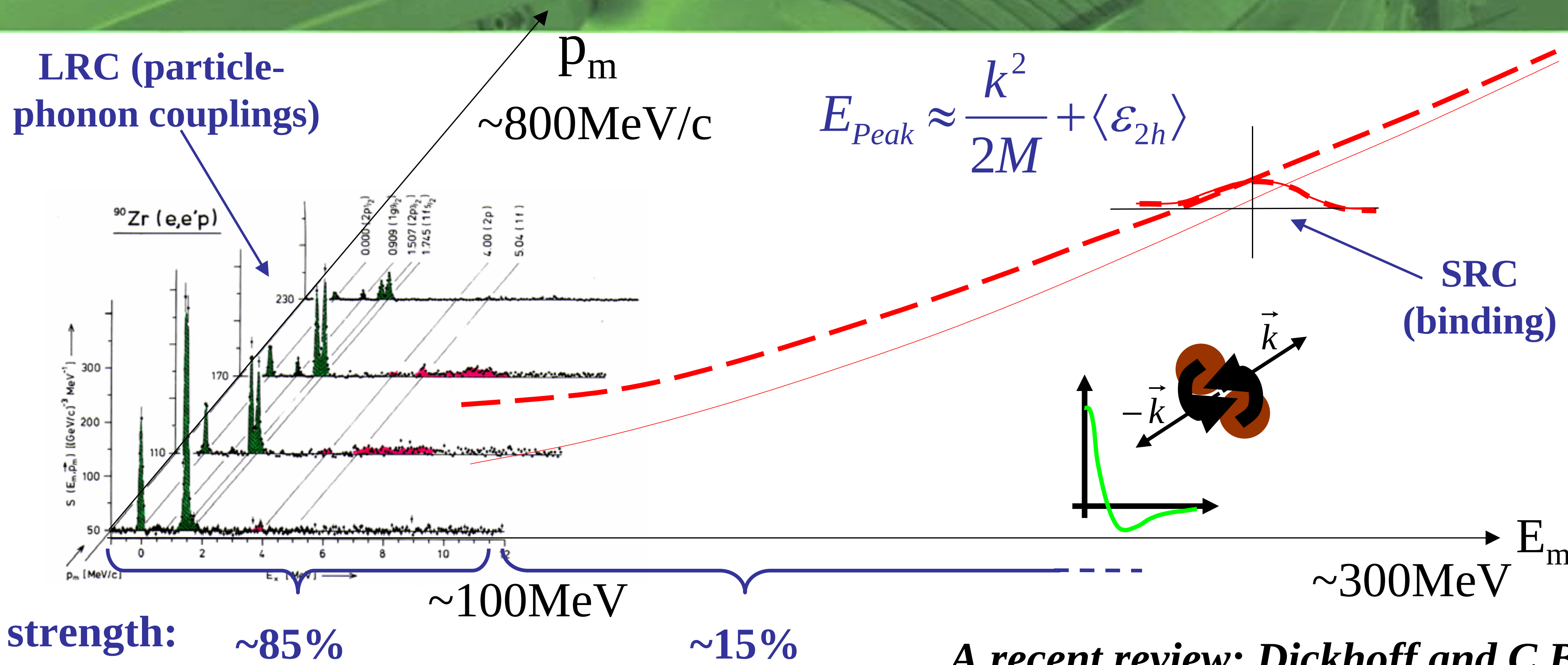


[Saclay data for ^{16}O]

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

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

Complete distribution of the nuclear strength

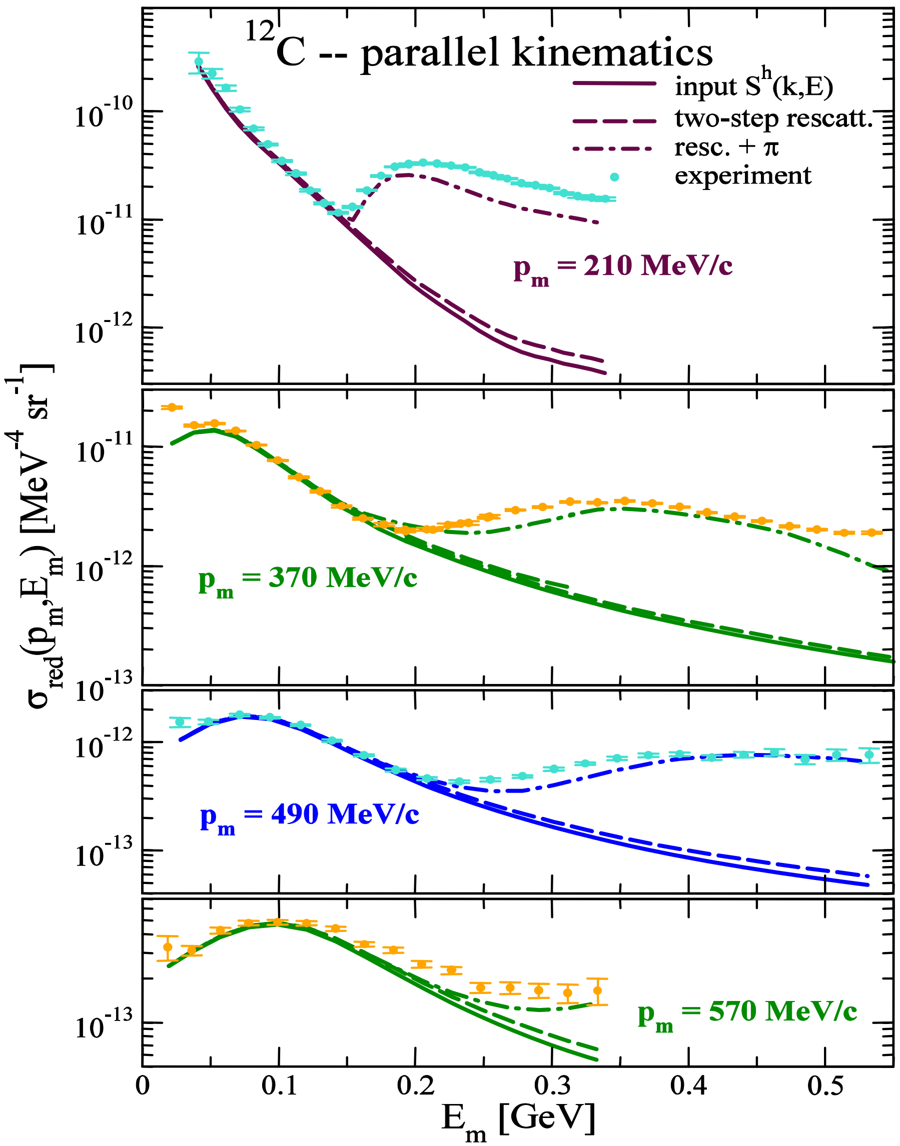


A recent review: Dickhoff and C.B., Prog. Part. Nucl. Phys. 52 (2004) 337.

Short range correlated region:

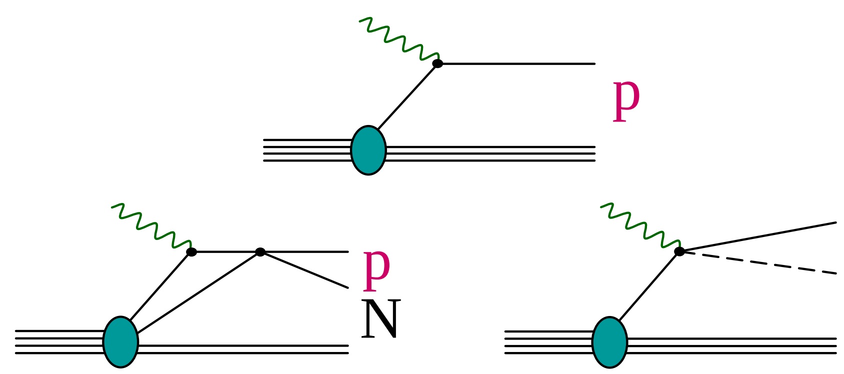
- a *fraction* of the total number of nucleons:
  - ~10% in light nuclei (VMC, FHNC, Green's function on light nuclei)
  - ~15% in heavy systems (CBF, Green's function on nuclear matter)
- can explain up to *2/3 of the binding energy* (!) [see eg. PRC51, 3040 ('95)]

High missing energy/momentum strength -- SRC



Observation of high momentum components:

- signature of SRC
- possible in parallel kinematics
- parallel kinematics (and ^{12}C) described in a MC cascade model + delta excitation

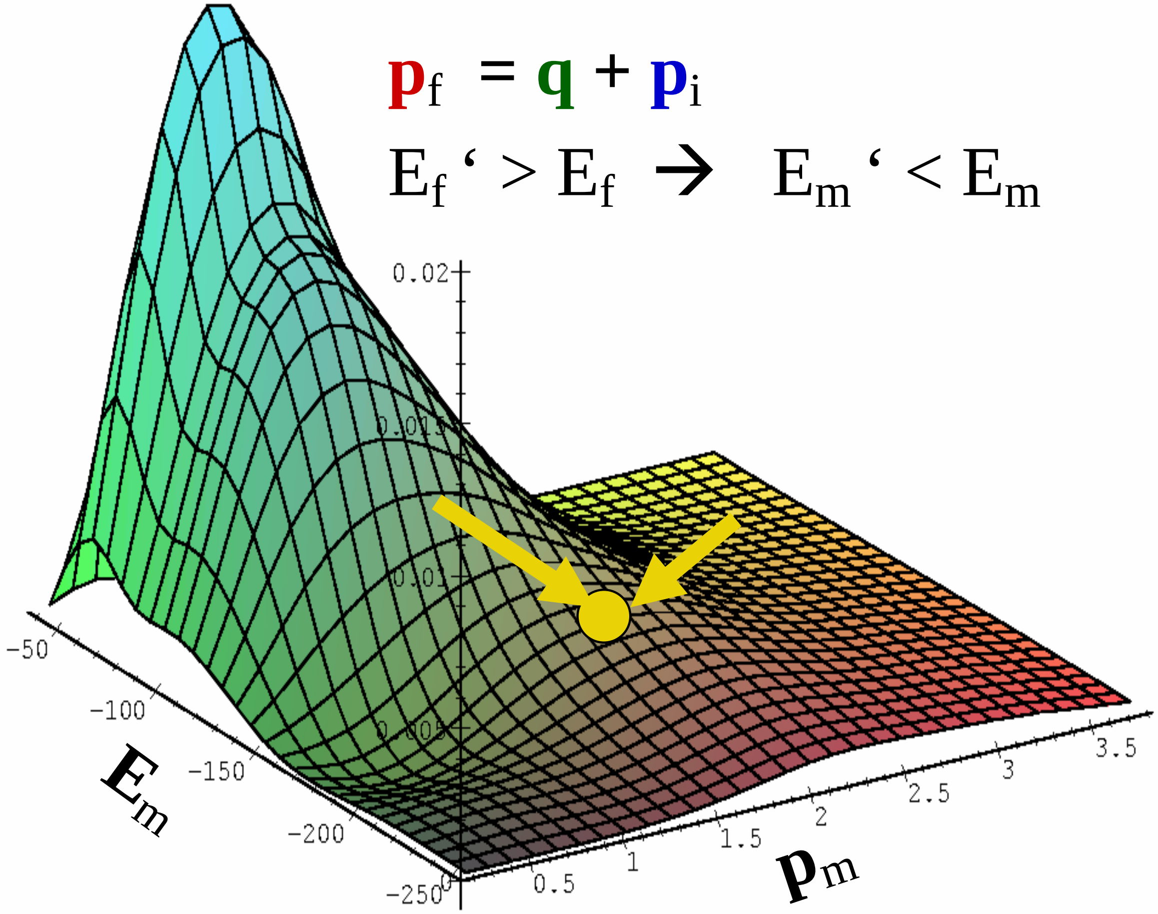


Measurement:
D. Rohe, et. al, Phys. Rev. Lett. 93, 182501 (2004)
FSI:
CB, L. Lapikás, Phys. Rev. C70, 054612 (2004)
CB, Nuclear Physics B (Proc. Suppl.) 159 (2006) 174

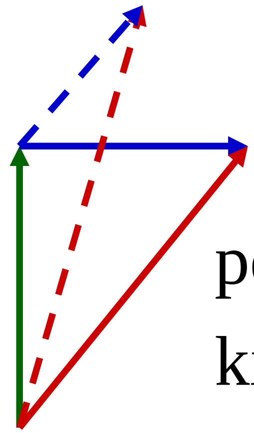
Dependence of rescatt. on kinematics

$\mathbf{p}_f = \mathbf{q} + \mathbf{p}_i$

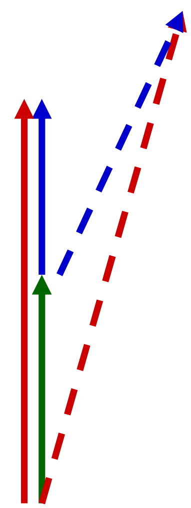
$E_f' > E_f \rightarrow E_m' < E_m$



The kinematics are defined in terms of the angle between the final ($\mathbf{p}_f$) and initial ($\mathbf{p}_i = -\mathbf{p}_m$) momentum of the proton



perpendicular kinematics

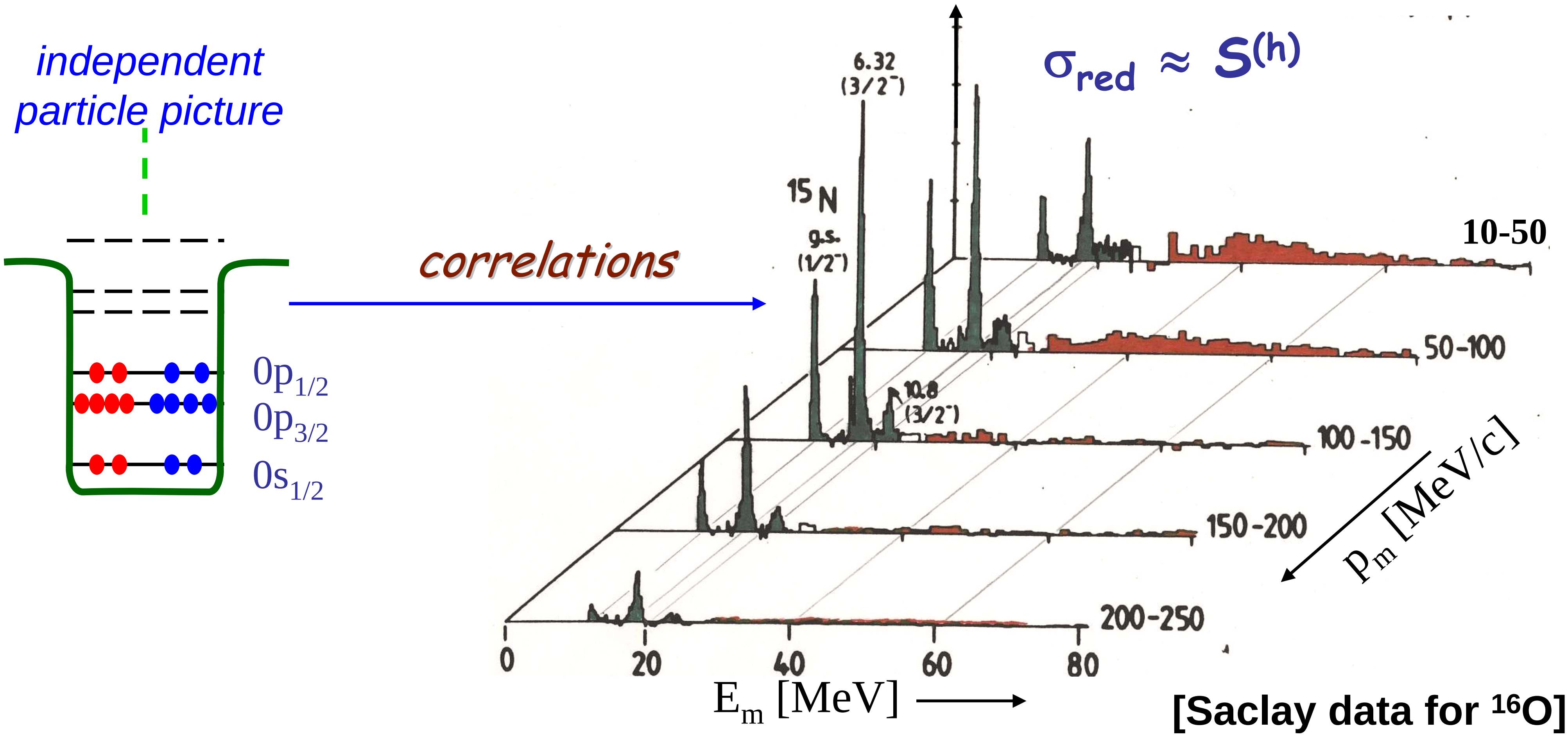


parallel kinematics

(picture credit: D.Rohe, habilitaion thesis)

CB, Rohe, Sick, Lapikás, Phys. Lett. B608 47 (05)

One-hole spectral function -- example



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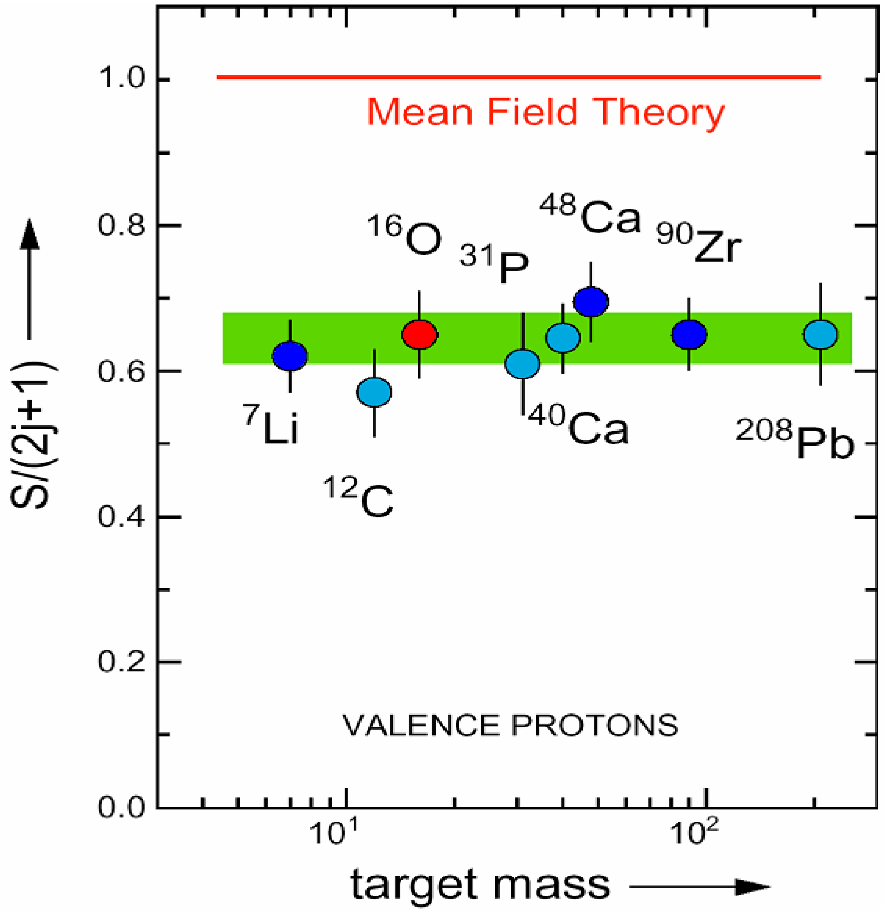
$$S^{(h)}(p_m, E_m) = \sum_n \left| \langle \Psi_n^{A-1} | c_{\vec{p}_m} | \Psi_0^A \rangle \right|^2 \delta(E_m - (E_0^A - E_n^{A-1}))$$

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

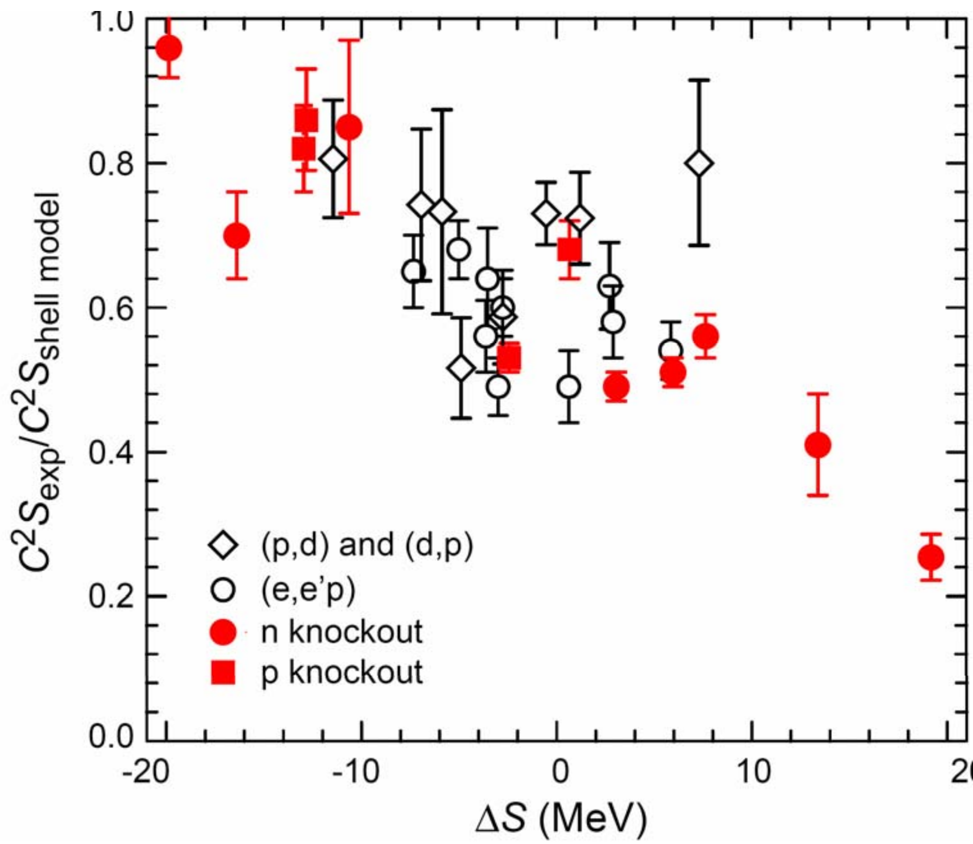
Experimental spectroscopic factors

NIKHEF



Nucl. Phys. A553 (1993) 297c

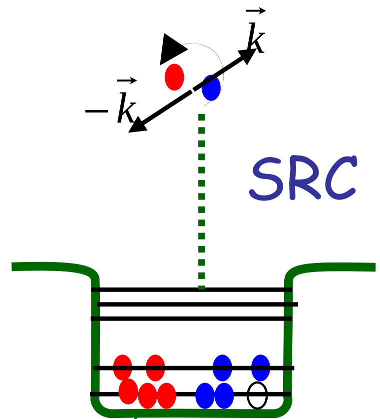
MSU/NSCL

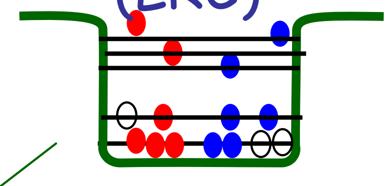


PRL93, 042501 (2004)

Correlations and spect. factors

$$S = \left| \langle \Psi_0^A | c_{-n}^+ | \Psi_n^{A-1} \rangle \right|^2$$

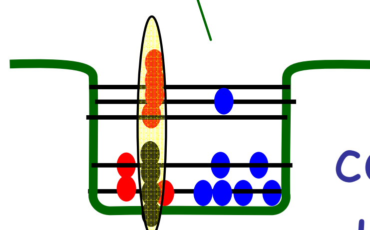




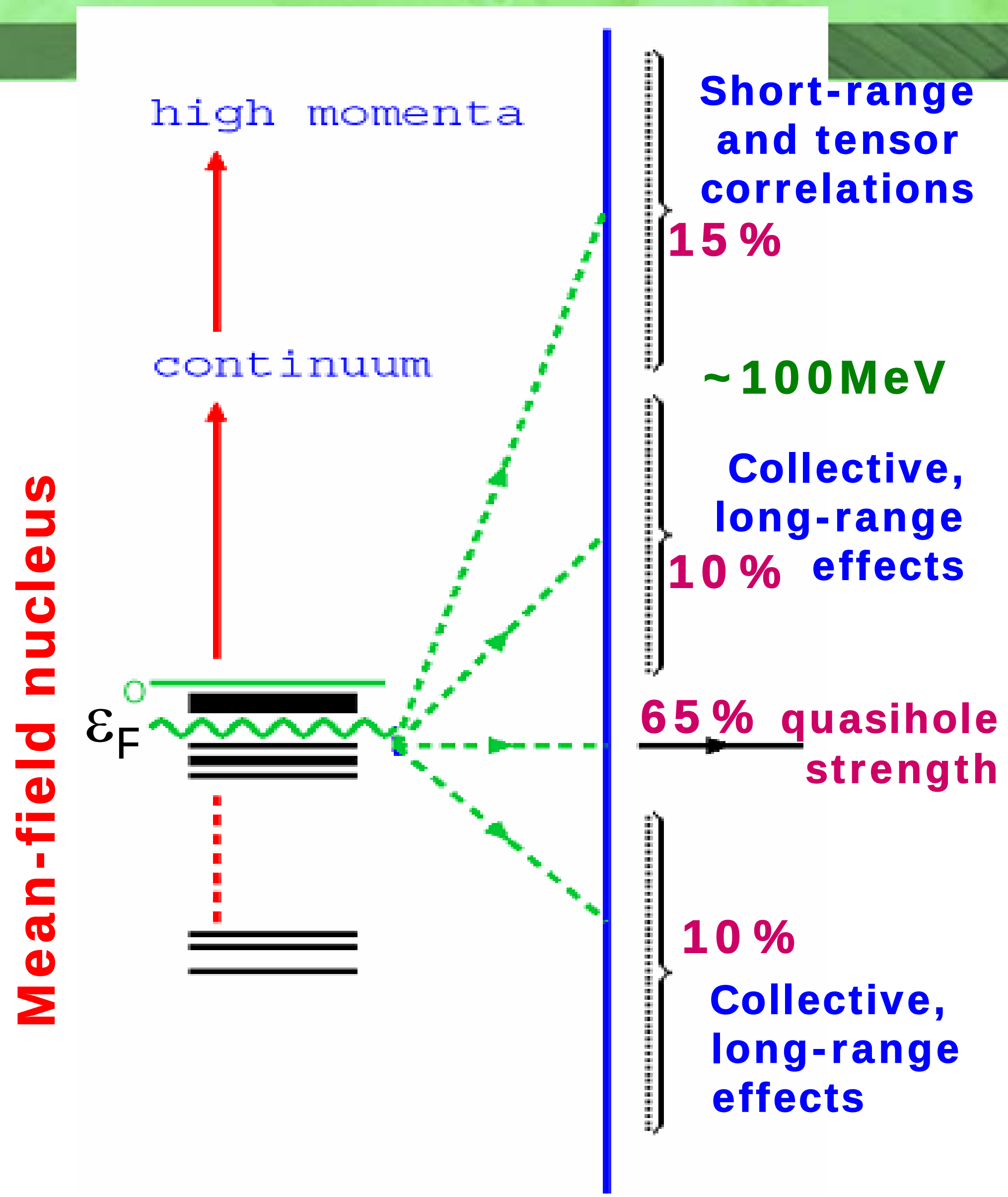
Schematically:

$$|\Psi_0^A\rangle \approx \alpha c_{-n}^+ |\Psi_n^{A-1}\rangle + \sum c_m^+ c_n^+ c_i |\Psi_n^{A-1}\rangle + \sum c_m^+ c_n^+ c_p^+ c_i c_j |\Psi_n^{A-1}\rangle + \ldots$$

$\alpha^2 \rightarrow$ spectroscopic factor



Correlations and spect. factors



Spectral strength for a correlated nucleus

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):

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

Principal Many-body Green's functions

Quasiparticle and phonon excitations can be described with many-body Green's functions:

$$g_{\alpha\beta}(\omega) = \langle \Psi_o^A | c_\alpha \frac{1}{\omega - H + i\eta} c_\beta^+ | \Psi_o^A \rangle + \ldots$$ one-body propagator

$$G^{II}_{\alpha\beta,\,\gamma\delta}(\omega) = \langle \Psi_o^A | c_\alpha c_\beta \frac{1}{\omega - H + i\eta} c_\delta^+ c_\gamma^+ | \Psi_o^A \rangle + \ldots$$ two-body propagator

$$\Pi_{\alpha\beta,\,\gamma\delta}(\omega) = \langle \Psi_o^A | c_\alpha^+ c_\beta \frac{1}{\omega - H + i\eta} c_\delta^+ c_\gamma | \Psi_o^A \rangle + \ldots$$ polarization (ph) propagator

Principal Many-body Green's functions

Quasiparticle and phonon excitations can be described with many-body Green's functions:

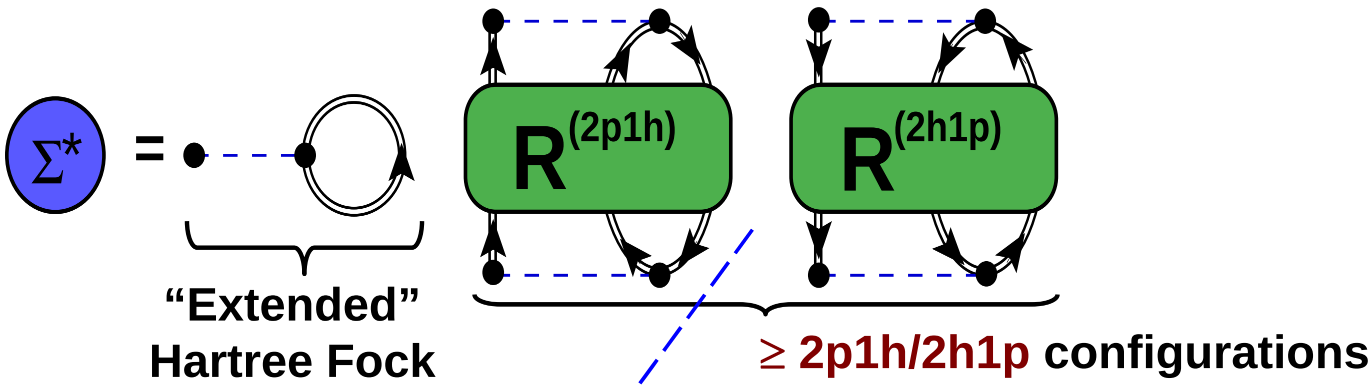
$g_{\alpha\beta}(\omega)$	addition removal of *one* particle, spectra of A±1 particle systems, one-body density, optical potential.
$G^{II}_{\alpha\beta,\,\gamma\delta}(\omega)$	addition removal of *two* particles, spectra of A±2 particle systems, two-body density
$\Pi_{\alpha\beta,\,\gamma\delta}(\omega)$	Spectrum of the A particle systems, one-body response

→ linked to a lot of exp. Information

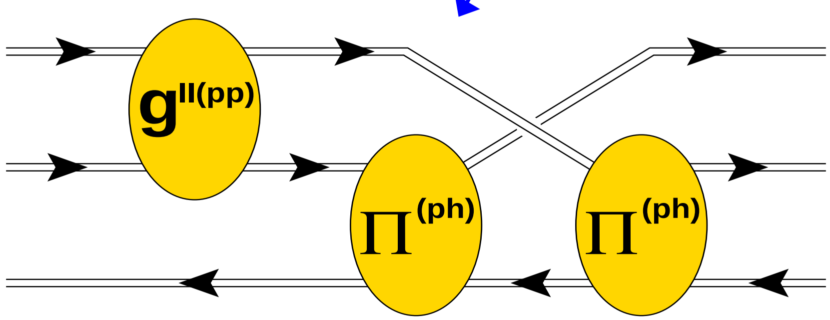
→ "efficiency" with information, only transition amplitudes are generated

Coupling single particle to collective modes

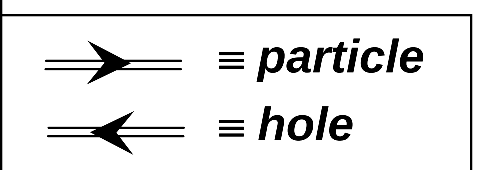
- Non perturbative expansion of the self-energy:



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

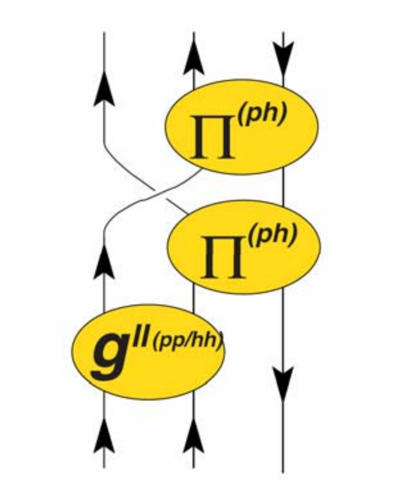


- Both pp (ladder) and ph (ring) modes included
- Pauli exchange at 2p1h/2h1p level

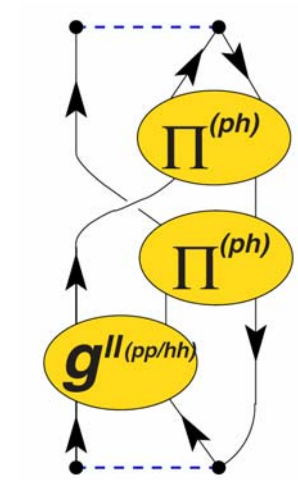


PRC63, 034313 (2001)
PRC65, 064313 (2002)
PRA76, 052503 (2007)

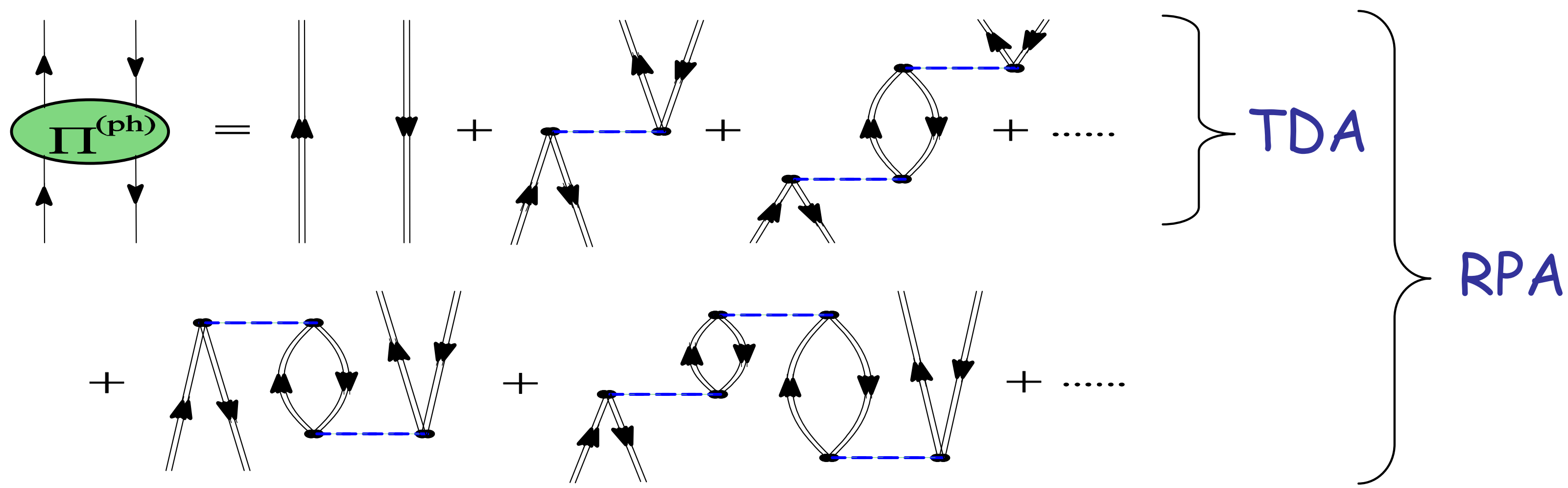
FRPA: Faddeev summation of RPA propagators



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



where:

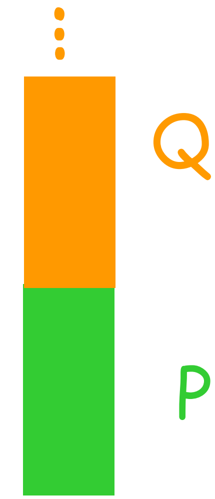


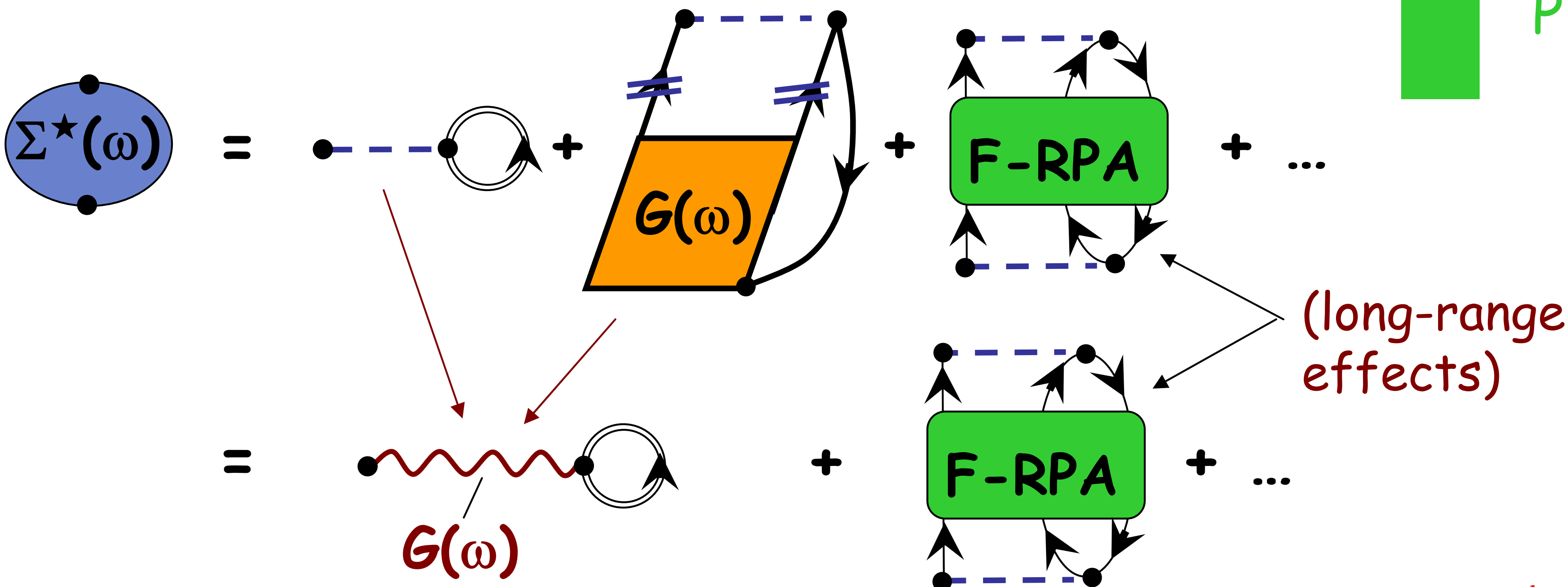
References: CB, et al., Phys. Rev. C63, 034313 (2001); Phys. Rev. A76, 052503 (2007)

Treating short-range corr. with a G-matrix

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

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

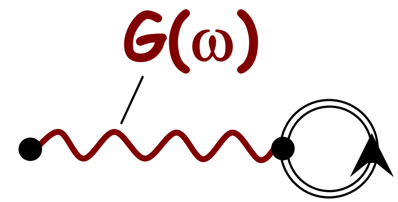


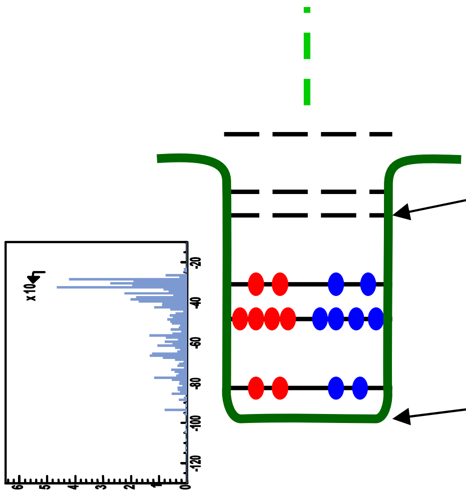


Treating short-range corr. with a G-matrix

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

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

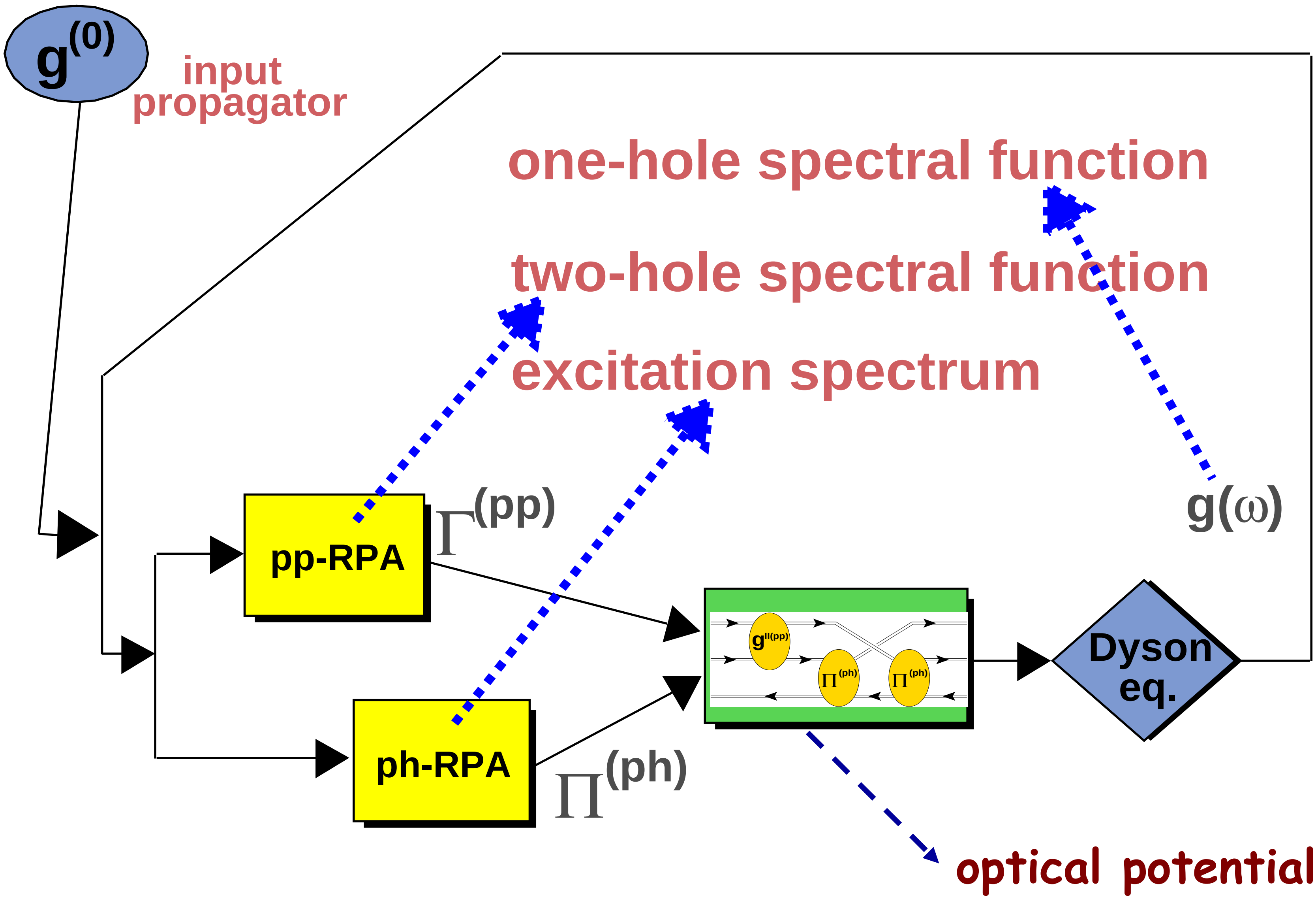




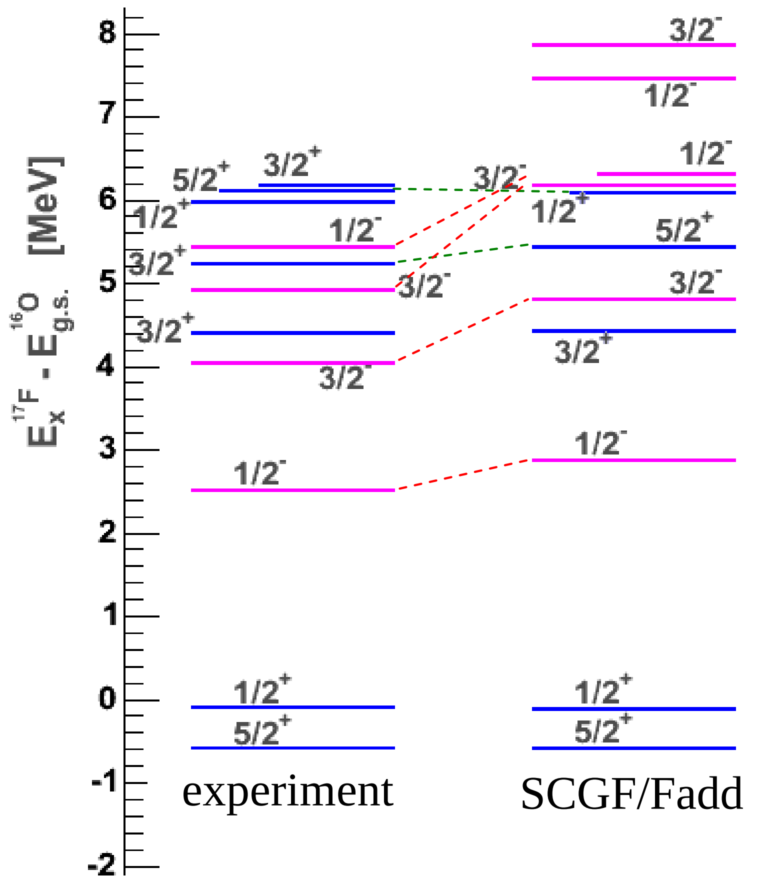
Near E_F: long-range / SM-like physics
→ stronger eff. interaction

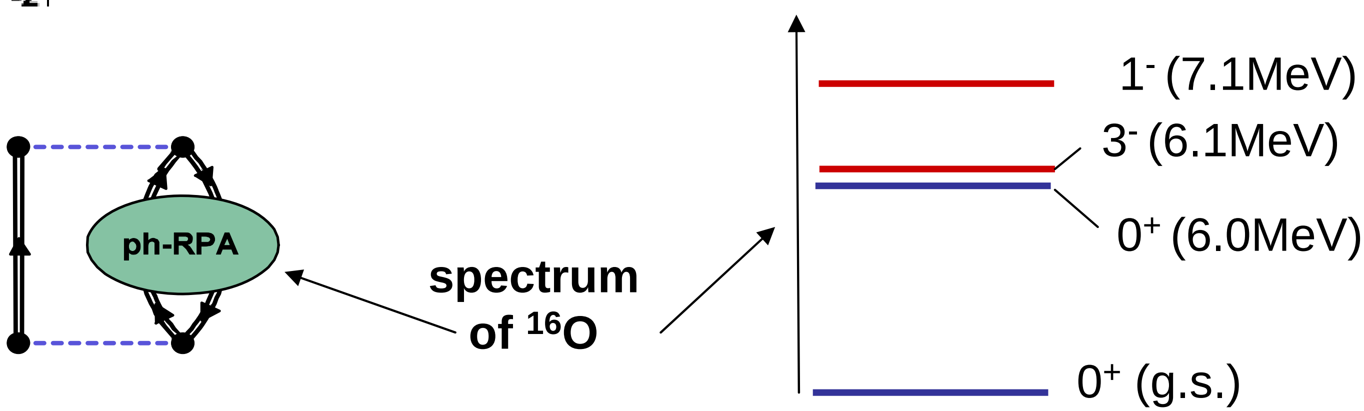
Deeply bound "orbits": binding!
the HF mean-field is weaker

Self-consistent Green's function approach



Quasiparticle spectrum of ^{16}O (i.e. ^{17}F)





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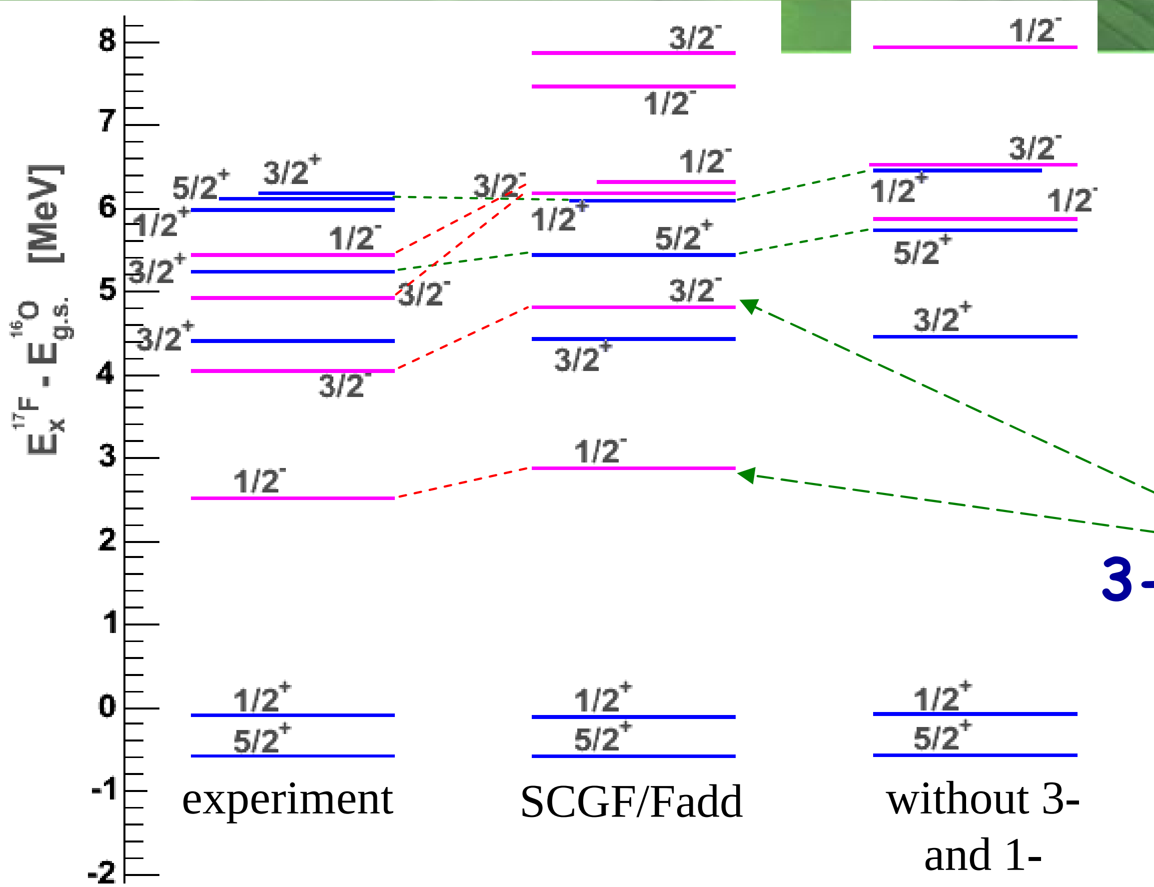
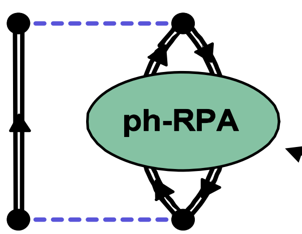
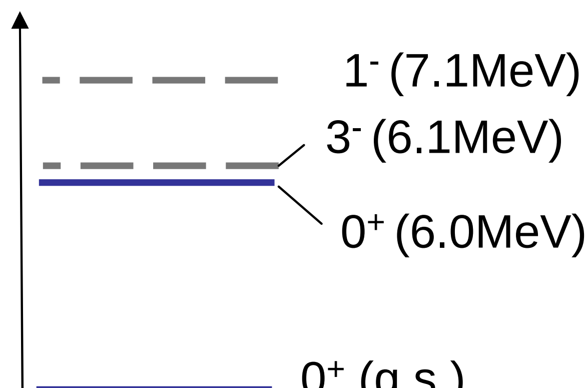


coupling a proton to
3- and 1- phonons in ^{16}O



spectrum of ^{16}O



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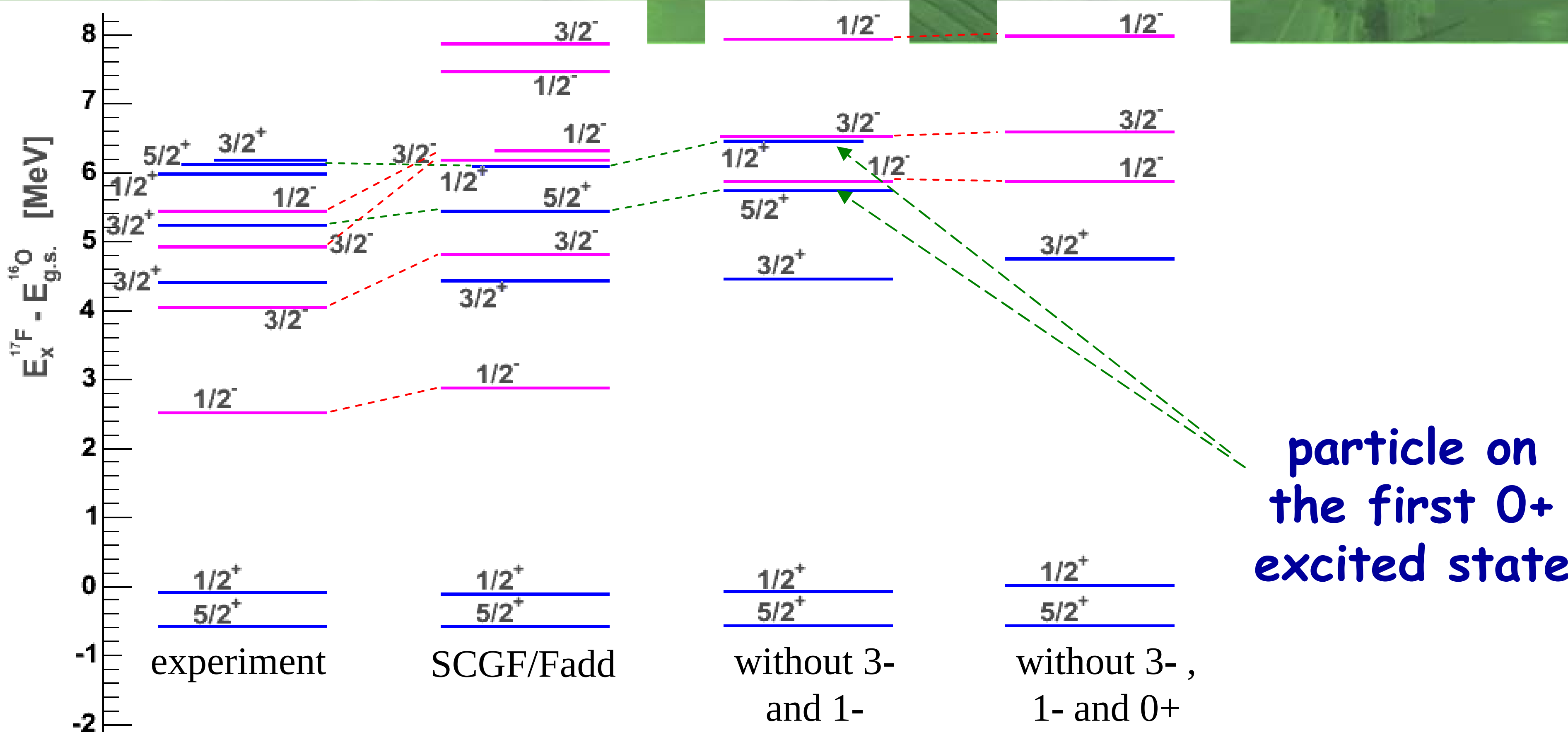
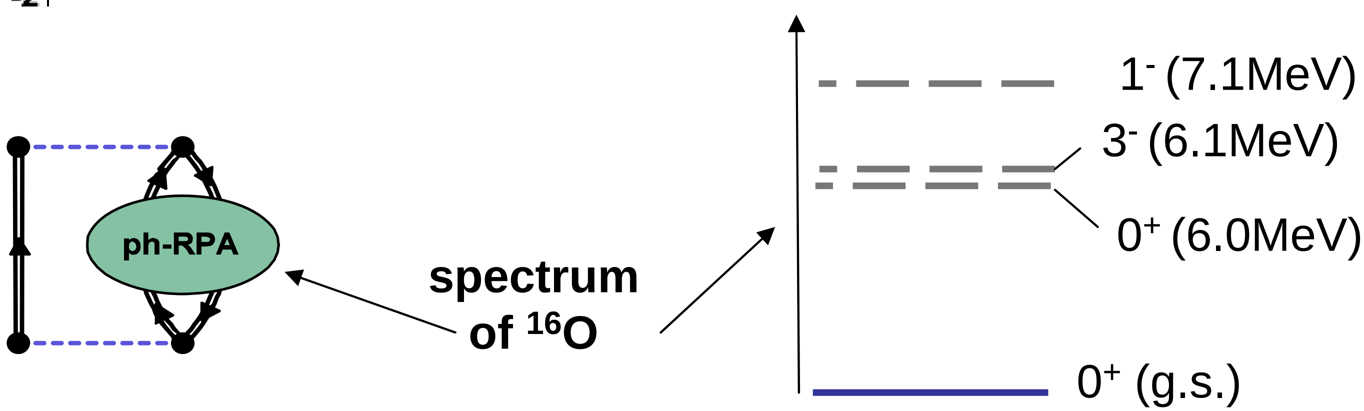
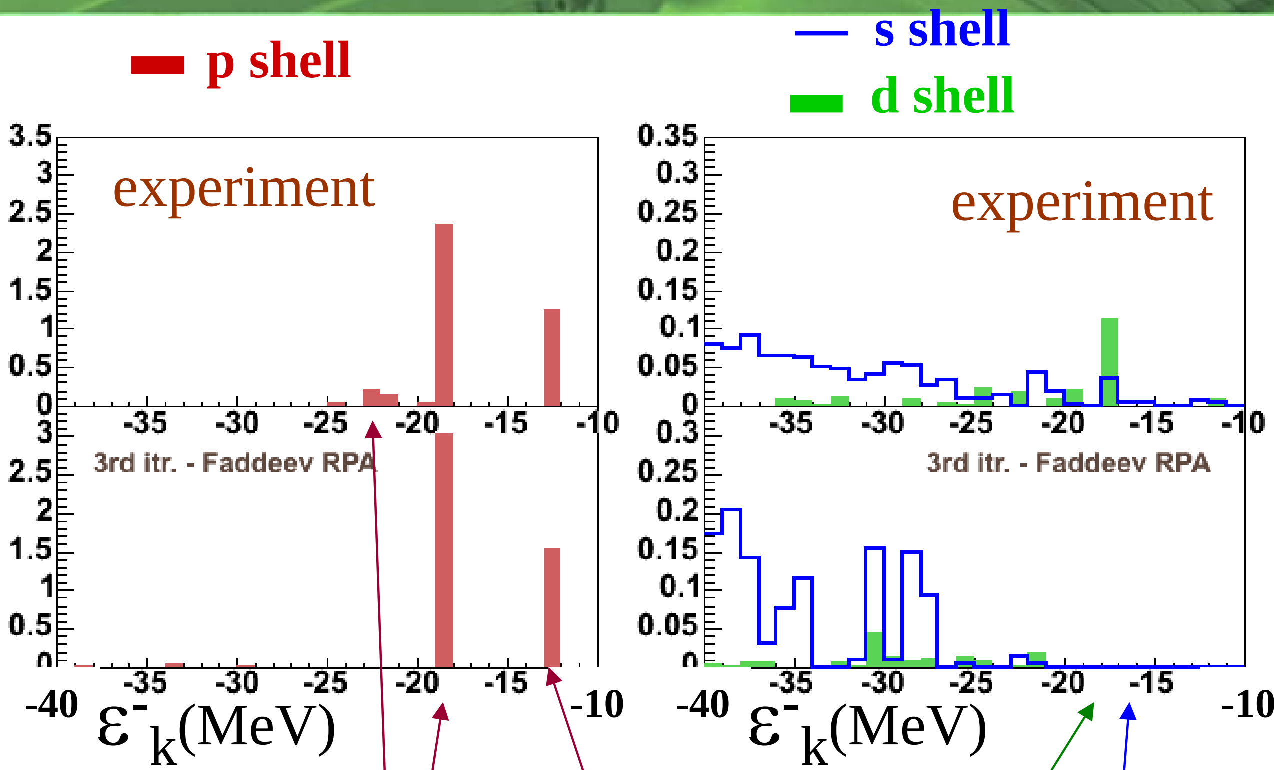




Results for the hole spectral function of 16O



Experiment from NIKHEF, Leuschner et. al., PRC59, 655 (94)

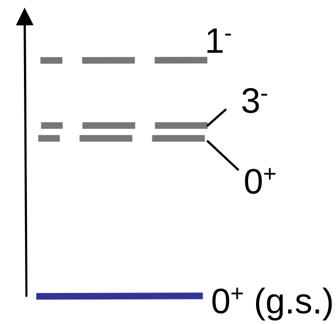
← Results from Faddeev expansion and SCGF

$p_{1/2}$ (g.s.)

$p_{3/2}$ (E_x≈6.3MeV)

$S_{1/2}$ (E_x≈5.2MeV)

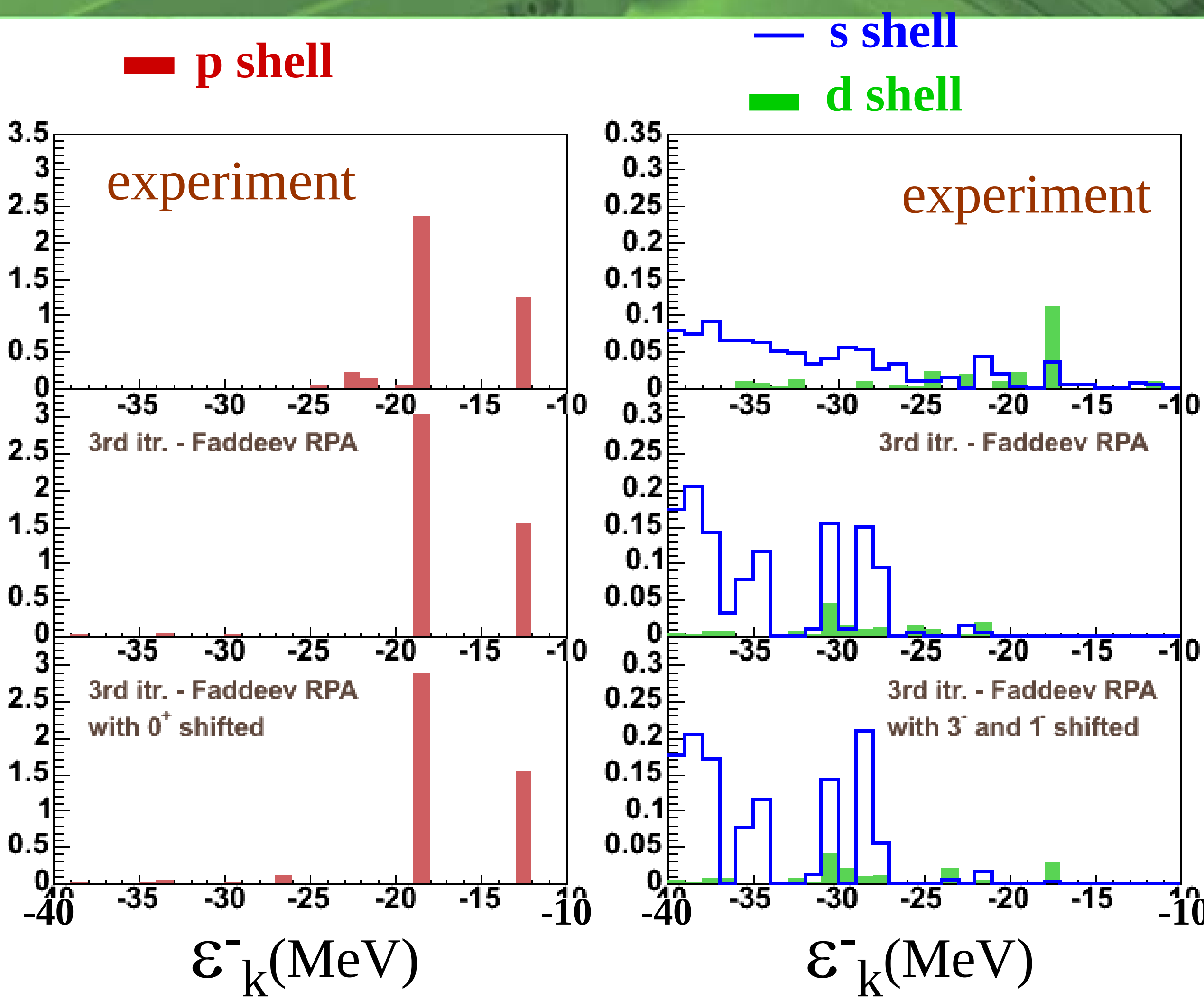
$d_{5/2}$ (E_x≈5.2MeV)



C.B. et. al., PRC65, 064313 (2002)

Results for the hole spectral function of 16O

C.B. and WD, PRC65, 064313 (02)



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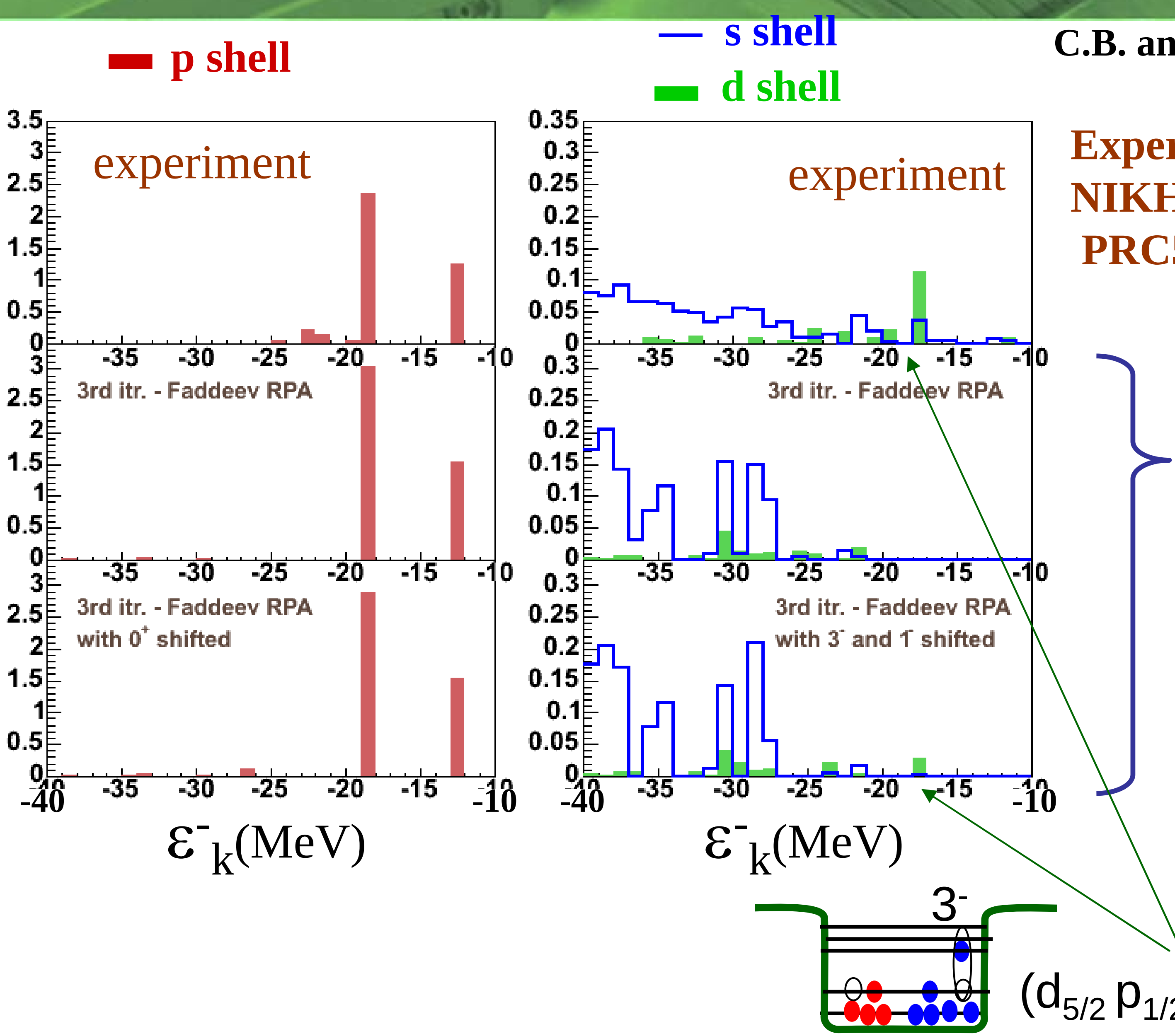

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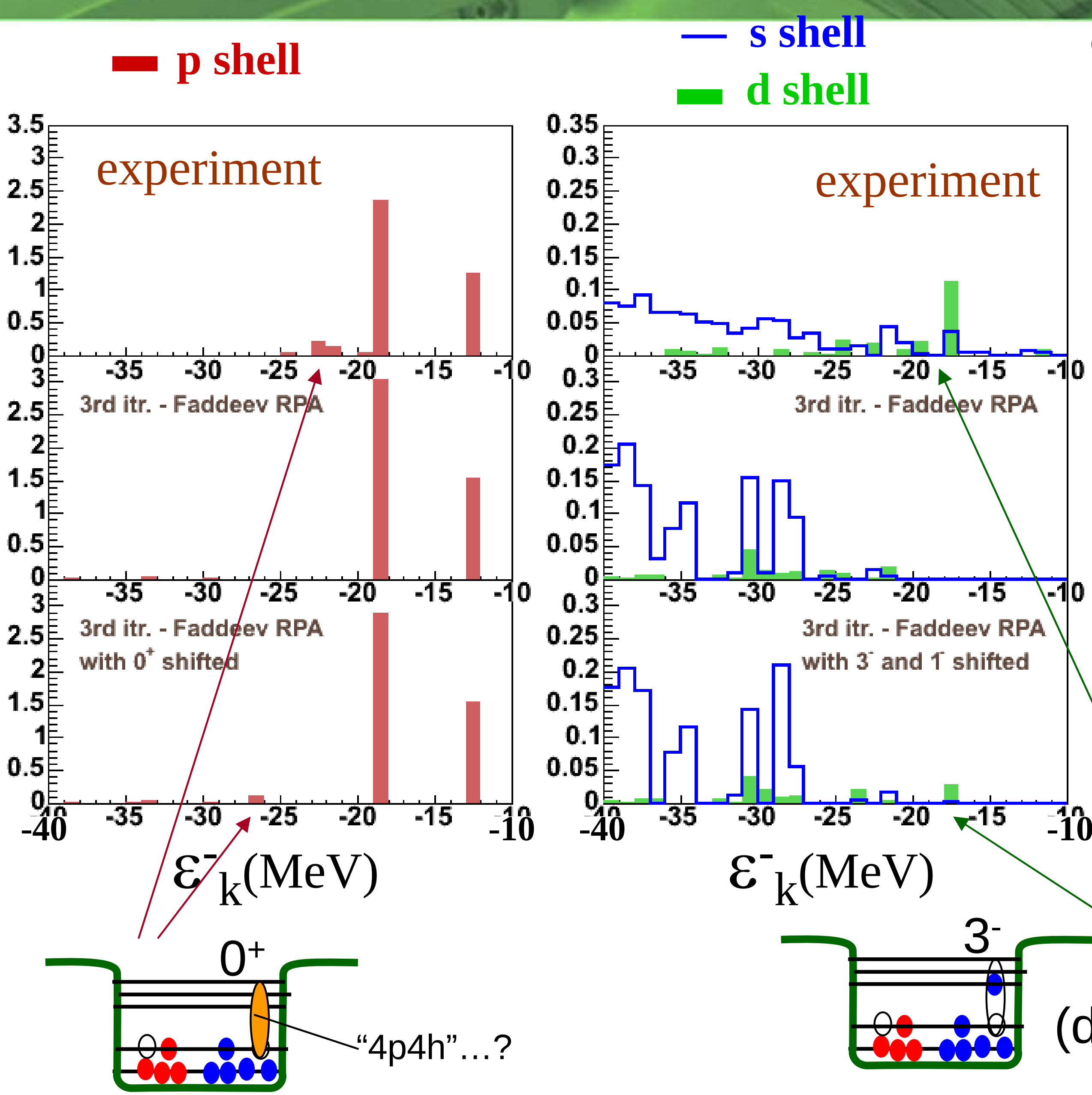
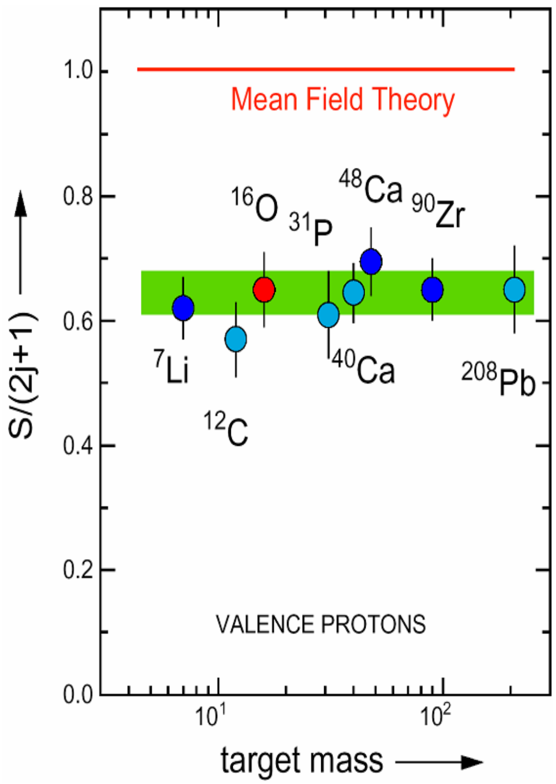


Experiment from NIKHEF, Leuschner et. al., PRC59, 655 (94)

- Results from Faddeev expansion and SCGF

$(d_{5/2}\,p_{1/2}^{-1})\;p_{1/2}^{-1} \approx d_{5/2} \otimes 3^-$

Quasihole fragments in ^{16}O (spectroscopic factors)



	$S_{p1/2}$	$S_{p3/2}$	
• Short-range correlations oriented methods:			
– VMC [Argonne, '94]	0.90		
– GF(SRC) [St.Louis-Tübingen '95]	0.91	0.89	
– FHNC/SOC [Pisa '00]	0.90		
• Including particle-phonon couplings:			
– GF(Faddeev) [St.Louis '01]	0.77	0.72	
[CB et al., Phys. Rev. C**65**, (02)]			
• Experiment:	0.63	0.67	±0.05 (estimated uncertainty)

→ most elaborated calculations for ^{16}O

→ relevance of collective modes (but still need to do better)

Details of calculations

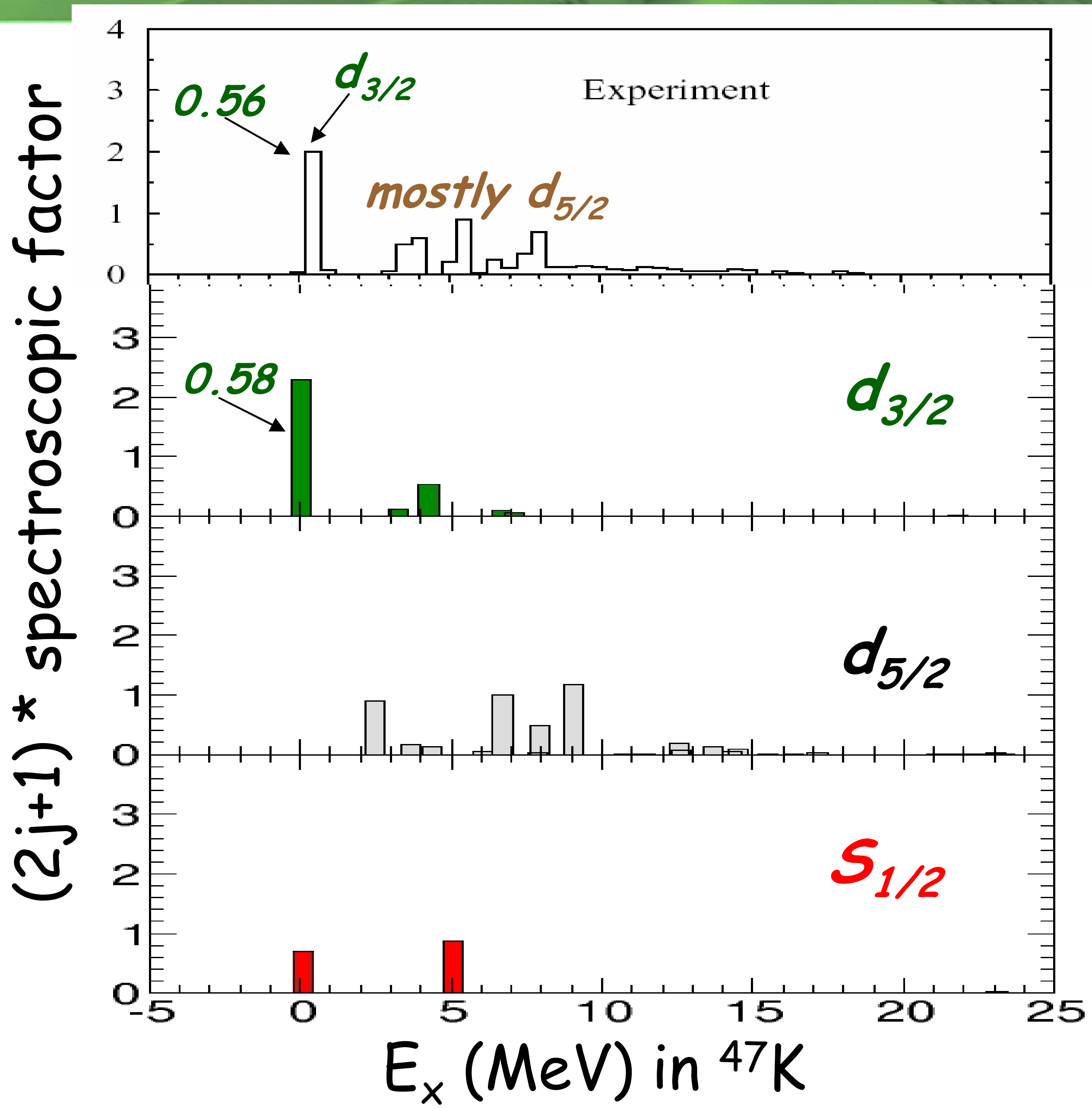
^{16}O →

- 4 major oscillator shells
- G-matrix derived from Bonn-C
- Full self-consistency

^{48}Ca, ^{56}Ni, etc… →

- Up to 8 major oscillator shells (more possible)
- G-matrix derived from N3LO + Coulomb
- Partial self-consistency only for the mean-field

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



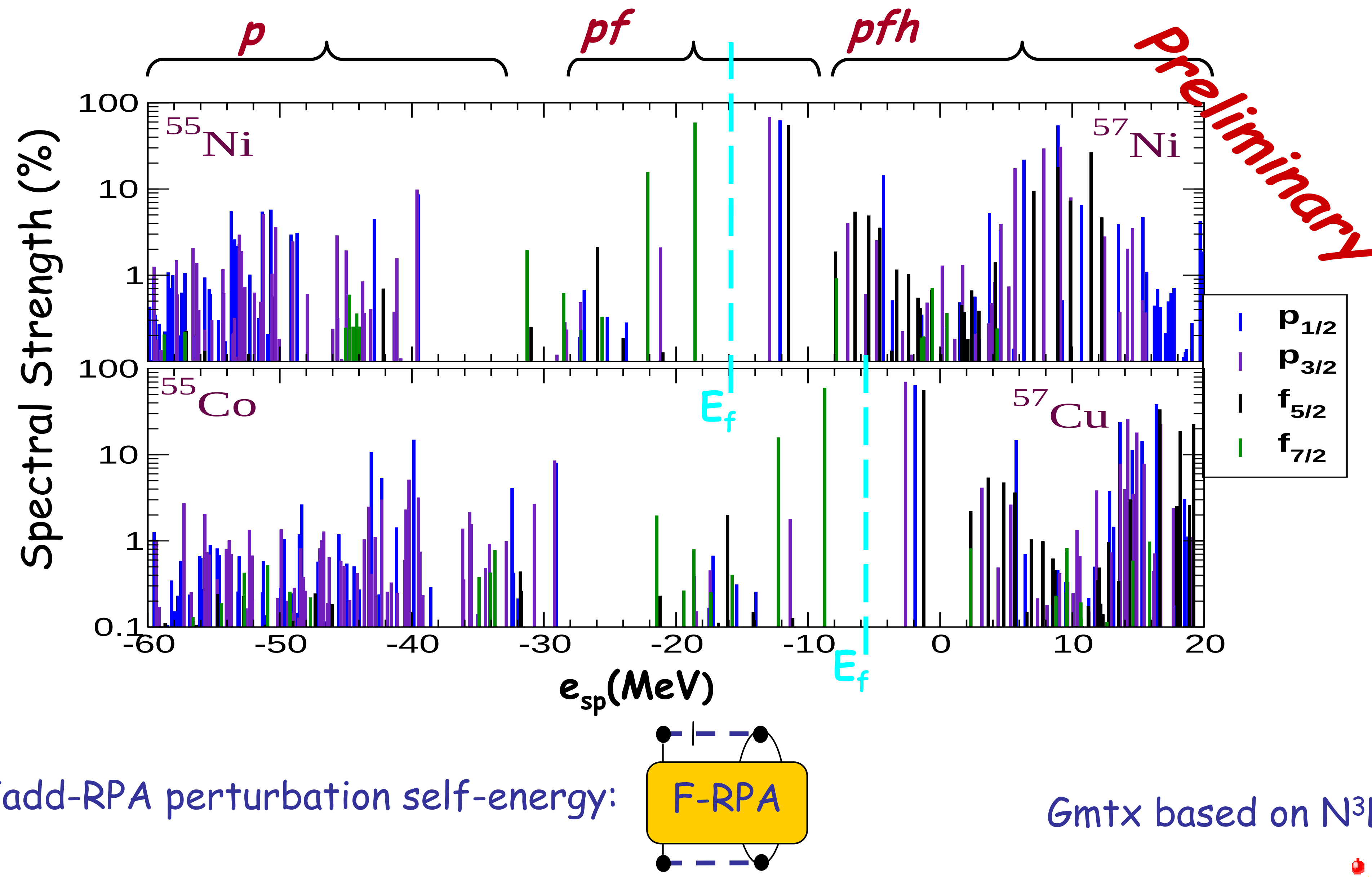
NIKHEF
G. Kramer, Thesis

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

high-energy mixing
☑ short-range correlations

CB, to be published

Example of calculated spectral function around ^{56}Ni



Fadd-RPA perturbation self-energy:

F-RPA

Gmtx based on N³LO

Applications to Electron Systems

Why RPA?

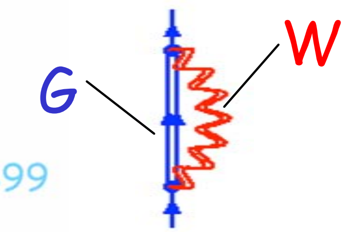
Describing phonons in RPA theory:

- Nuclei → collective modes

- Electron gas → screening of long-range Coulomb, correlation energies

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



- Quasiparticle-DFT (D. van Neck) → needs a consistent description of both small and extended e- systems.

Comparison with coupled-cluster theory

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: $1h$	Ω: $2h$-$1p$	E_0	Scaling[a]
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

Phys. Rev. A76, 052503 (2007).

+ CB and van Neck, work in progress

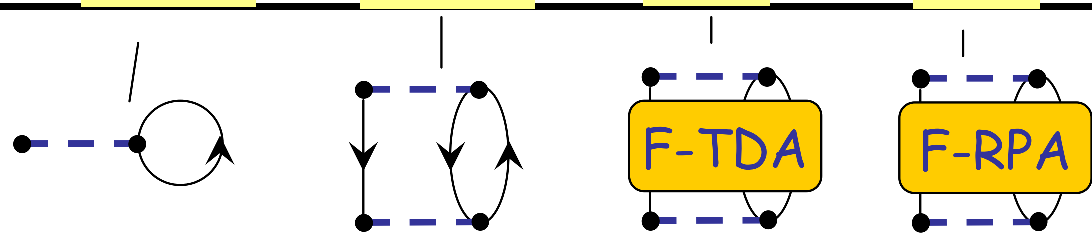
Energies in Hartree /

Relative to the experiment in mH

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

Valence Ionization Energies

	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

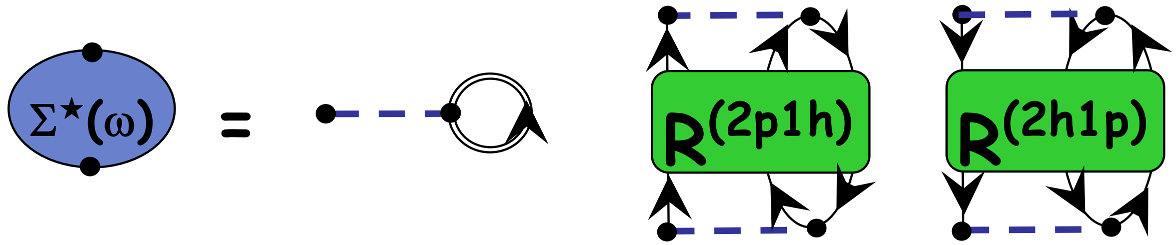


Systematic improvement of ionization energies when including RPA propagators: about 4mH for valence orbits

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

cc-pV(TQ)Z basis, extrapolated

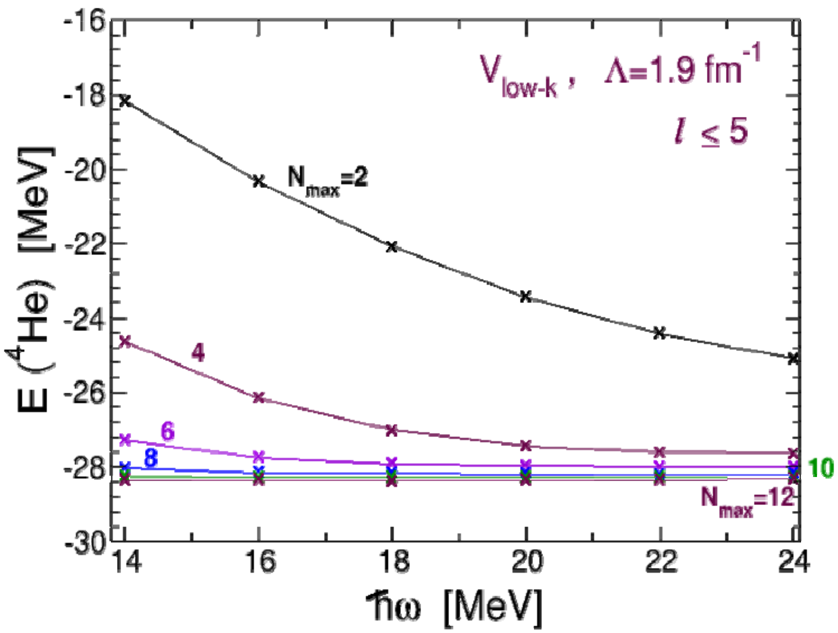
Binding energy – ^{4}He case

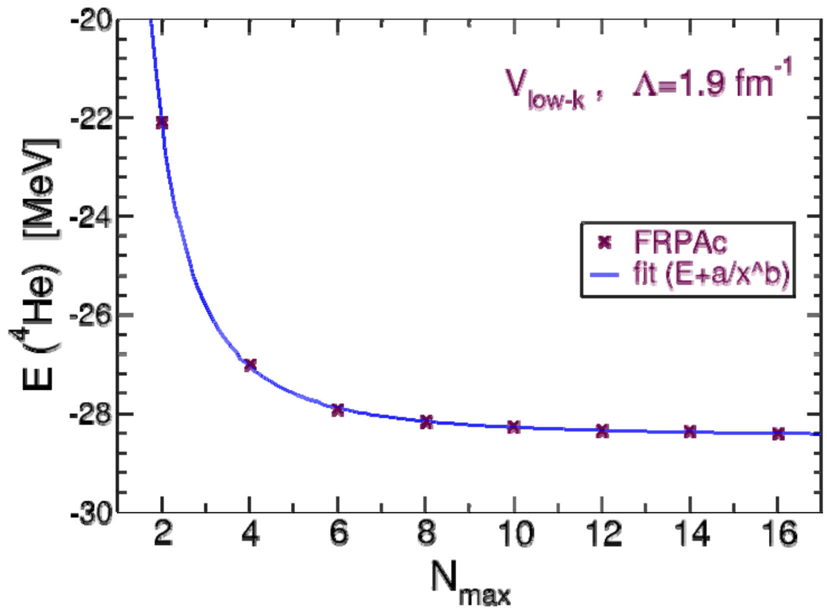


$H_{int} = T + V - T_{int}$

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

binding energy
(Migdal-Galitski-Koltun)





$E_{g.s.}$(GF) = -28.49 MeV ,   ≈700keV from the exact result (-29.19 MeV)

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.

- Spectroscopic factors:
  - large scale microscopic calculations are now possible
  - work to investigate effects of correlations as a function of asymmetry is underway!

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

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

} work in progress…

...THANKS for your attention!