Applications of Green's function theory to medium-mass nuclei

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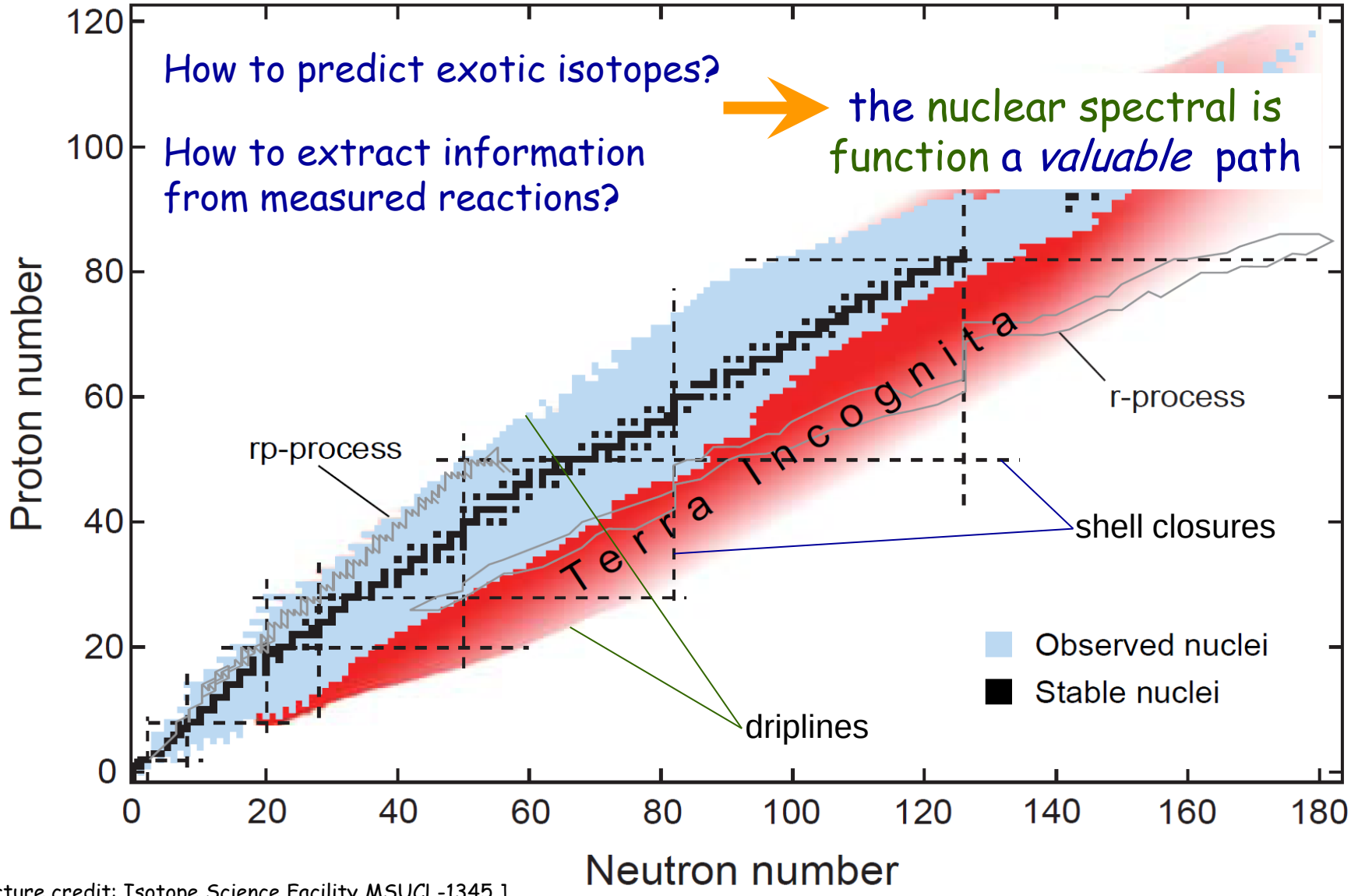
JAPAN-ITALY EFES Workshop, 6-8 September 2010

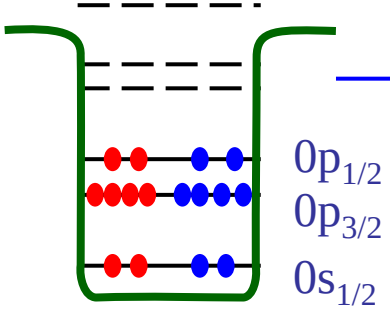
Future Challenges in Nuclear Structure



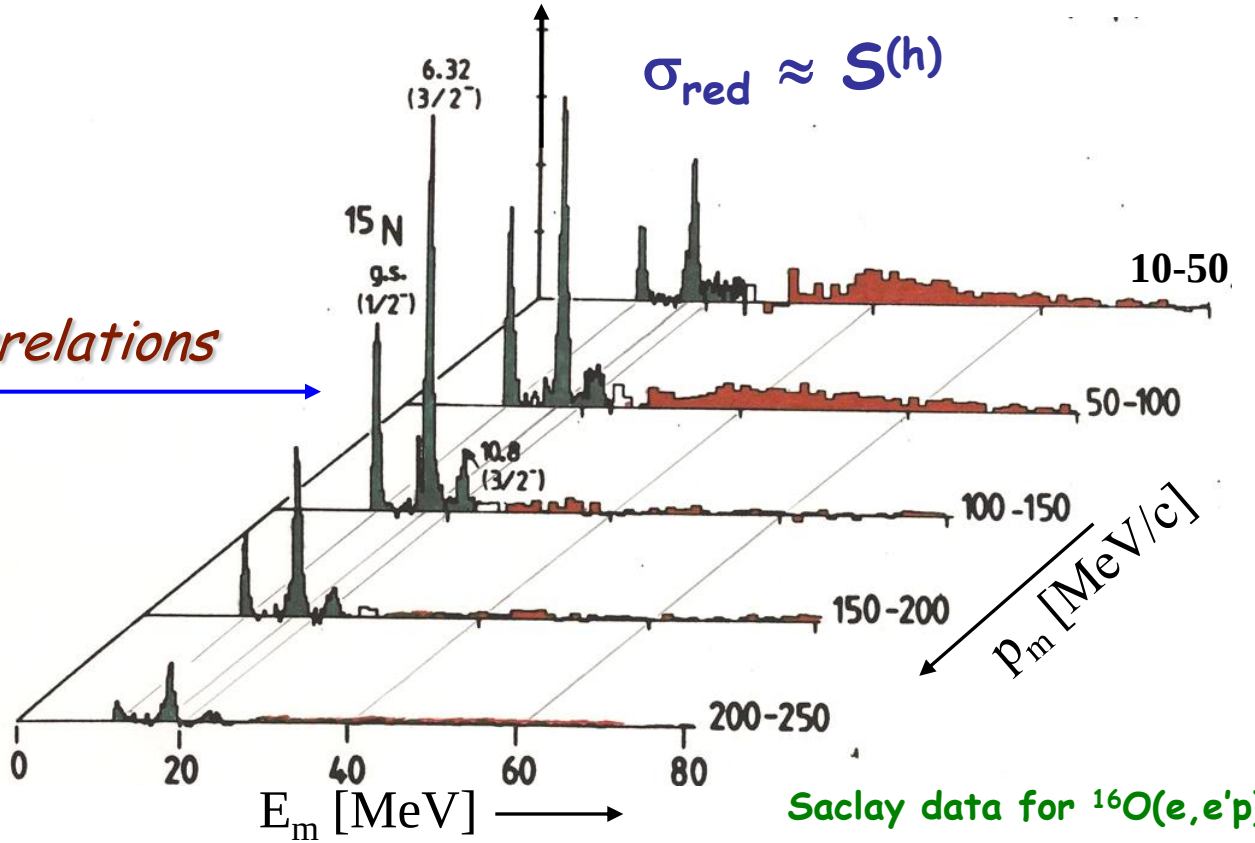
[Picture credit: Isotope Science Facility MSUCL-1345]

One-hole spectral function -- example

independent particle picture



correlations



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

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

→ distribution of momentum ($\mathbf{p_m}$) and energies ($\mathbf{E_m}$)

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??

Theory Features:

- Fully microscopic → "ab-initio" approach
- Linked diags. → *size extensivity*
- hierarchy of equations—can improve systematically
- The computational cost *scales gently* with increasing *A*
- Suitable for parallel computing
- *Self-consistency* :
  - fulfillment of *conservation laws*
  - *"no"* reference state

Links to Physics:

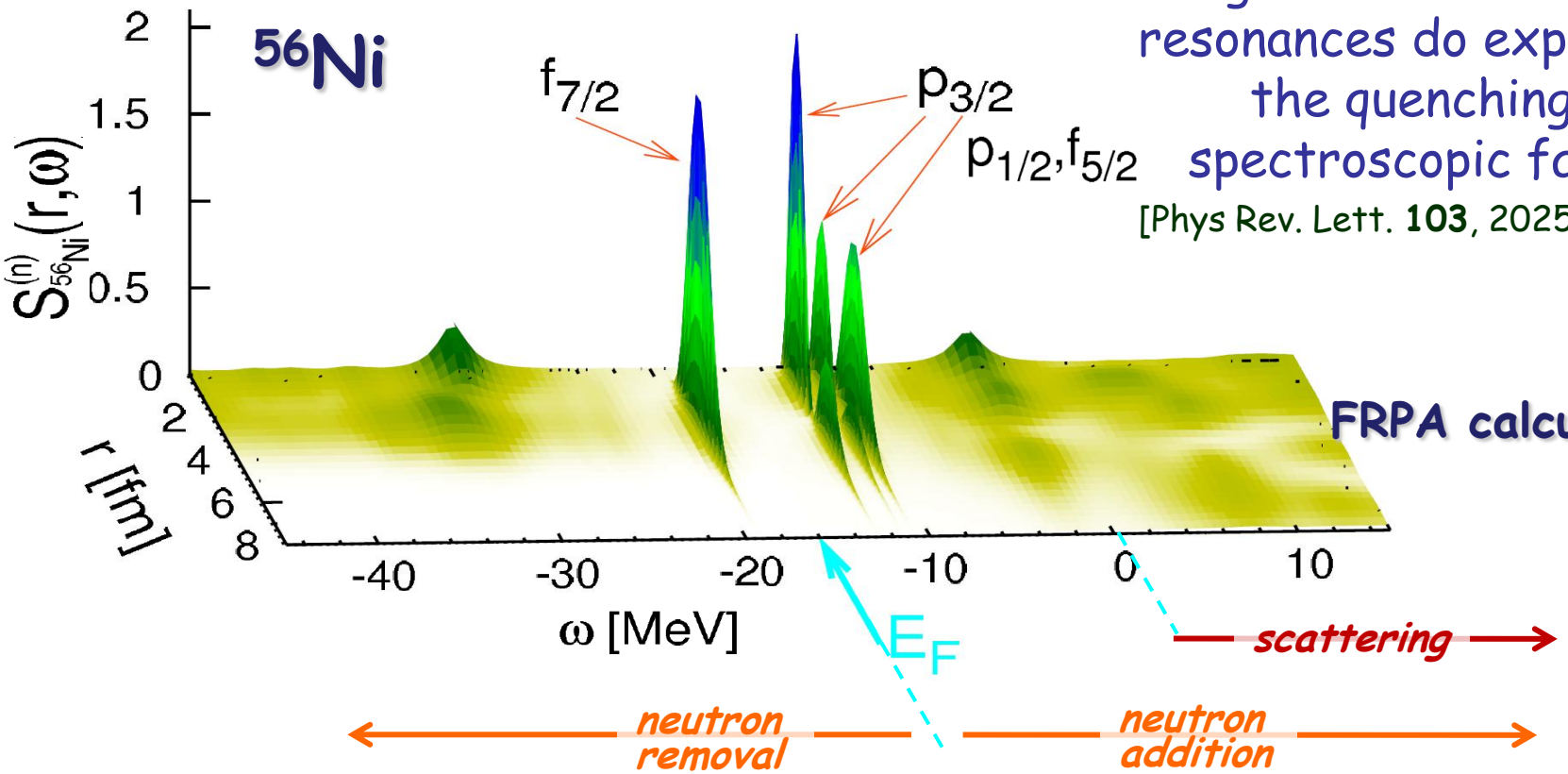
- Closely related to *spectroscopy* ←→ experiments
- "phonons" are the low-energy degrees of freedom←→ *phenomenological apps. possible*
- The self-energy is a nucleon-nucleus *optical potential* (see, e.g. DOM applications)

GFs are the *method of choice* for a *global picture* of nuclear dynamics

…and, yes, of course lots of information requires hard work…

Spectral Function of ^{56}Ni

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



Large bases & coupling to resonances do explain well the quenching of spectroscopic factors

[Phys Rev. Lett. **103**, 202502 (2009)]

FRPA calculations

Faddeev-RPA (FRPA) is a ***many-body*** method:
random phase approx. (RPA) for collective vibrations
Faddeev eqs. for particle-vibration coupling

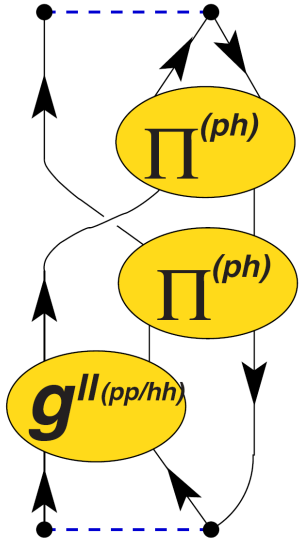
- up to $A \approx 56$ (for now)
- $^{100\text{-}132}$Sn, ^{78}Ni possible (parallelization)

Faddeev-RPA in two words…

Particle vibration coupling is the main cause driving the distribution of particle strength

Finite Systems (& nuclei) are *special*, they require ***all types*** of particle-vibration coupling:

- ✓ pairing effects, two-nucleon transfer
- ✓ collective motion, resonances, Gamow-Teller
- ✓ interference among them

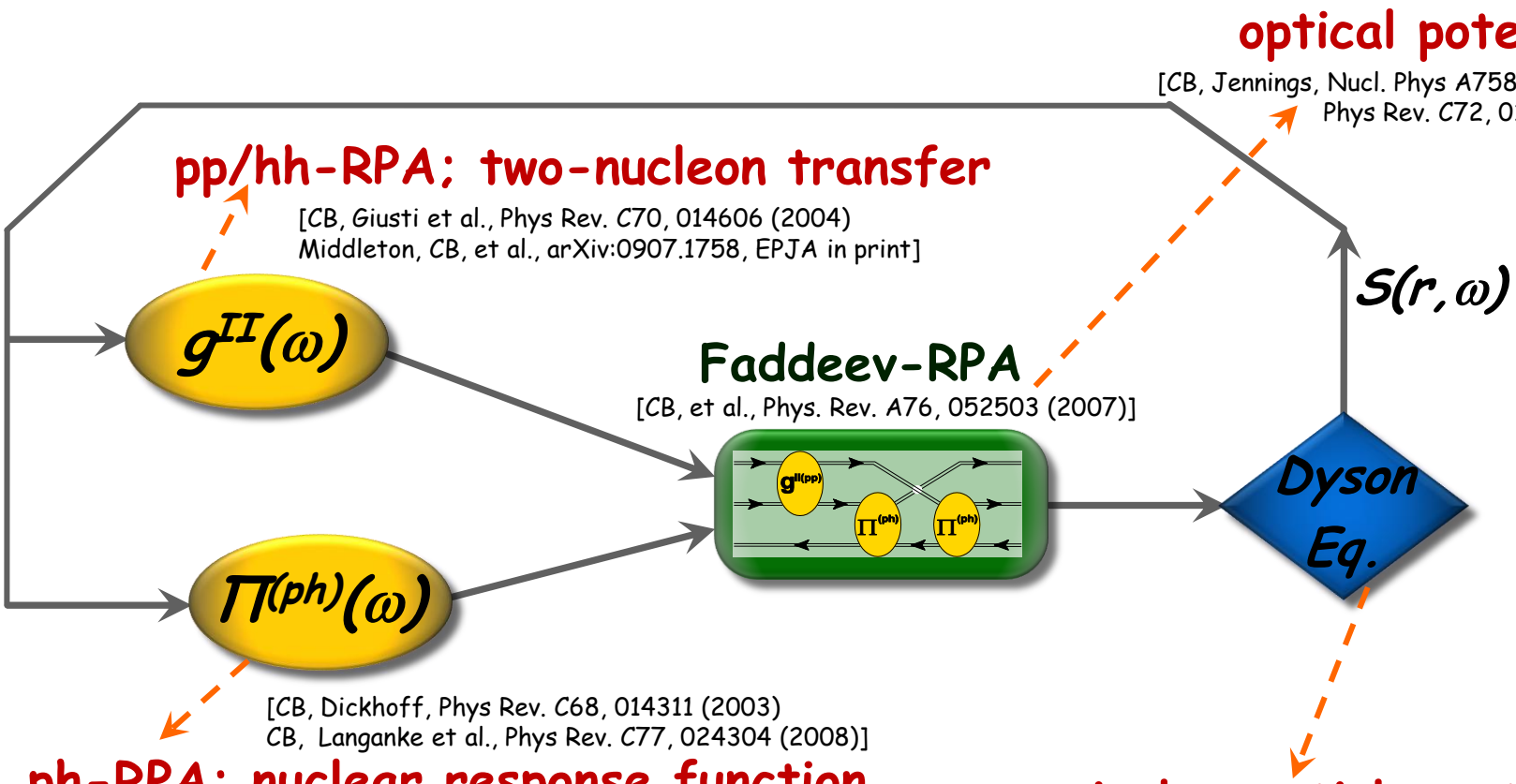


- Use *random phase approximation* (RPA) to get response functions of vibrations ($g^{II}(\omega)$, $\Pi^{(ph)}(\omega)$)
- Use Faddeev's equation to couple them

Faddeev-RPA

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

Self-Consistent Green's Function Approach



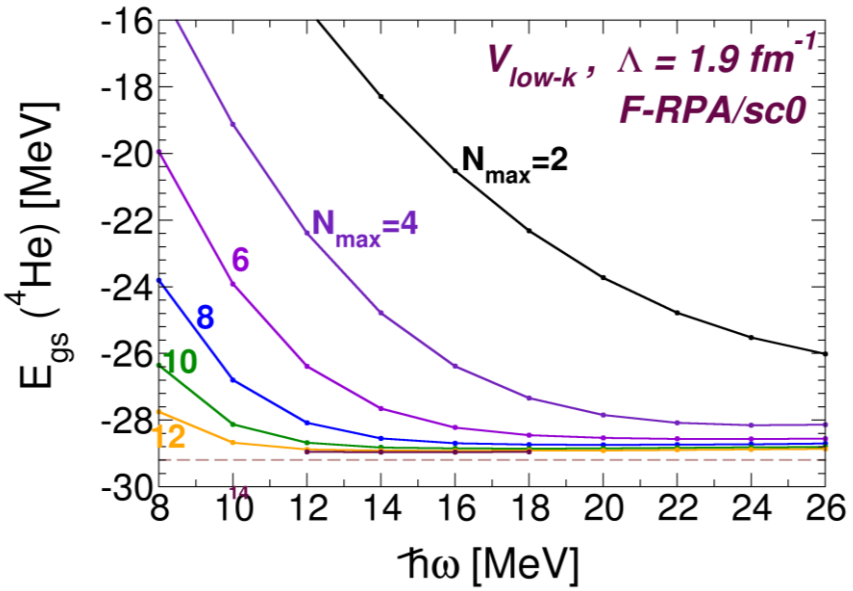
Faddeev-RPA is a ***many-body*** method:

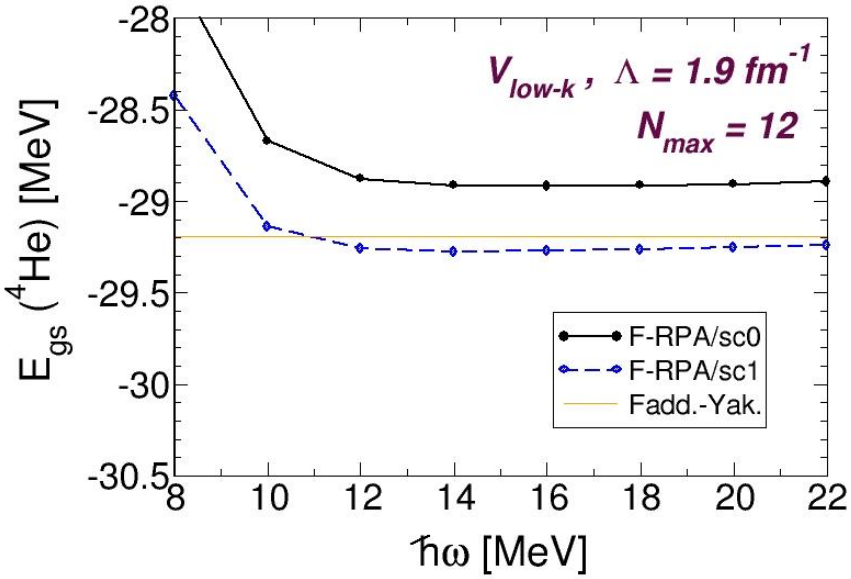
✓random phase approx. (RPA) for collective vibrations

✓Faddeev eqs. for particle-vibration coupling

Binding Energy – ^{4}He Case

[C. B., arXiv:0909.0336; to be submitted]





➔ 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. *C***70**, 061002 (2004)

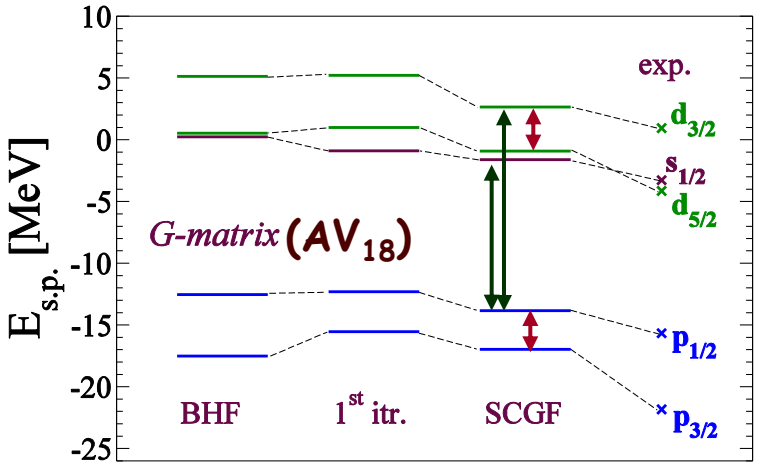
self-consistency in the mean field only

estimates from different approx. to self-consistency -- **preliminary**

Some applications to nuclei…

- quenching of absolute spect. factors (^{56}Ni)
- optical potentials
- two nucleon correlations ^{16}O(e,e'pn)

Single neutron levels around ^{16}O with FRPA



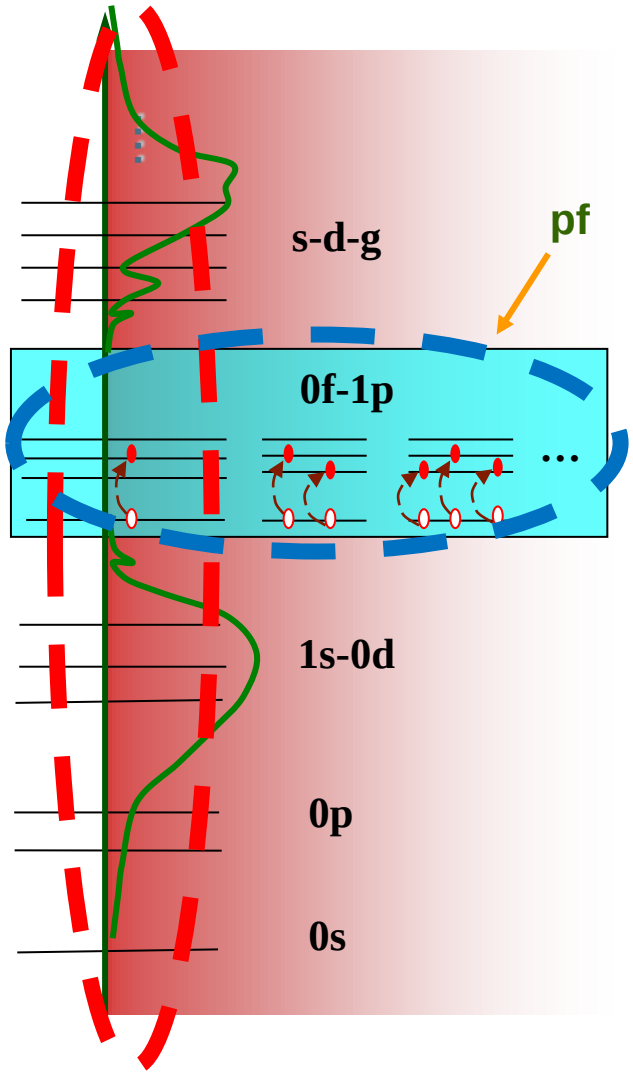
[CB, Phys. Lett. B643, 268 (2006)]

	Theory(MeV)	Exp.[MeV]
spin-orbit:		
$E_{d3/2}$-$E_{d5/2}$	3.5	5.08
$E_{p1/2}$-$E_{p3/2}$	3.1	6.18
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 agrees with ≈3.4MeV from variational Monte Carlo (VMC) [S. Pieper et al. Phys. Rev. Lett. 70 ('93) 2541, using AV_{14}]

Correlations & model space (RPA and SM)



Particle-vibration coupling dominates the quenching of spectroscopic factors

Relative strength among fragments requires shell-model approach

[see, e.g. Utsuno et al., AIP Conf. Proc. 1120, 81 (2009). Tsang et al., Phys. Rev. Lett. 102, 062501 (2009)]

		10 osc. shells			Exp. [30]	$1p0f$ space		
		FRPA (SRC)	full FRPA	FRPA $+\Delta Z_\alpha$		FRPA	SM	ΔZ_α
	^{57}Ni:							
^{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:							
^{55}Ni	$\nu 0f_{7/2}$	0.95	0.72	0.69		0.89	0.86	-0.03
	^{57}Cu:							
^{57}Cu	$\pi 1p_{1/2}$	0.96	0.66	0.62		0.80	0.76	-0.04
	$\pi 0f_{5/2}$	0.96	0.60	0.58		0.80	0.78	-0.02
	$\pi 1p_{3/2}$	0.96	0.67	0.65		0.81	0.79	-0.02
	^{55}Co:							
^{55}Co	$\pi 0f_{7/2}$	0.95	0.73	0.71		0.89	0.87	-0.02

[CB, Phys. Rev. Lett. ***103***, 202502 (2009)]

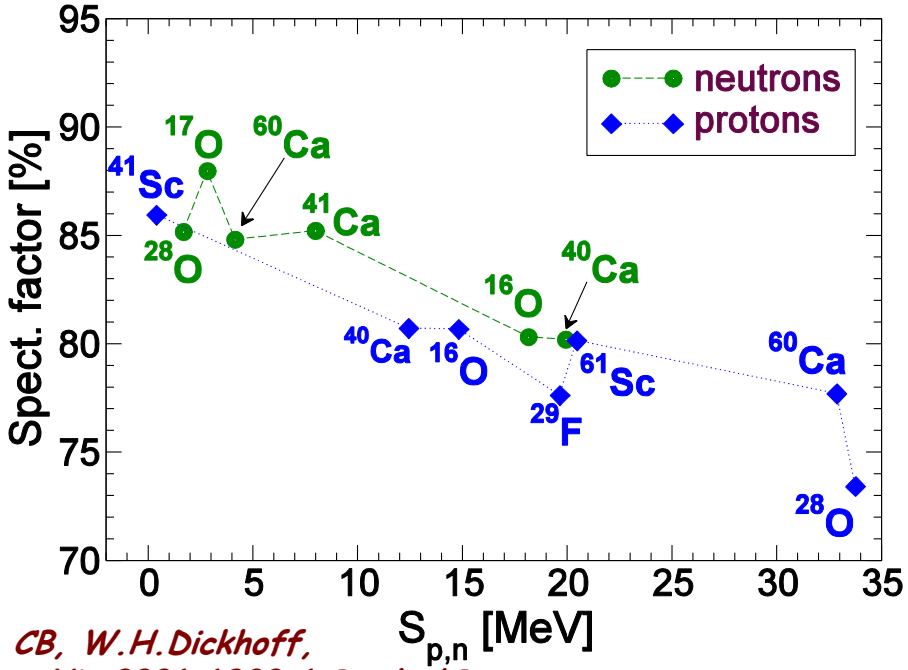
Asymmetry dependence: F-RPA estimate…

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

- in agreement with other calculations
- in disagreement with experimental analysis

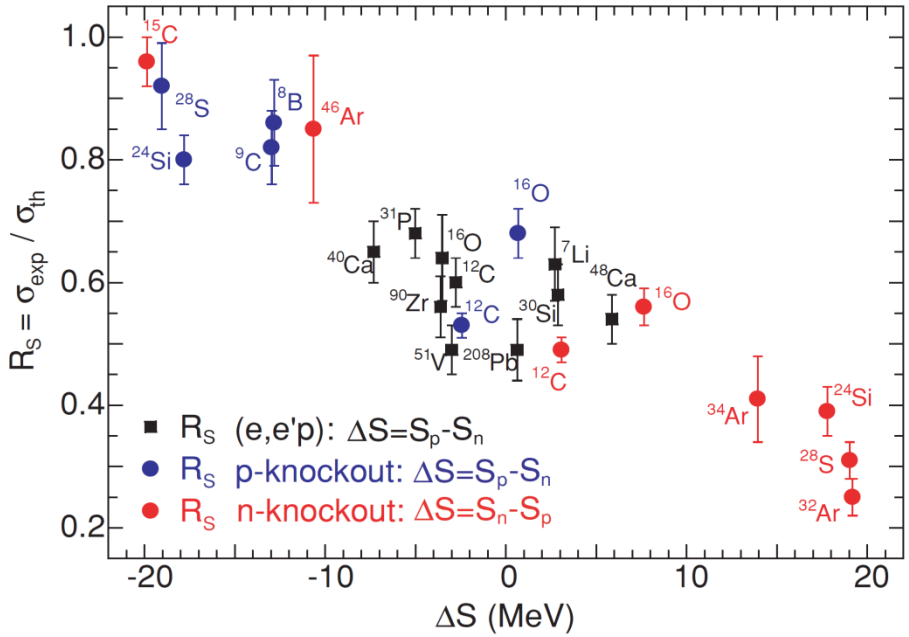
} → *OPEN PUZZLE!!!*

- collective modes may not (yet) be fully realistic… (try Skyrme? phen. corr.?)



CB, W.H.Dickhoff, arXiv:0901.1920v1 [nucl-th]

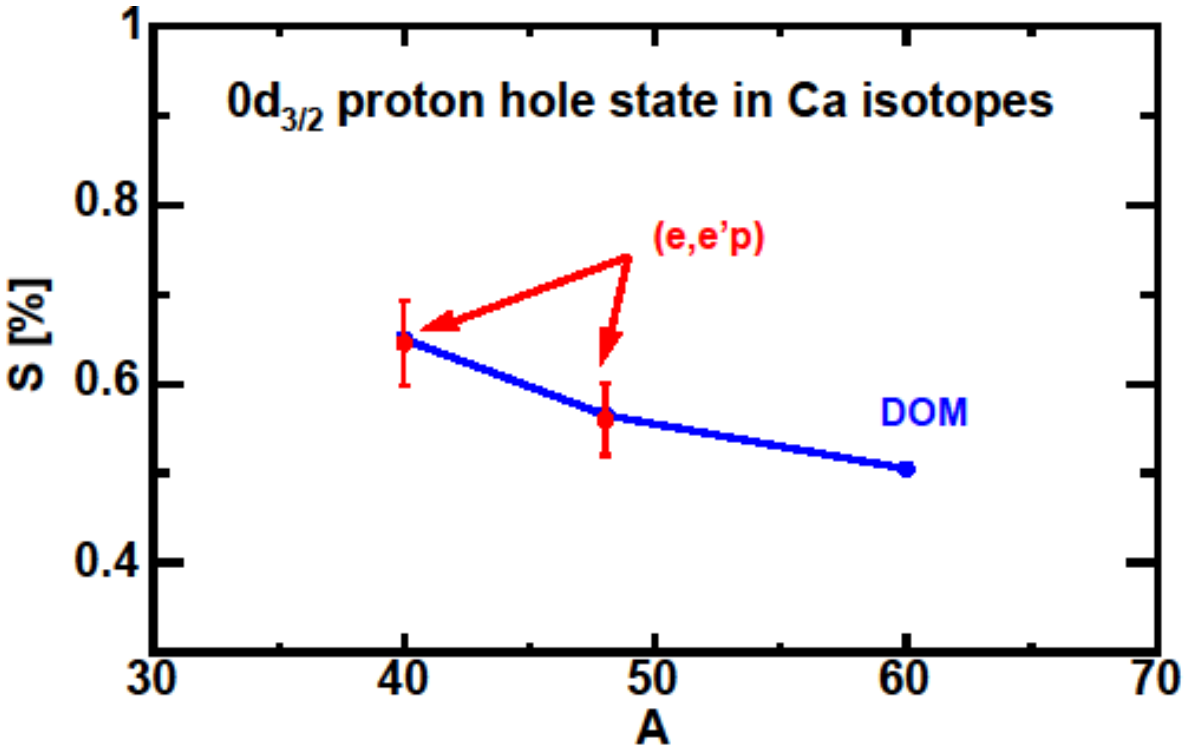
Int. Jour. Mod. Phys. A24, 2060 (2009).



Phys. Rev. C77, 044306 (2008)

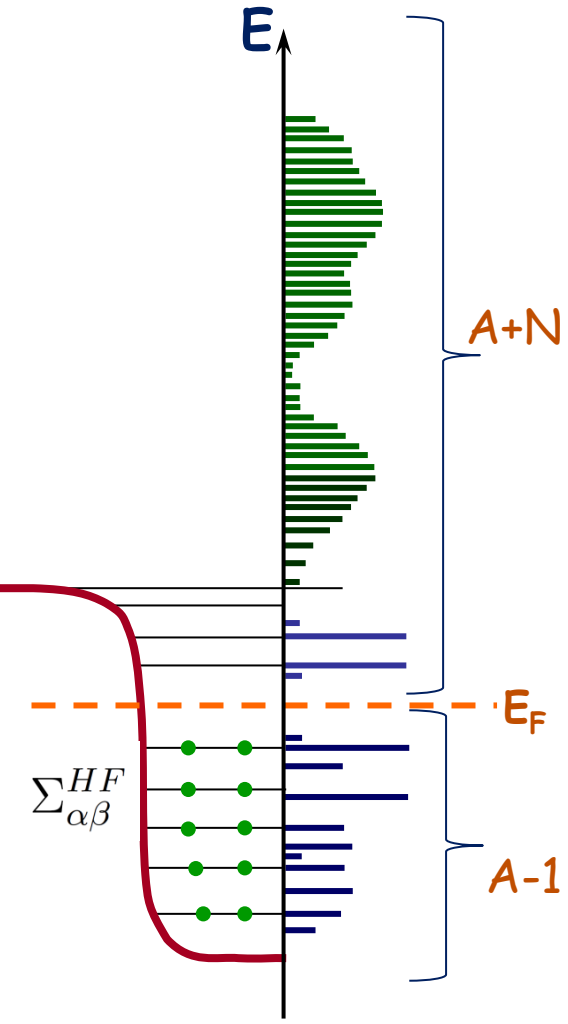
Asymmetry dependence: DOM estimate…

The dispersive opptical model (DOM) also predicts a "weak" asymmetry dependence for spectroscopic factors



[W.H.Dickhoff, communication]

Further away from E_F: elastic scattering…



Nuclear self-energy:

$$\Sigma^{\star}(\mathbf{r},\mathbf{r}';\varepsilon) = \Sigma^{HF}_{\alpha\beta} - \frac{1}{\pi}\int_{\varepsilon_T^{>}}^{\infty} dE' \, \frac{Im\,\Sigma^{\star}(\mathbf{r},\mathbf{r}';E')}{\varepsilon - E' + i\eta} + \frac{1}{\pi}\int_{-\infty}^{\varepsilon_T^{<}} dE' \, \frac{Im\,\Sigma^{\star}(\mathbf{r},\mathbf{r}';E')}{\varepsilon - E' - i\eta}$$

mean-field

correlations beyond mean-field/absorption

- it is *proven* to be a Feshbach's microscopic optical potential
- satisfies the dispersion relation (causality):

DOM in 2 words…

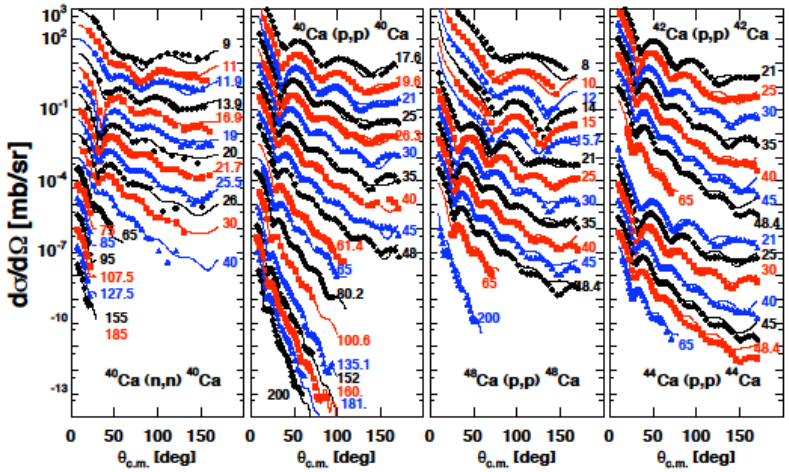
The dispersive optical model (DOM) is a *parameterization of the self-energy* based on theory. In particular it is made to satisfy the dispersion (i.e. parameterize ONLY $\mathcal{V}_{\rm HF}(r,E)$ and $\mathcal{W}(r,E)$) !!

$$\mathcal{U}(r,E) = \mathcal{V}(r,E) + i\mathcal{W}(r,E)$$

$$\mathcal{V}(r,E) = \mathcal{V}_{\rm HF}(r,E) + \Delta\mathcal{V}(r,E)$$

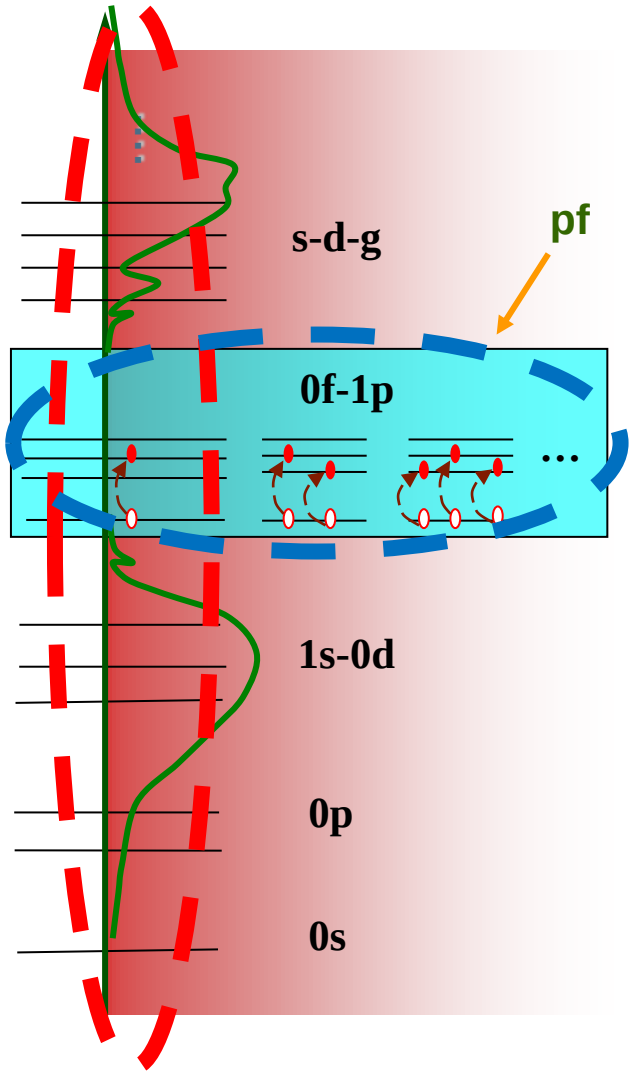
$$\Delta\mathcal{V}(r,E) = \frac{1}{\pi} P \int \mathcal{W}(r,E') \left(\frac{1}{E'-E} - \frac{1}{E'-E_F} \right) dE'$$

Recent developments:
global model around
the ^{A}Ca chain (St.Louis):



•R. J. Charity et al., Phys. Rev. Lett. **97**, 162503 (2006); Phys. Rev. *C* **76**, 044314 (2007)

Correlations in sp energies and strengths



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[CB, Phys. Rev. Lett. ***103***, 202502 (2009)]

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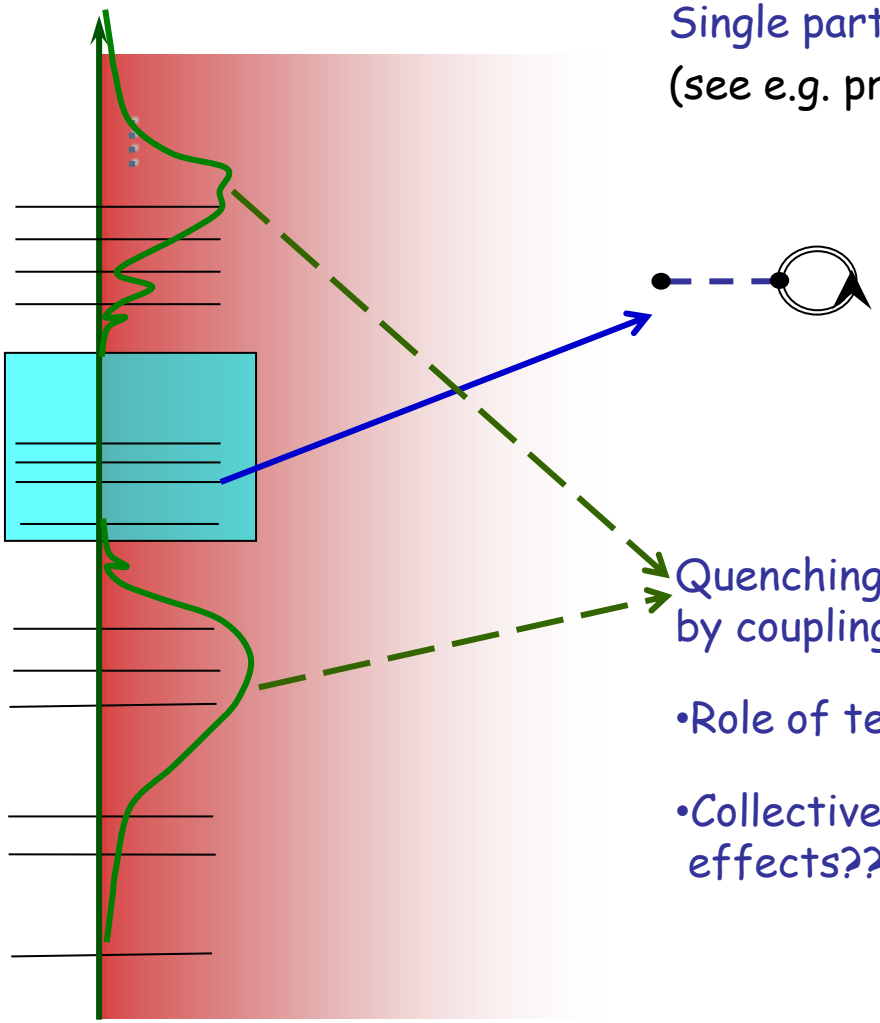
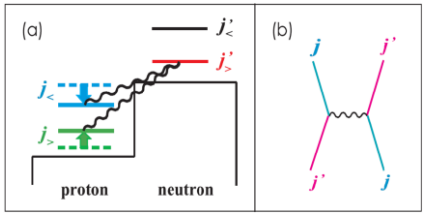
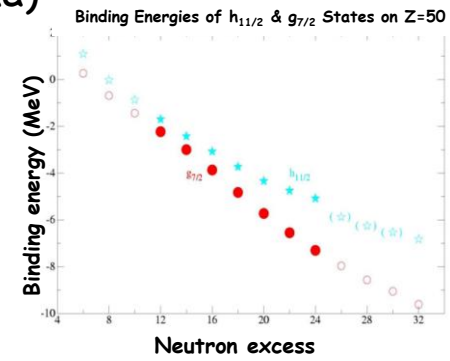


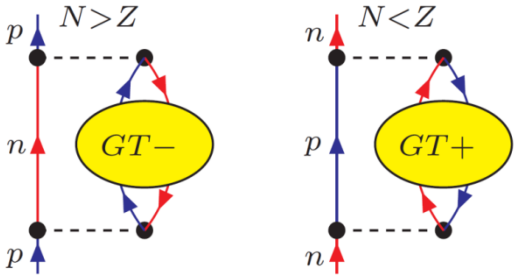
Single particle energies – driven by tensor + 3N force…
(see e.g. previous talk by T. Otsuka)





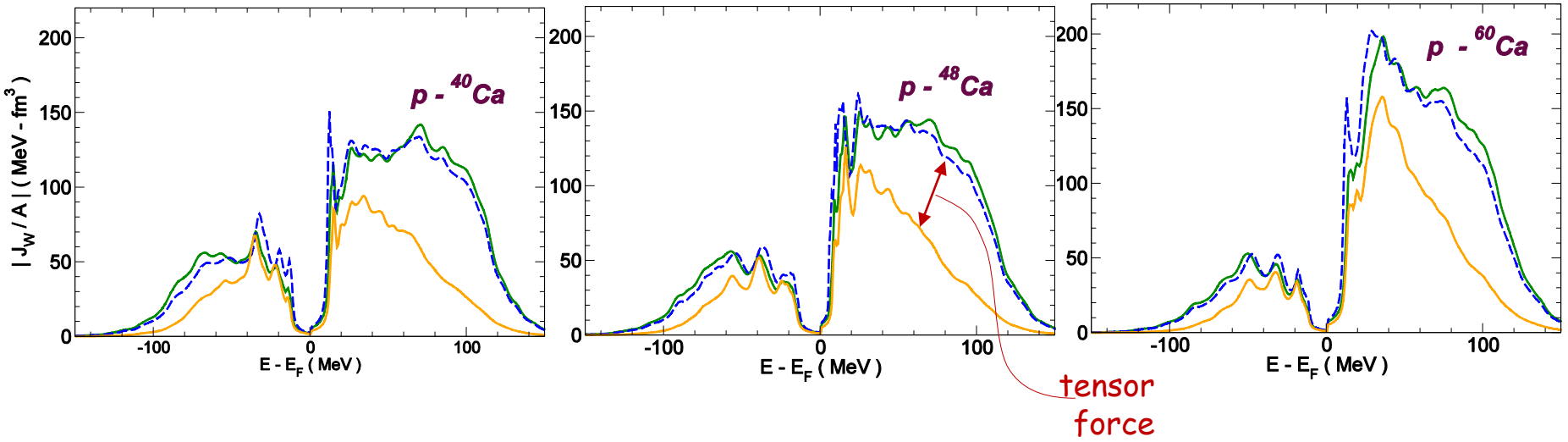
Quenching of spectral strength (spect. factor) – driven by coupling to collective modes…

- Role of tensor force??
- Collective, charge exchange effects???



Microscopic Optical Potential from FRPA

- absorption away from E_F is enhanced by the tensor force
- little effects from charge exchange (e.g. p-^{48}Ca <-> n-^{48}Sc)



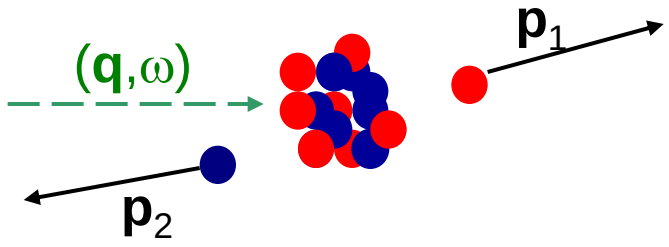
J_W: integral over the imaginary opt. pot (overall absorption)

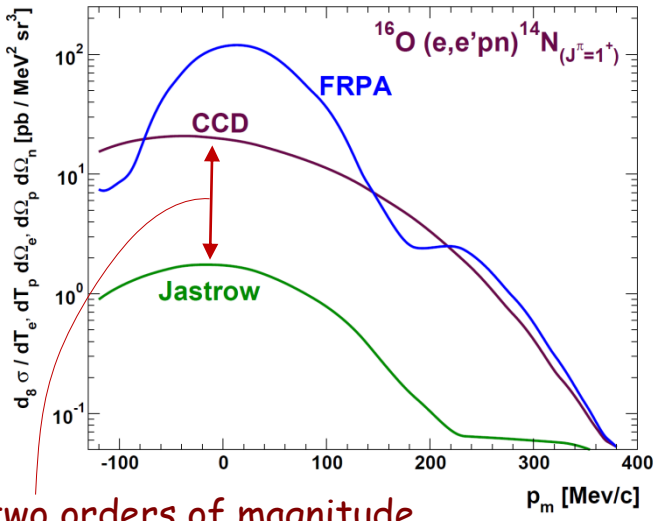
Full FRPA result (w/ av18)
Charge-exchange d.o.f. suppressed
Tensor force suppressed

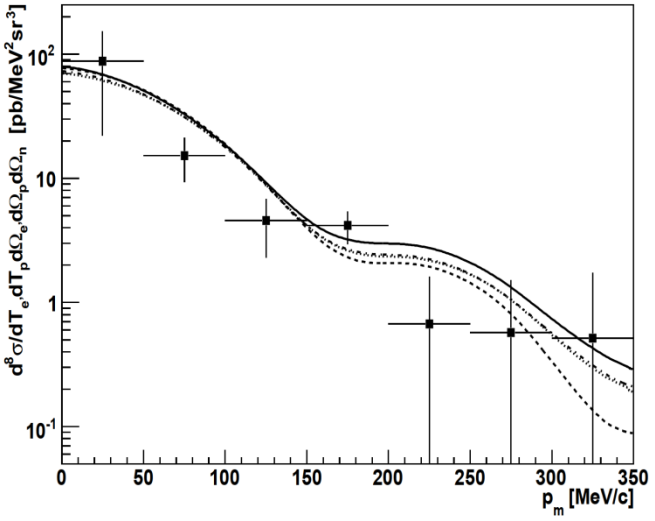
S. Waldecker, CB, W.Dickhoff -- in preparation

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.

arXiv:1004.4568v1 [nucl-th]

C. Giusti et al., Eur. Phys. J. A 33, 29 (2007) [theory]

D. G. Middleton et al., Eur. Phys. J. A 29, 261 (2006); ibid., 43, 137 (2010) [experiment]

Atoms and molecules…

- Ne as a test case
- Performance of FRPA for atoms and molecules

Spectral strength of Neon

Example of sole "ladder" or "ring" and full mixing

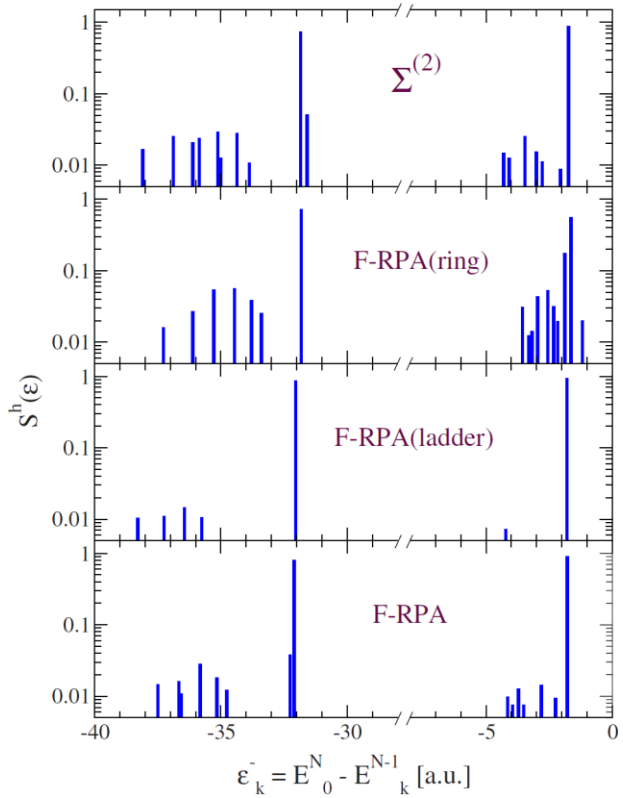


FIG. 4. (Color online) Spectral function for the s states in Ne obtained with various self-energy approximations. From the top down: the second-order ($\Sigma^{(2)}$), the FRPA (ring), the FRPA (ladder), and the full FRPA self-energies. The strength is given relative to the Hartree-Fock occupation of each shell. Only fragments with strength larger than $Z>0.005$ are shown.

Atom of Ne
(10 electrons problem)

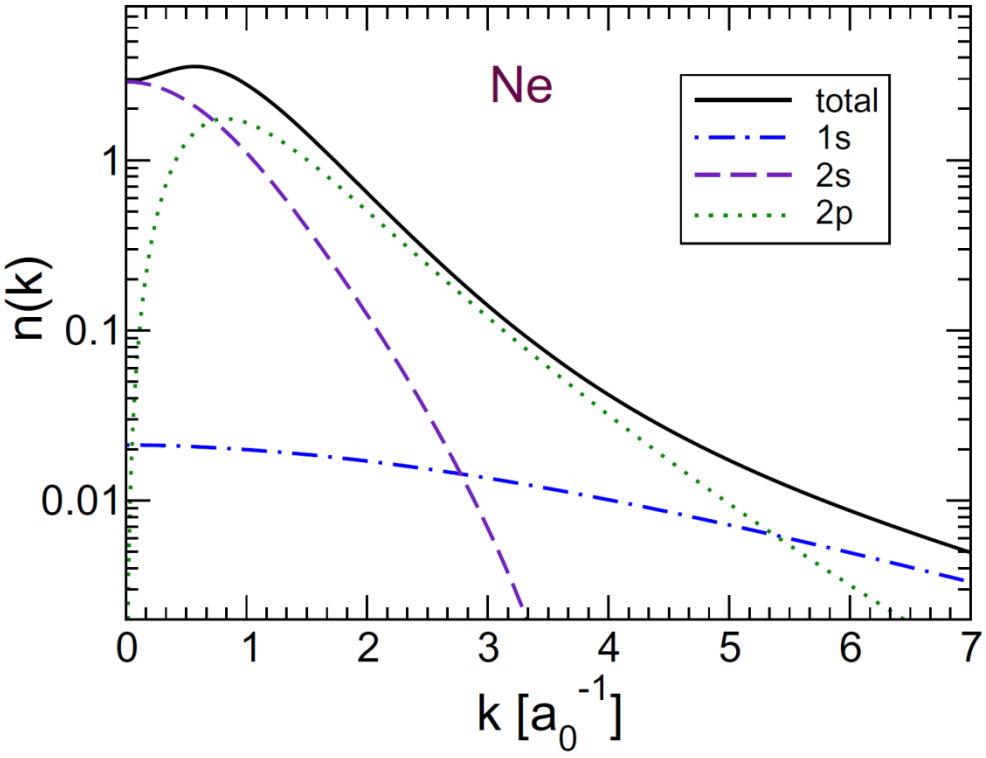
TABLE IV. Energy (in a.u.) and strength (numbers in parentheses) of the main fragments in the spectral function of neon, generated by different self-energies. Results for the HF+continuum basis. Consecutive rows refer to (1) HF; (2) second-order self-energy; (3) G_0W_0 results from Ref. [14]; (4) FRPA self-energy with only *ph* rings retained; (5) FRPA self-energy with only *pp-hh* ladders retained; (6) complete FRPA self-energy. In all FRPA results the self-energy was corrected at third order through Eq. (8). The static self-energy was pure HF (no partial self-consistency). The experimental values are taken from Refs. [32,33].

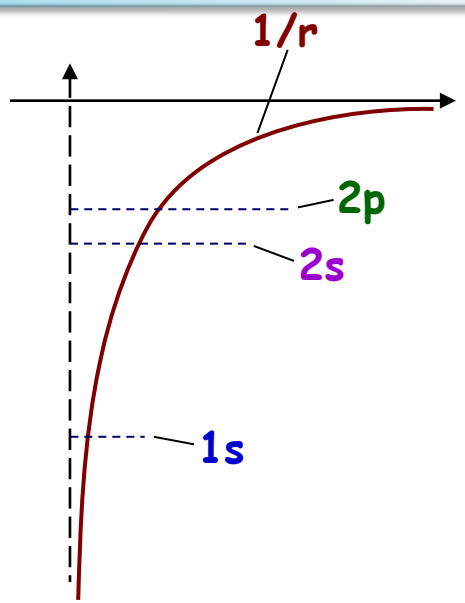
	1*s*	2*s*	2*p*
HF	−32.77 (1.00)	−1.931 (1.00)	−0.850 (1.00)
$\Sigma^{(2)}$	−31.84 (0.74)	−1.736 (0.88)	−0.747 (0.91)
G_0W_0	−31.14 (0.85)	−1.774 (0.91)	−0.801 (0.94)
FRPA (ring)	−31.82 (0.73)	−1.636 (0.56)	−0.730 (0.80)
FRPA (ladder)	−32.04 (0.87)	−1.802 (0.95)	−0.781 (0.96)
FRPA	−32.10 (0.81)	−1.792 (0.91)	−0.799 (0.94)
Expt.	−31.70	−1.782 (0.85)	−0.793 (0.92)

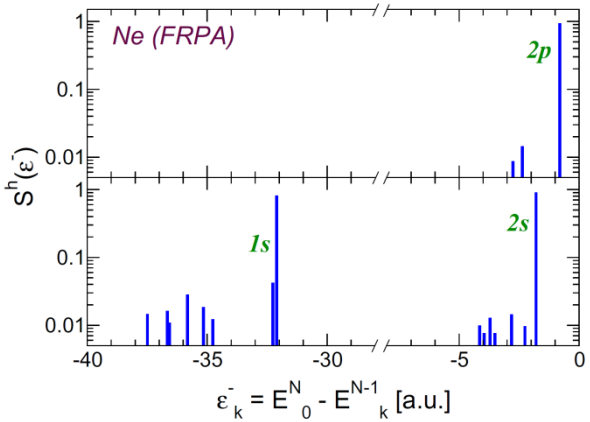
Phys. Rev. A76, 052503 (2007)

Spectral strength of Neon

Momentum distribution:







[CB, Van Neck, AIP Conf.Proc.1120, 104 ('09)]

FIGURE 2. Hole spectral function (right) and momentum distribution (left) of the Ne atom. The dotted, dashed and dot-dashed lines are the contributions coming from the main $2p$, $2s$ and $1s$ quasihole peaks seen on the right side.

Accuracy of FRPA for atoms

Binding energy

	Hartree-Fock	FTDAc	FRPAc	CCSD	Experiment
He	-2.8617 (+42.0)	-2.9028 (+0.9)	-2.9029 (+0.8)	-2.9039 (-0.2)	-2.9037
Be^{2+}	-13.6117 (+43.9)	-13.6559 (-0.3)	-13.6559 (-0.3)	-13.6561 (-0.5)	-13.6556
Be	-14.5731 (+94.3)	-14.6438 (+23.6)	-14.6436 (+23.8)	-14.6522 (+15.2)	-14.6674
Ne	-128.5505 (+387.8)	-128.9343 (+4.0)	-128.9381 (+0.2)	-128.9353 (+3.0)	-128.9383
Mg^{2+}	-198.83 7 (+444)	-199.226 (-5)	-199.228 (-7)	-199.225 (-4)	-199.221
Mg	-199.616 (+438)	-200.048 (+6)	-200.052 (+2)	-200.050 (+4)	-200.054
Ar	-526.820 (+724)	-527.543 (+1)	-527.548 (-4)	-527.536 (+8)	-527.544
σ_{rms} [mH]	392	9.5 (3.6)	9.5 (3.4)	6.9 (4.2)	

[CB, Van Neck, Degroote, arXiv.1004.yyyy; J. Phys. Chem. Submitted]

Accuracy of FRPA for atoms

Binding energy

		Hartree-Fock	(2^{nd} order)c	FTDAc/ ADC(3)c	FRPAc	Experiment [51, 52]
He:	1s	0.918 (+14)	0.9012 (-2.5)	0.9025 (-1.2)	0.9008 (-2.9)	0.9037
Be^{2+}:	1s	5.6672 (+116)	5.6542 (-1.4)	5.6554 (-0.2)	5.6551 (-0.5)	5.6556
Be:	2s	0.3093 (-34)	0.3187 (-23.9)	0.3237 (-18.9)	0.3224 (-20.2)	0.3426
	1s	4.733 (+200)	4.5892 (+56)	4.5439 (+11)	4.5405 (+8)	4.533
Ne:	2p	0.852 (+57)	0.752 (-41)	0.8101 (+17)	0.8037 (+11)	0.793
	1s	1.931 (+149)	1.750 (-39)	1.8057 (+24)	1.7967 (+15)	1.782
Mg^{2+}:	2p	3.0068 (+56.9)	2.9217 (-28.2)	2.9572 (+7.3)	2.9537 (+3.8)	2.9499
	1s	4.4827	4.3283	4.3632	4.3589	
Mg:	3s	0.253 (-28)	0.267 (-14)	0.272 (-9)	0.280 (-1)	0.281
	2p	2.282 (+162)	2.117 (-3)	2.141 (+21)	2.137 (+17)	2.12
Ar:	3p	0.591 (+12)	0.563 (-16)	0.581 (+2)	0.579 (≈0)	0.579
	3s	1.277 (+202)	1.111 (+36)	1.087 (+12)	1.065 (-10)	1.075
	3s		1.840	1.578	1.544	
σ_{rms} [mH]		81.4	29.3	13.7	10.6	

TABLE IV: Ionization energies obtained with Hartree-Fock, second-order perturbation theory for the self-energy, FTDAc and with the full Faddeev-RPAc (in Hartrees). All results are extrapolated from the cc-p(c)vQz and cc-p(c)v5z basis sets (see Table III). The deviations from the experiment (indicated in parentheses) and the *rms* errors are given in mHartrees. The experimental energies are from Ref. [51, 52].

[CB, Van Neck, Degroote, arXiv.1004.yyyy; J. Phys. Chem. Submitted]

Accuracy of FRPA for atoms

Diatomic molecules

		FTDAc	FRPAc	CCSD(T)	Expt.
N_2					
	E_0	−109.258	−109.272	−109.276	-
	r_0	1.104	1.106	1.119	1.098
	I	0.565	0.544	0.602[a]	0.573
BF					
	E_0	−124.365	−124.368	−124.380	-
	r_0	1.284	1.285	1.295	1.267
	I	0.395	0.402	0.406	-
CO					
	E_0	−113.037	−113.048	−113.055	-
	r_0	1.130	1.123	1.145	1.128
	I	0.503	0.494	0.550[a]	0.515

[a] Only up to CCD

[Degroote, Van Neck, CB, to be submitted]

Future Directions

- Nuclear structure studies:

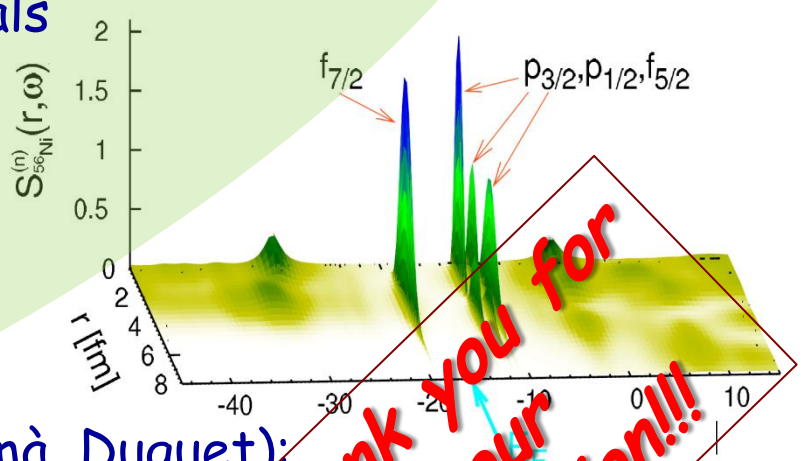
  Calculations of main chains (O, Ca, Ni…) to address:

  - quenching of spectroscopic factors vs. N/Z
  - origin shell closures and driplines location
  - SHELL MODEL's basis states, interactions and charges
  - properties of global optical potentials

- *"Ab-initio"* & tech. advances:
  - parallelization (→ ^{100}Sn, ^{78}Ni)
  - inclusion of 3NF
  - extension to Gorkov-formalism (Somà, Duguet):

    → open-shell nuclei

    → structure of next generation EDF



Thank you for your attention!!!