"Advances in Many-Body Theory: From Nuclei to Molecules"

@INT,2-5 April 2013

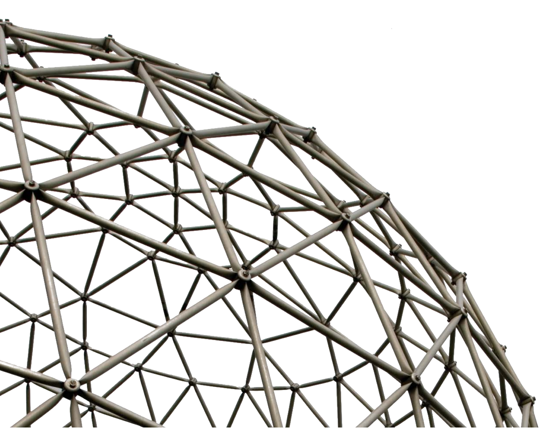
Three-Body Forces in Green's Function Theory and First Application to Isotopic Chains

Andrea Cipollone

&

Carlo Barbieri

Collaborator: Petr Navrátil



Title: **"Green Function"**
Artist: Dr. **Regina Valluzzi**
Exibition: **Mathematical Art Galleries**

Outline

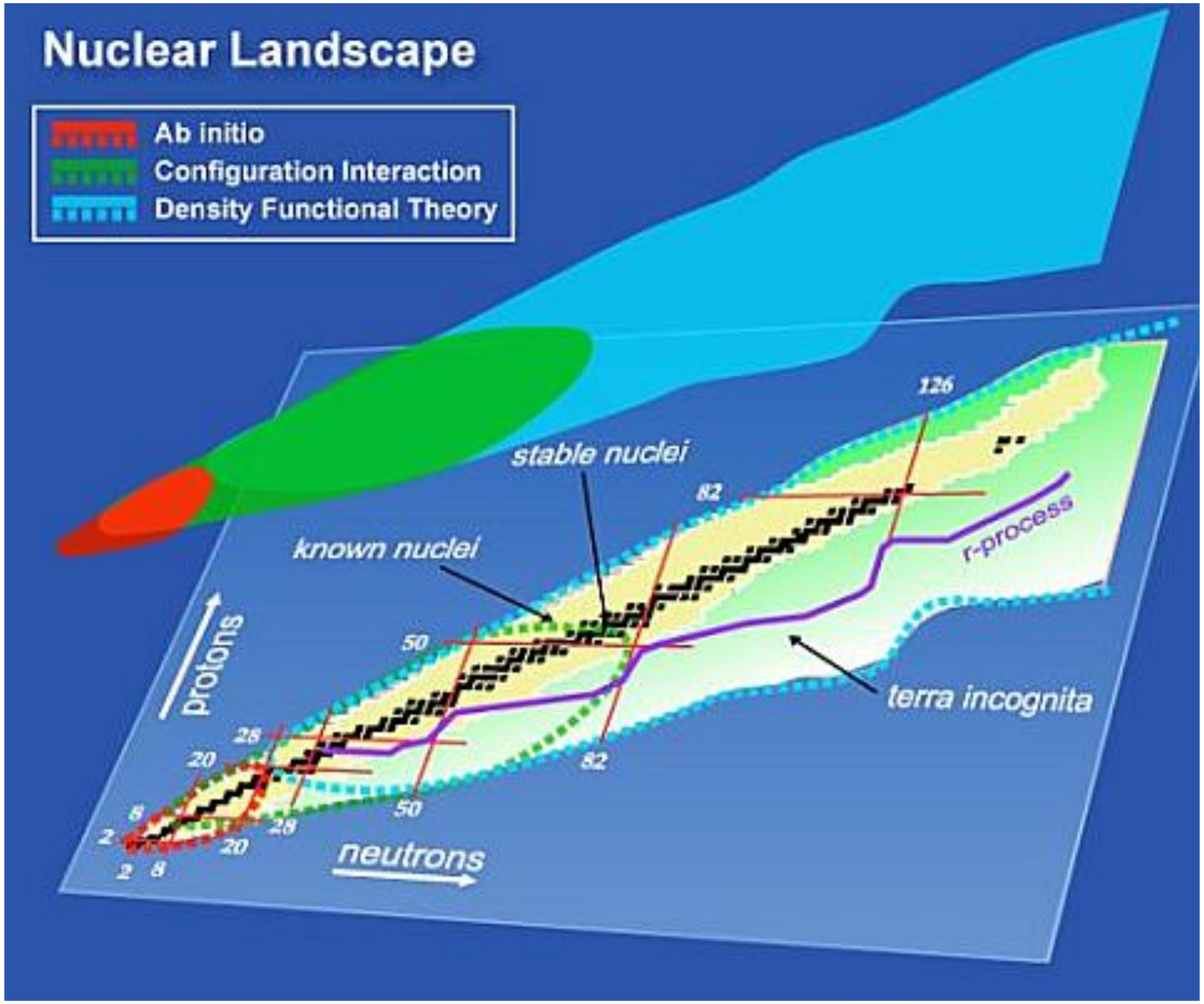
- Introduction :
  - physical content in a GF
  - Why we need 3NF?
- Green's Function formalism with 3NF
  - Approximation for Self-Energy (Optical potential)
  - Extended Koltun Sum-Rule
  - What is next??
- Results
  - Driplines in O, F, N
  - "Ionization energies and affinities"

Green's Function in the nuclear chart

Open Issues

- Need a good nuclear hamiltonian
- Structure calculations are limited to ~~closed-shell nuclei~~ or $(A \pm 1, 2)$

  $\longrightarrow$ Vittorio's talk
- Ab-initio link between structure and reactions



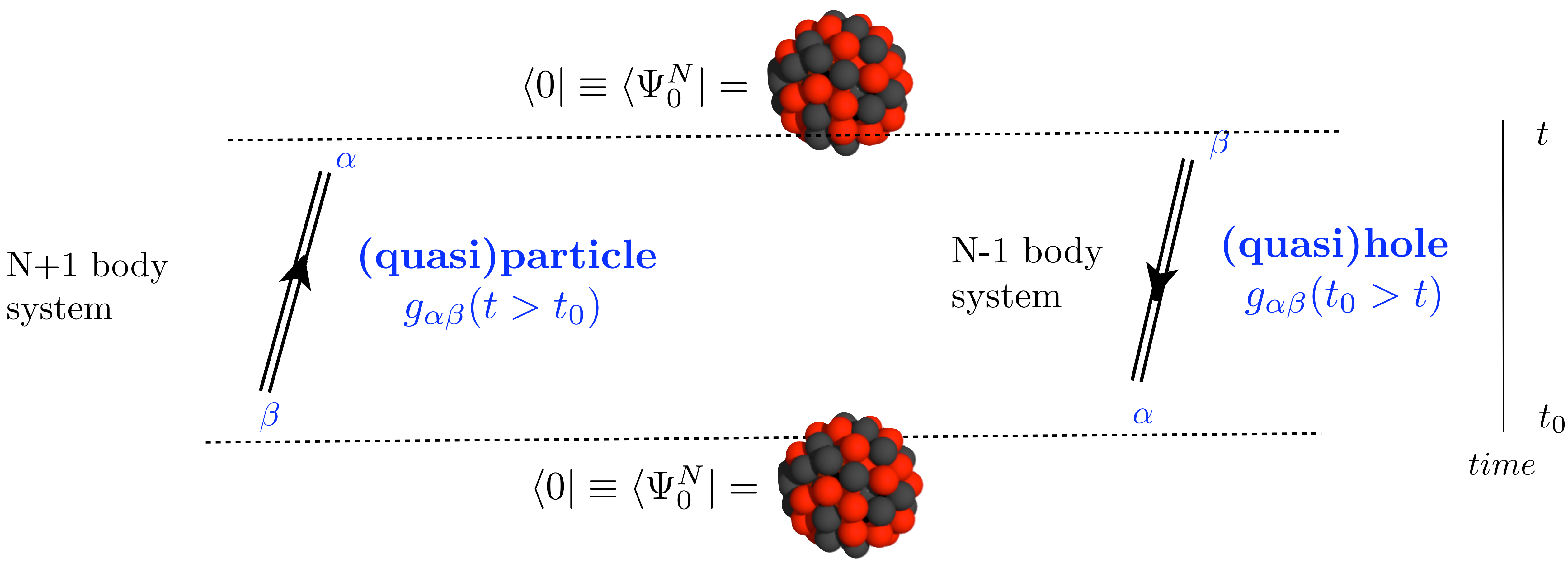
Introduction

- One-body system: excitation from "*vacuum*" $|0\rangle$

G.F.

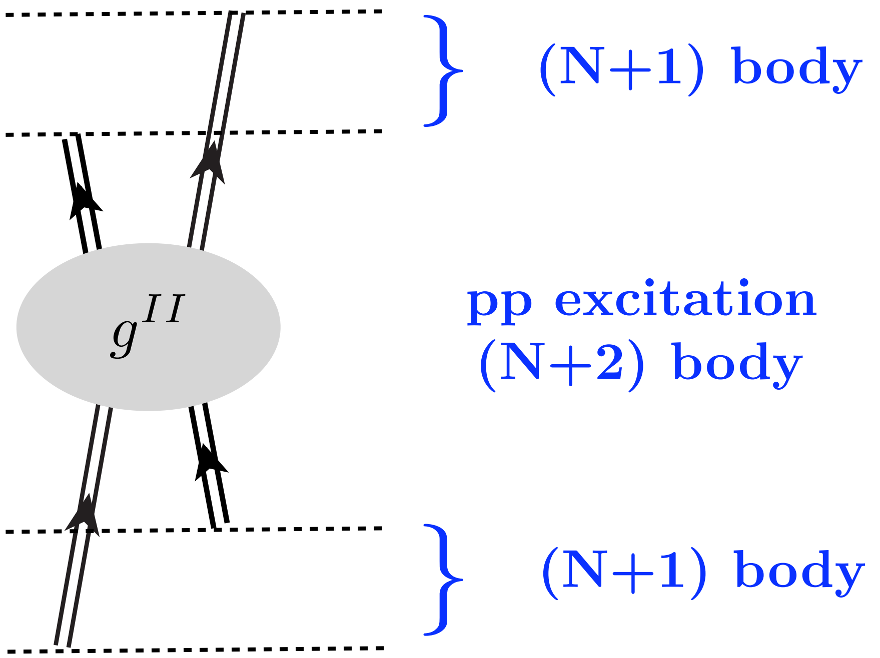
$$\psi(\mathbf{r},t)=\langle\mathbf{r}|\alpha,t_0,t\rangle = \langle\mathbf{r}|e^{-\frac{i}{\hbar}H(t-t_0)}|\alpha,t_0,t\rangle = \int dr' \, \langle 0|a_{\mathbf{r}}e^{-\frac{i}{\hbar}H(t-t_0)}a^\dagger_{\mathbf{r}'}|0\rangle \, \langle\mathbf{r}'|\alpha,t_0,t\rangle$$

- M-B system: propagation through an *interacting* $|0\rangle$

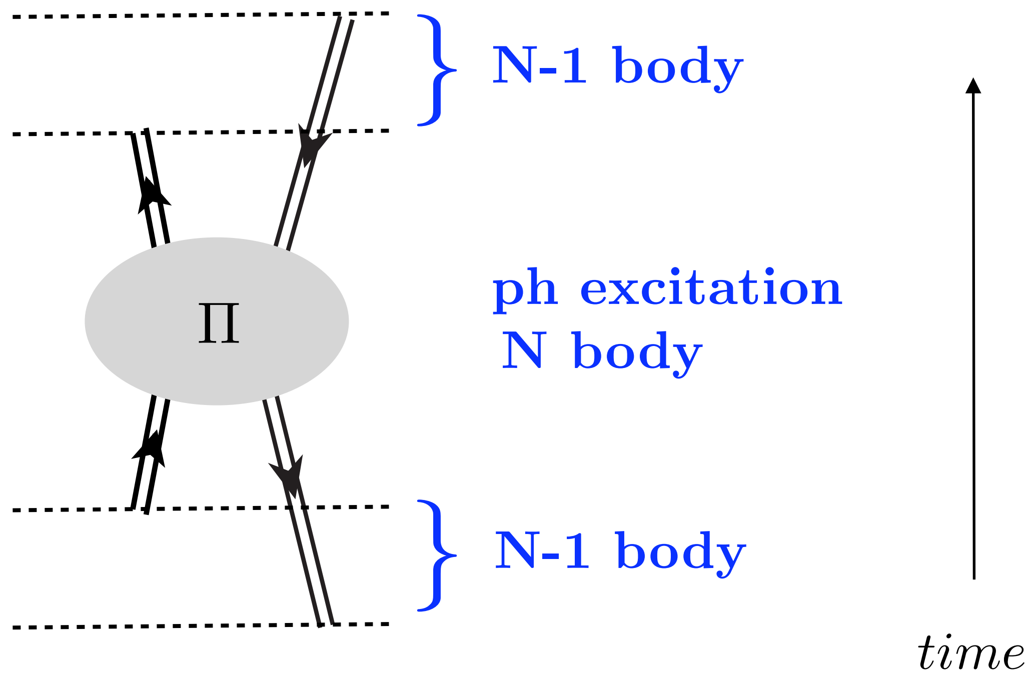


Introduction

- Two-body green functions



pair correlations,
access to N+2 system

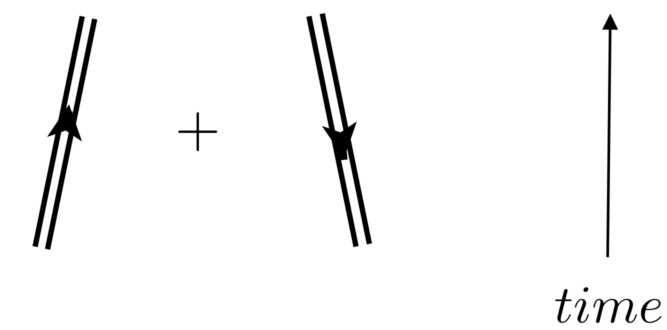


collective modes,
phonons,
ecc.

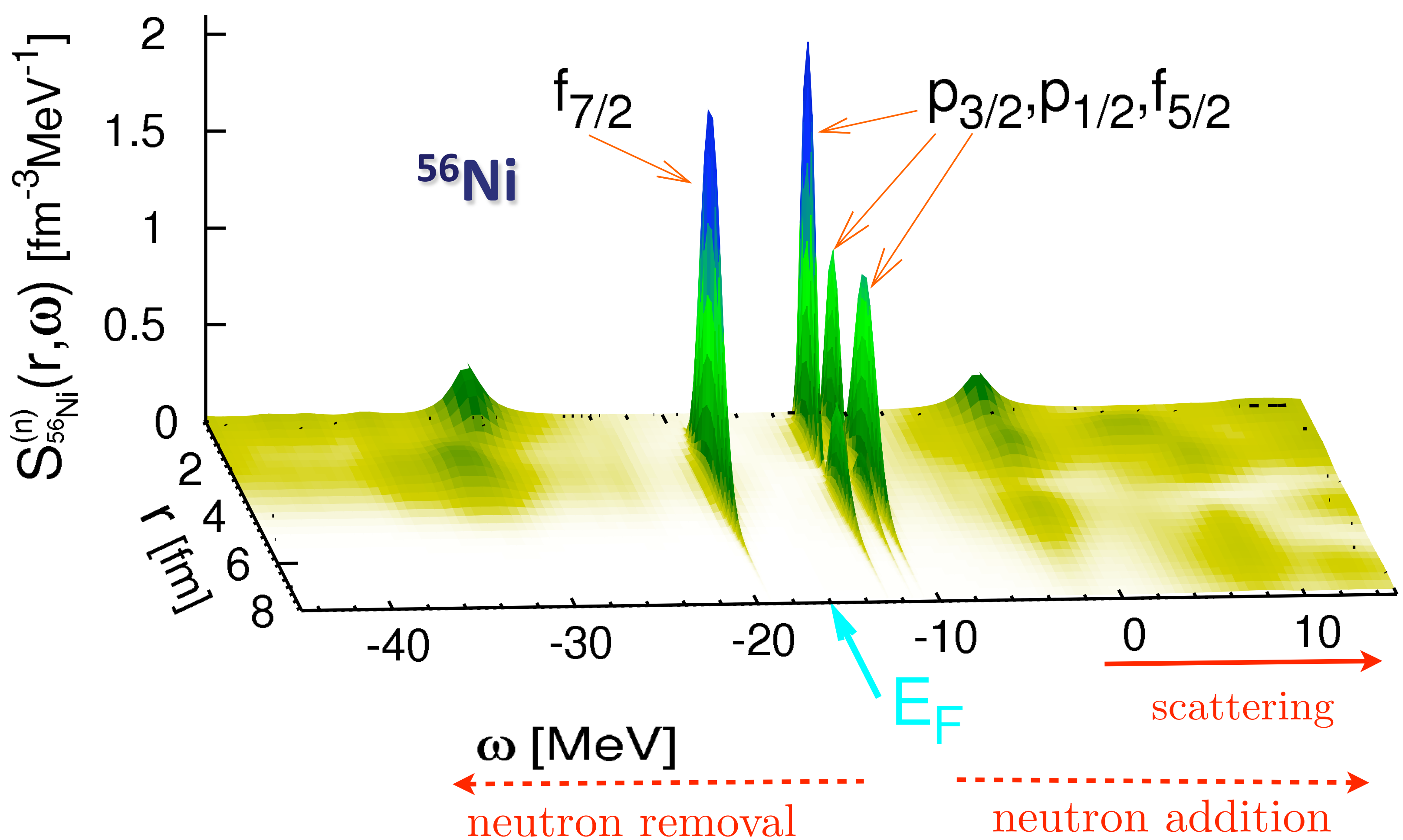
- and so on...

The single-particle green function

$$g_{\alpha\beta}(\omega) = \sum_n \frac{\langle\Psi_0^N|a_\alpha|\Psi_n^{N+1}\rangle\langle\Psi_n^{N+1}|a_\beta^\dagger|\Psi_0^N\rangle}{\omega-(E_n^{N+1}-E_0^N)+i\eta} + \frac{\langle\Psi_0^N|a_\beta^\dagger|\Psi_n^{N-1}\rangle\langle\Psi_n^{N-1}|a_\alpha|\Psi_0^N\rangle}{\omega-(E_0^N-E_n^{N-1})-i\eta} =$$

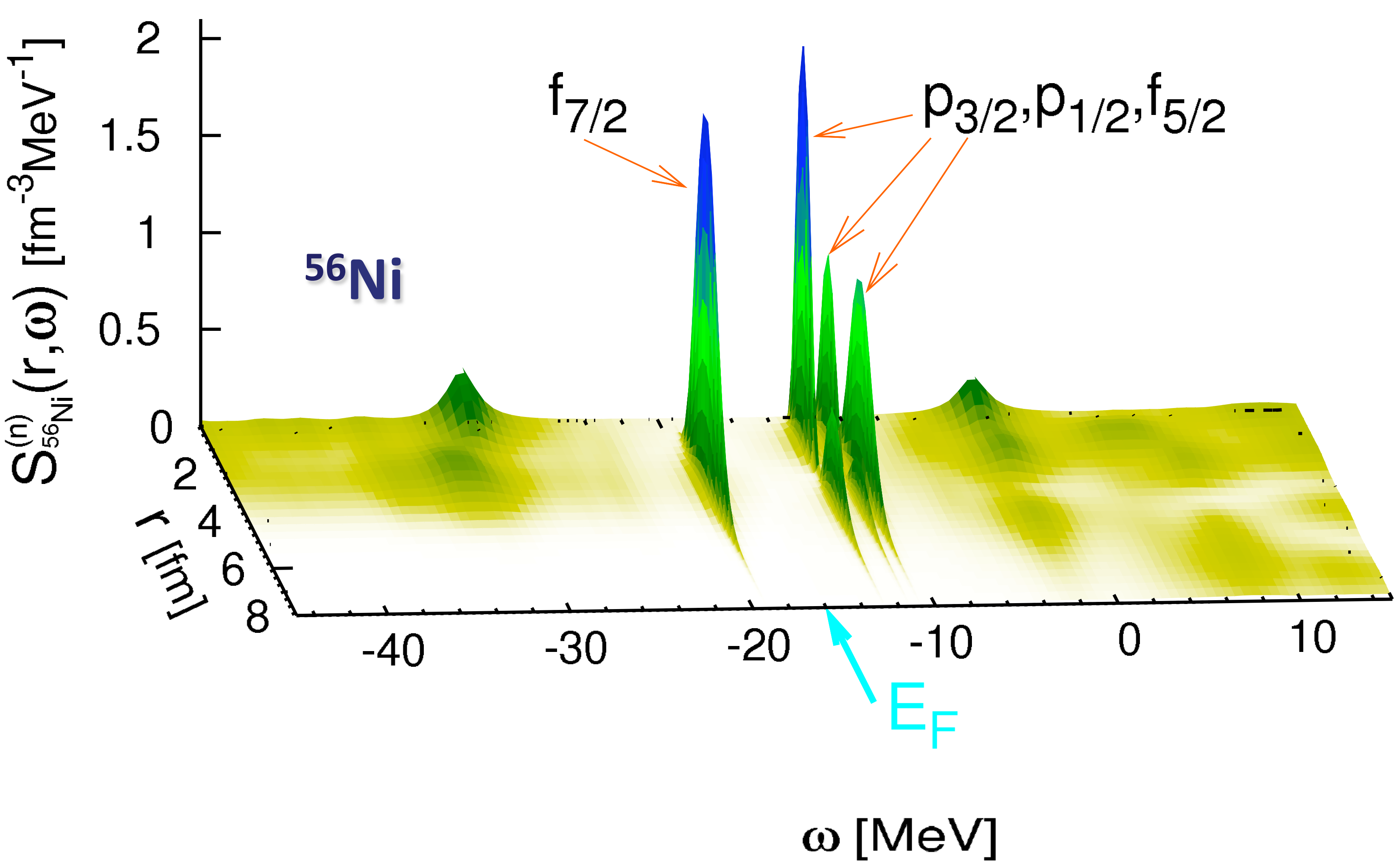


all the structure information probed by one-nucleon transfer



C. Barbieri, PRL **103**,202520 (2009)

- Details

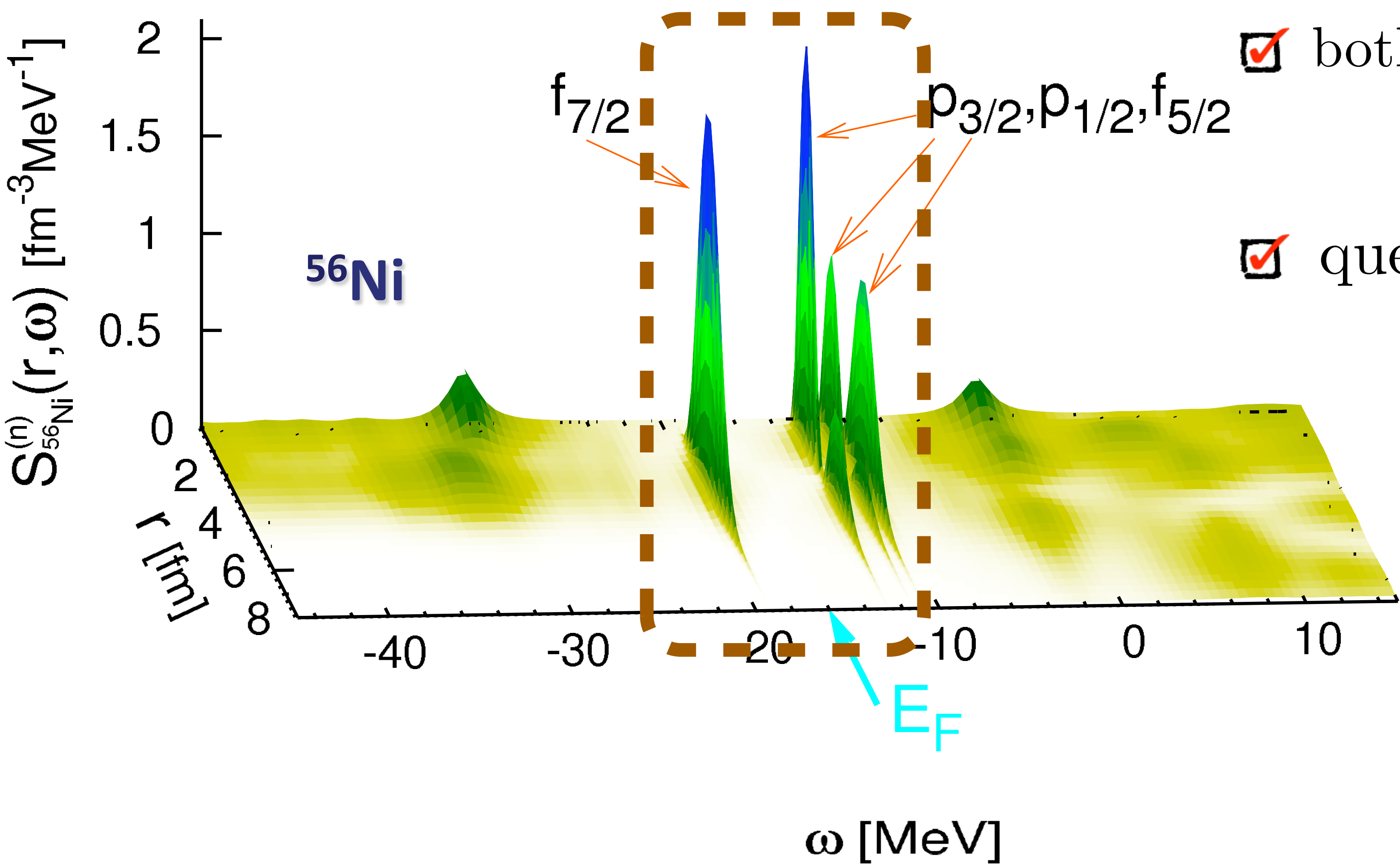


C. Barbieri, PRL **103**,202520 (2009)

Introduction

- Details

Role of E_F: ***M-B*** s.p. states



- ☑ shell model
- ☑ low-energy physics
- ☑ both *finite* and *infinite* system (Landau theory)
- ☑ quenching SP: SRC ∼ 10%

C. Barbieri, PRL **103**,202520 (2009)

Introduction

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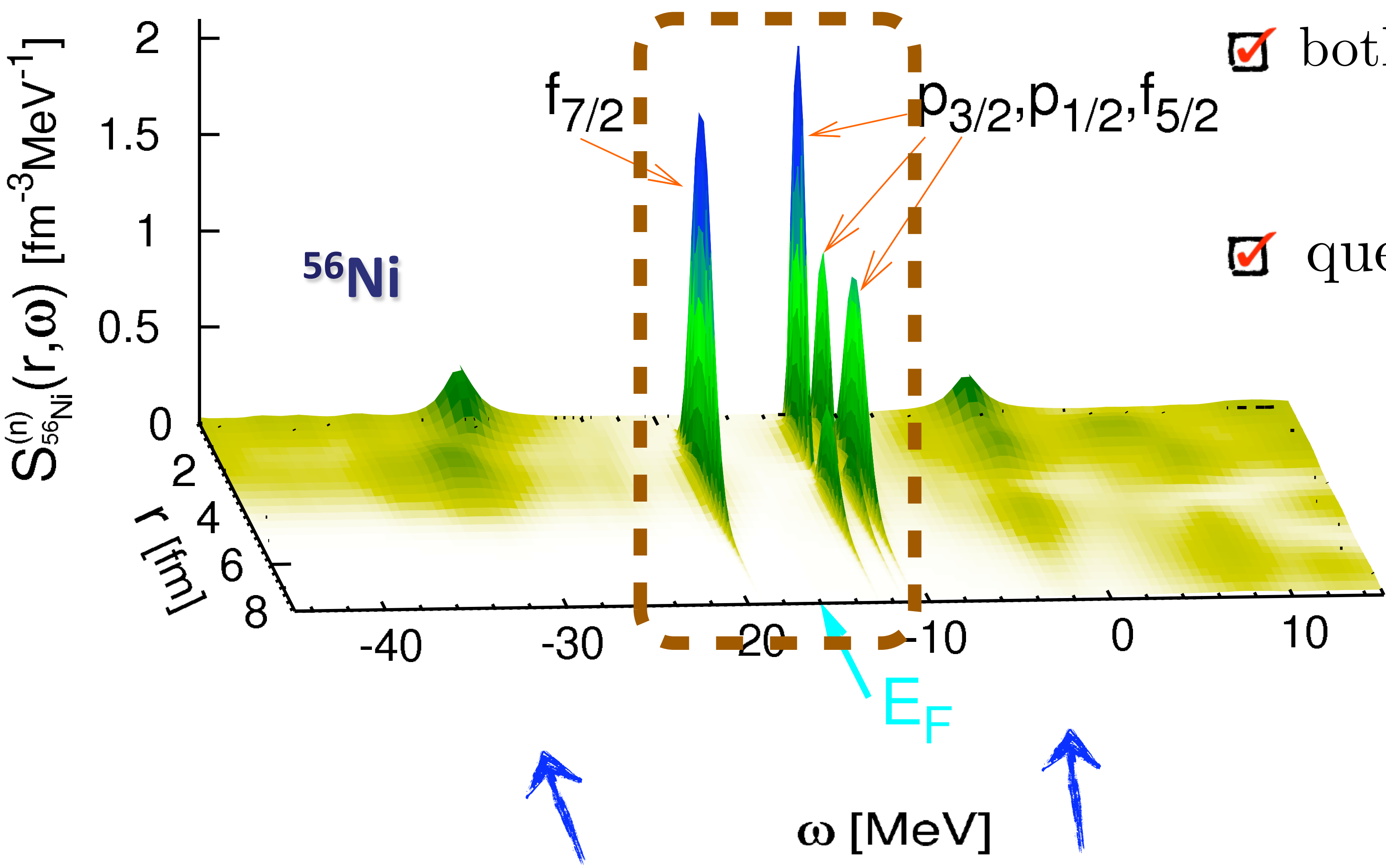
Role of E_F: ***M-B*** s.p. states



Particle-vibration coupling

- ☑ shell model
- ☑ low-energy physics
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- ☑ quenching SP: SRC $\sim 10\%$

C. Barbieri, PRL **103**,202520 (2009)

Introduction

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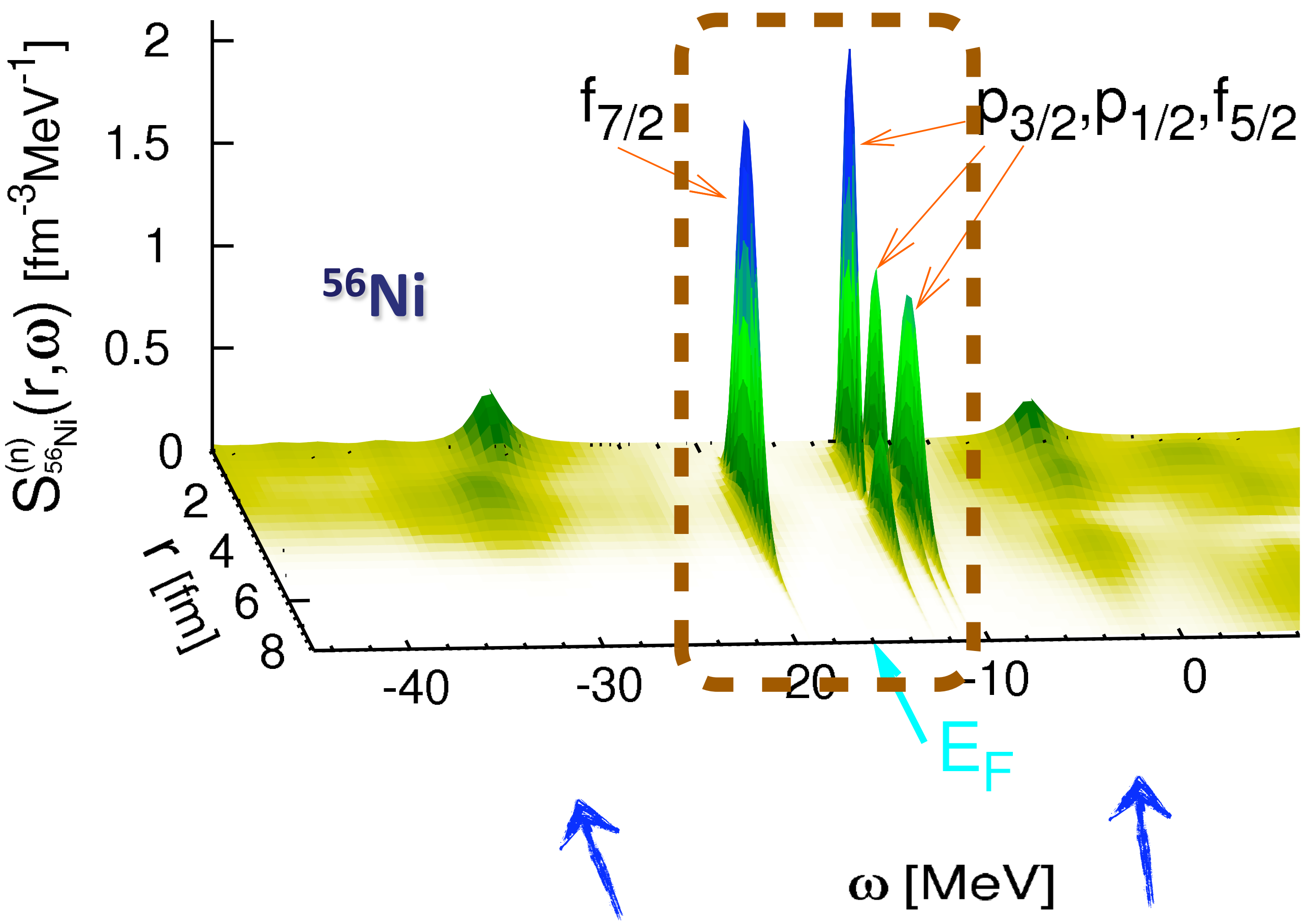
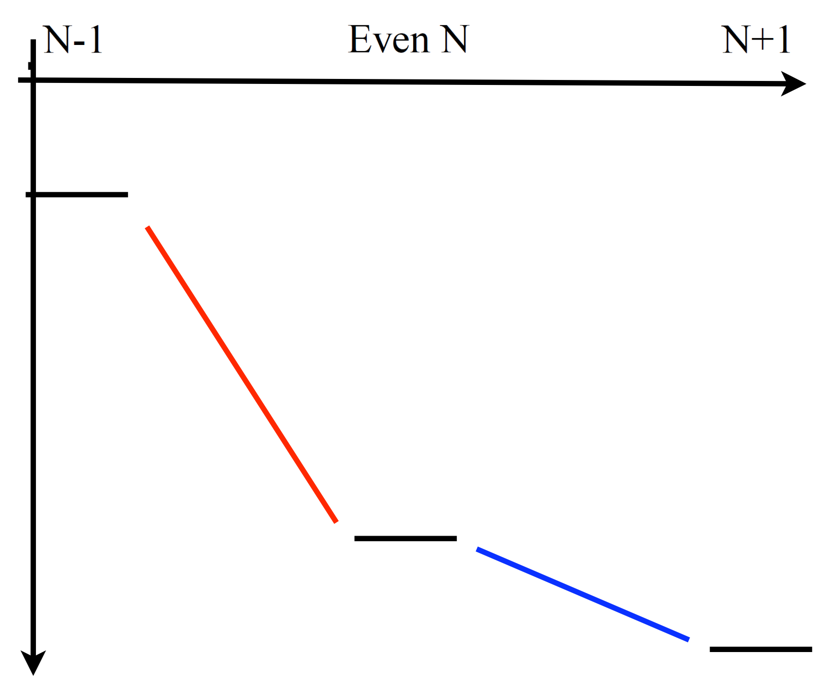
Role of E_F: ***M-B*** s.p. states



Particle-vibration coupling

- ☑ shell model
- ☑ low-energy physics
- ☑ both *finite* and *infinite* system (Landau theory)
- ☑ quenching SP: SRC ~ 10%

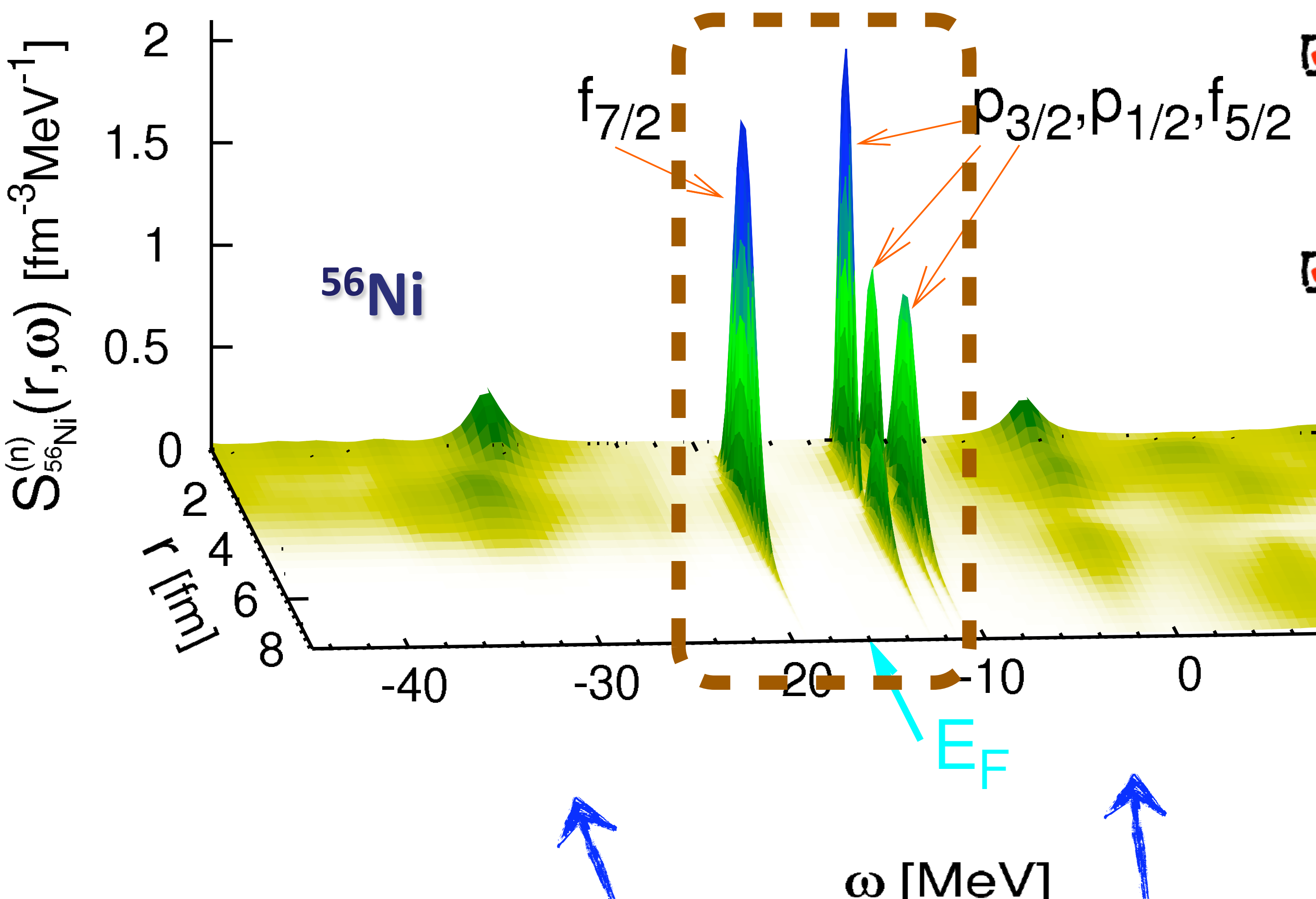


C. Barbieri, PRL **103**,202520 (2009)

Introduction

- Details

Role of E_F: *M-B* s.p. states



Particle-vibration coupling

C. Barbieri, PRL **103**,202520 (20

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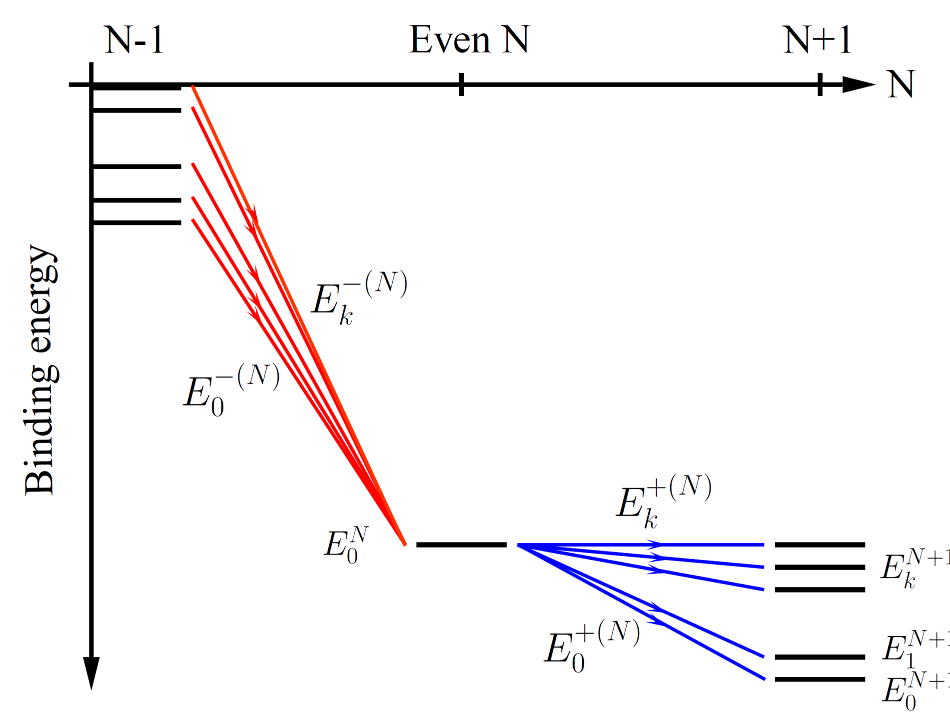
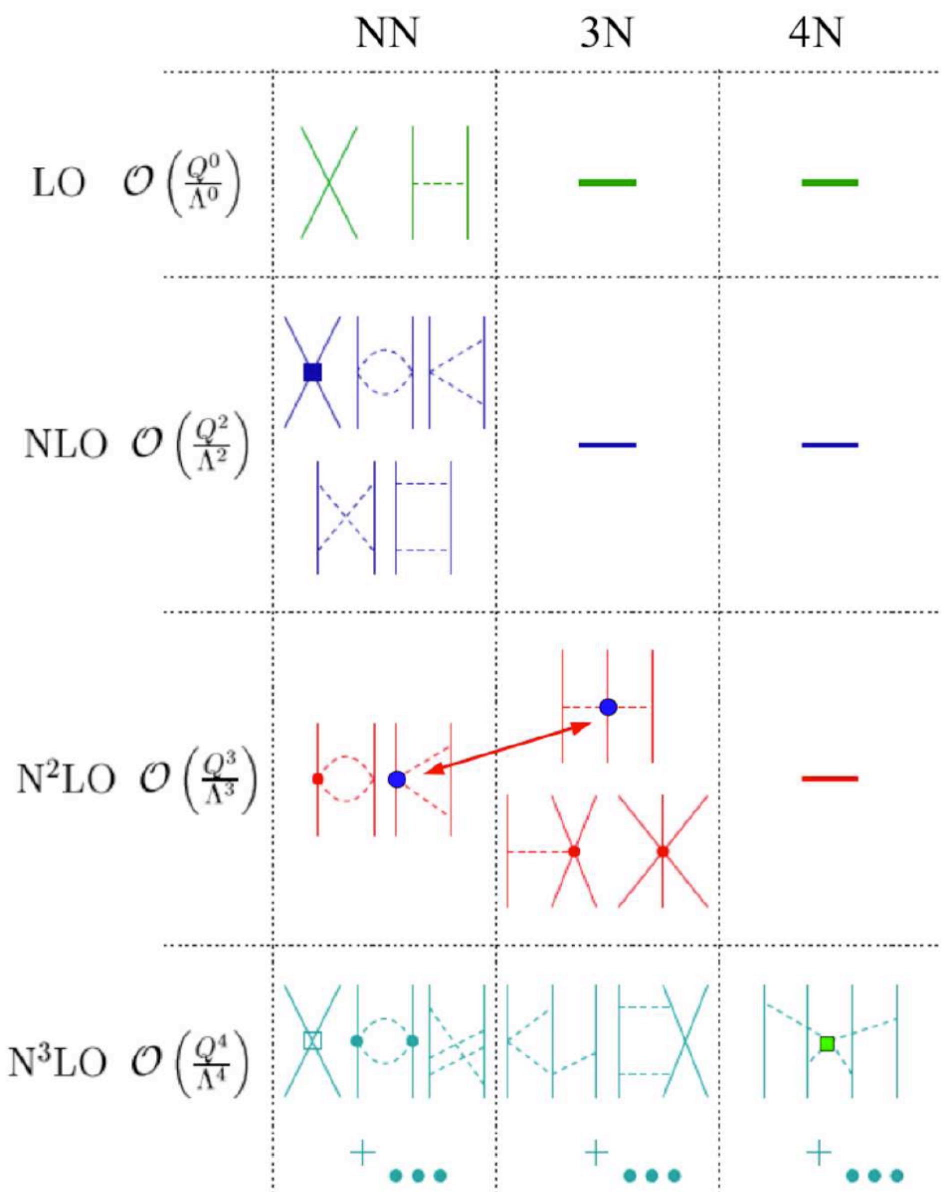
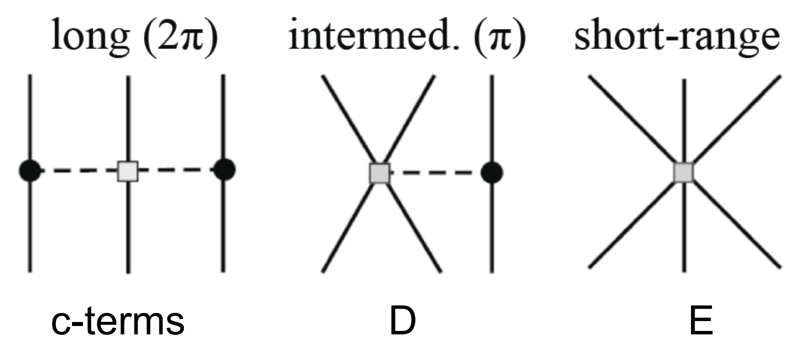


Courtesy of J. Sadoudi

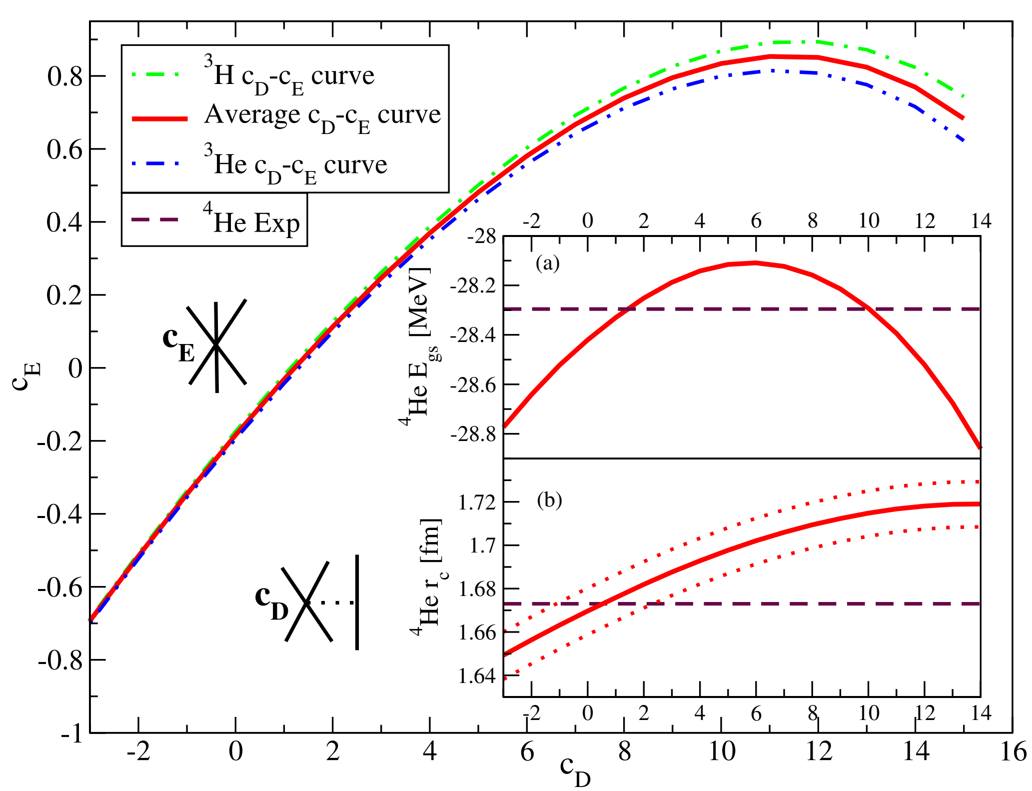
Bare *systematic* nuclear potential

- χPT theory: 3NF arise naturally at N^2LO





only two more constant to be fitted!



Navratil et al, PRL **99**,042501 (2007)

3BF in nuclear environment

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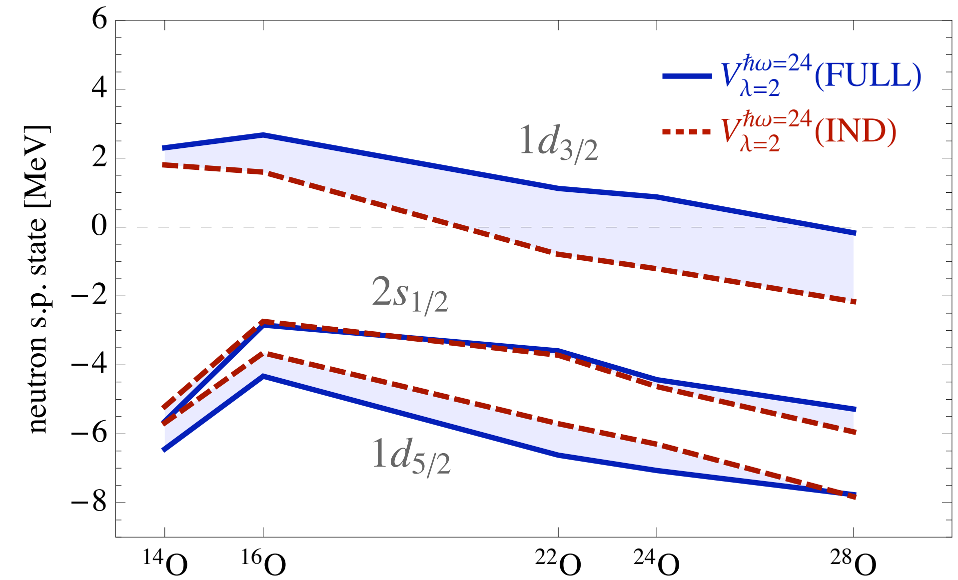
- sd-shell nuclei

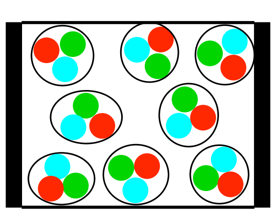
  AC, C. Barbieri & P. Navrátil, arXiv:1303.4900

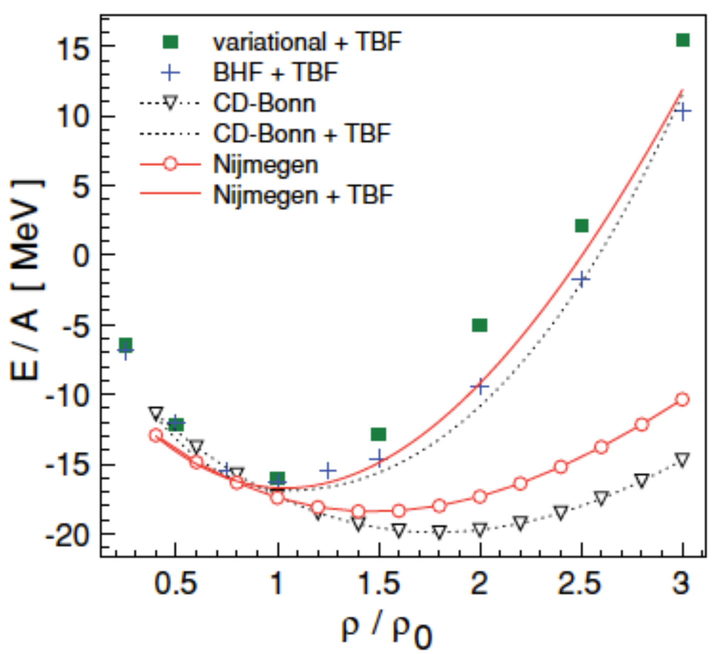
- Infinite Matter

Single particle spectrum at E_F

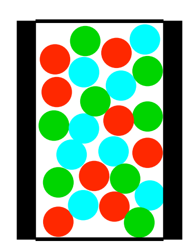


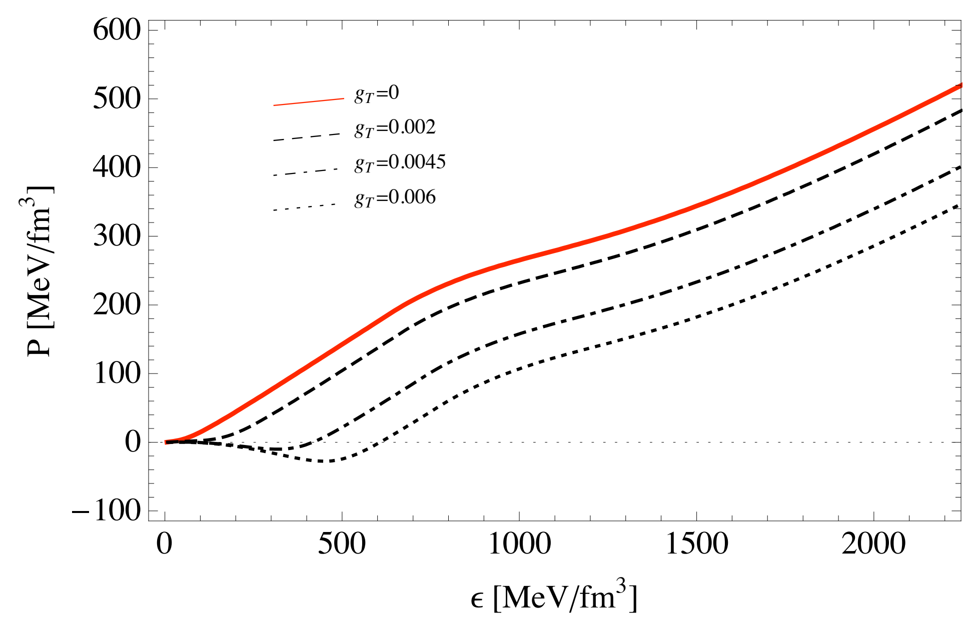
Saturation density for NSM





Quartk matter EoS (NJL model)





V.Somà and P. Bozek, PRC **78**, 054003 (2008)

O.Benhar and AC , A&A **525**, L1 (2011)

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”Green function or green’s function?”

M.C.M. Wright, Nature Physics **2**, 646 (2006)

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- Structure of Nuclear Hamiltonian

$$H = \sum_{\alpha\beta} T_{\alpha\beta}\, a^\dagger_\alpha a_\beta + \frac{1}{(2!)^2} \sum_{\alpha\beta\gamma\delta} V_{\alpha\beta,\gamma\delta}\, a^\dagger_\alpha a^\dagger_\beta a_\delta a_\gamma + \boxed{\frac{1}{(3!)^2} \sum_{\alpha\beta\gamma\delta\epsilon\zeta} W_{\alpha\beta\gamma,\delta\epsilon\zeta}\, a^\dagger_\alpha a^\dagger_\beta a^\dagger_\gamma a_\delta a_\epsilon a_\zeta}$$

Elements of Green Function theory

Structure of Nuclear Hamiltonian

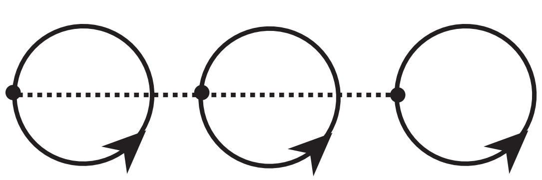
$$H = \sum_{\alpha\beta} T_{\alpha\beta}\, a^\dagger_\alpha a_\beta + \frac{1}{(2!)^2} \sum_{\alpha\beta\gamma\delta} V_{\alpha\beta,\gamma\delta}\, a^\dagger_\alpha a^\dagger_\beta a_\delta a_\gamma + \boxed{\frac{1}{(3!)^2} \sum_{\alpha\beta\gamma\delta\epsilon\zeta} W_{\alpha\beta\gamma,\delta\epsilon\zeta}\, a^\dagger_\alpha a^\dagger_\beta a^\dagger_\gamma a_\delta a_\epsilon a_\zeta}$$

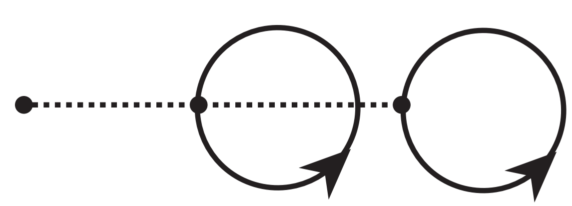
Decomposition in Normal Ordering

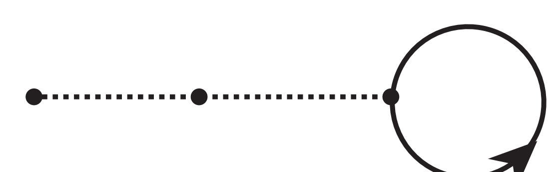
$$3BT = \widetilde{W}^0 + \widetilde{W}^1_{\gamma\zeta} : a^\dagger_\gamma a_\zeta : + \widetilde{W}^2_{\beta\gamma,\epsilon\zeta} : a^\dagger_\beta a^\dagger_\gamma a_\zeta a_\epsilon : + W_{\alpha\beta\gamma,\delta\epsilon\zeta} : a^\dagger_\alpha a^\dagger_\beta a^\dagger_\gamma a_\zeta a_\epsilon a_\delta :$$

$$\widetilde{W}^0 = \frac{1}{6} \sum_{n_1,n_2,n_3} W_{n_1 n_2 n_3, n_1 n_2 n_3} \qquad \widetilde{W}^1_{\gamma\zeta} = \frac{1}{2} \sum_{n_1,n_2} W_{n_1 n_2 \gamma, n_1 n_2 \zeta} \qquad \widetilde{W}^2_{\beta\gamma\epsilon\zeta} = \frac{1}{4} \sum_{n_1} W_{n_1 \beta\gamma, n_1 \epsilon\zeta}$$

n_i means occupied s.p. state of $|\Phi_{ref}\rangle$







Elements of Green Function theory

Structure of Nuclear Hamiltonian

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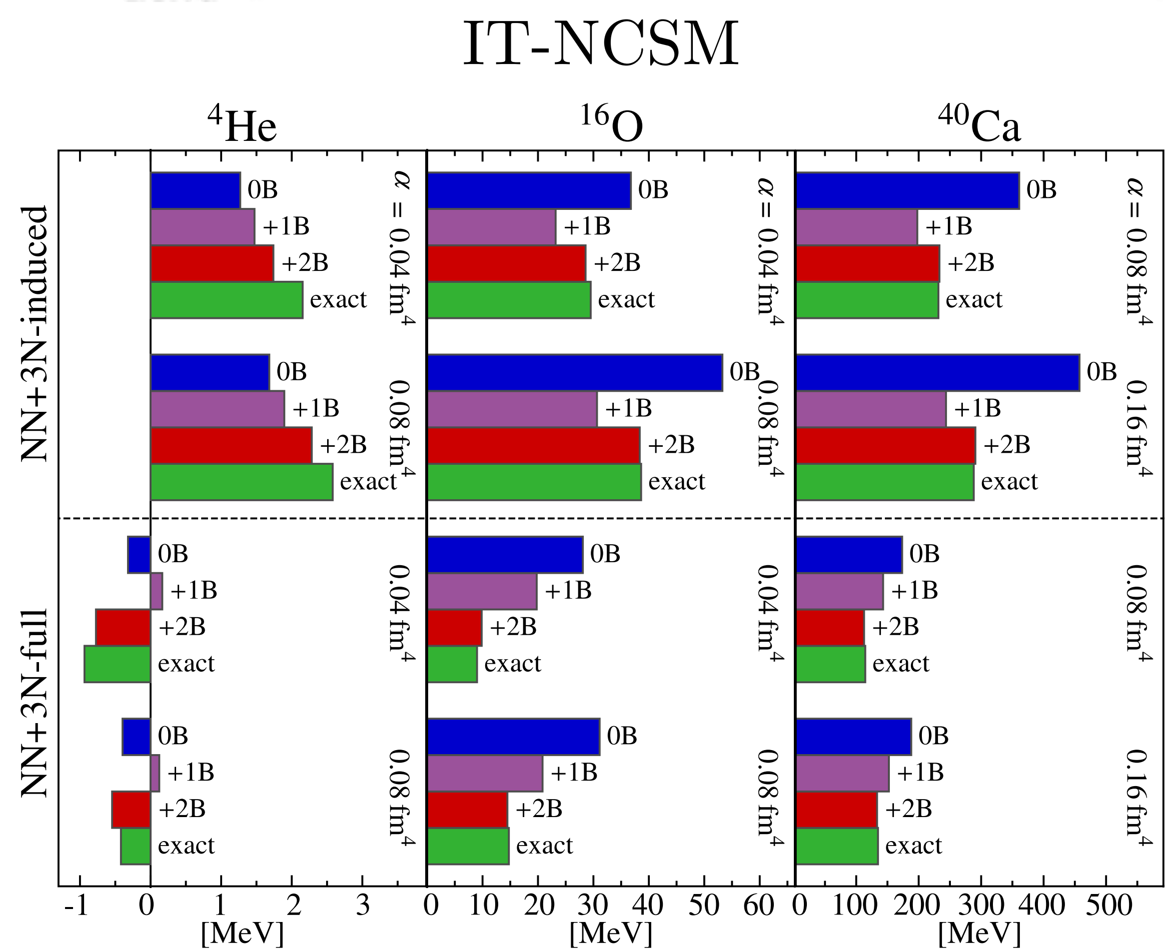
Decomposition in Normal Ordering



R. Roth et al., Phys. Rev. Lett. **109**,052501 (2012)

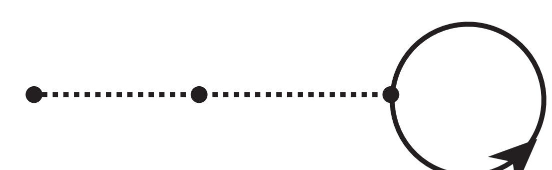
$\ldots a_\epsilon : +W_{\alpha\beta\gamma,\delta\epsilon\zeta} : a^\dagger_\alpha a^\dagger_\beta a^\dagger_\gamma a_\zeta a_\epsilon a_\delta :$

$\widetilde{W}^0$

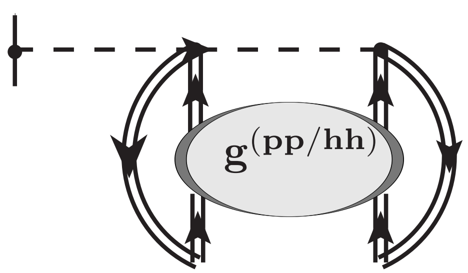
ζ

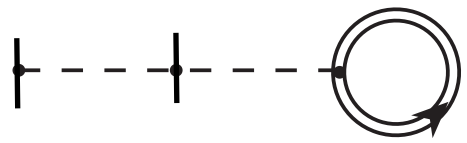
$$\widetilde{W}^2_{\beta\gamma\epsilon\zeta} = \frac{1}{4} \sum_{n_1} W_{n_1\beta\gamma,n_1\epsilon\zeta}$$

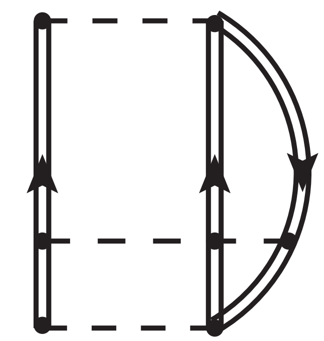
n



- 3NF can enter the diagrams in three different ways

$\frac{1}{4}$ 

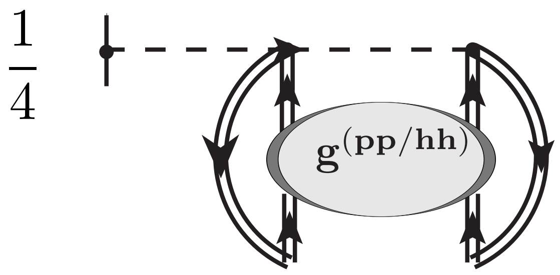


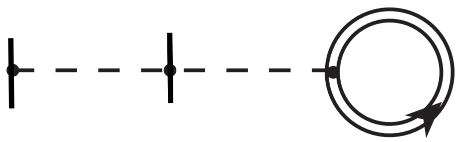


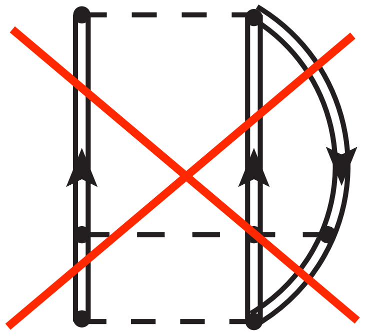
- Using *fully correlated density matrices* (BEYOND a normal ordering...)

Elements of Green Function theory

- 3NF can enter the diagrams in three different ways



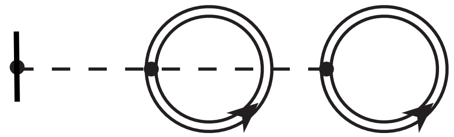


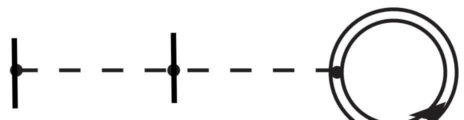


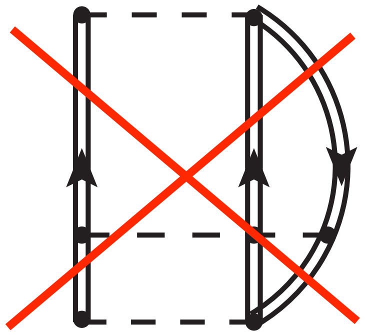
- [x] Using *fully correlated density matrices* (BEYOND a normal ordering...)

Elements of Green Function theory

- 3NF can enter the diagrams in three different ways

$\frac{1}{2}$ 



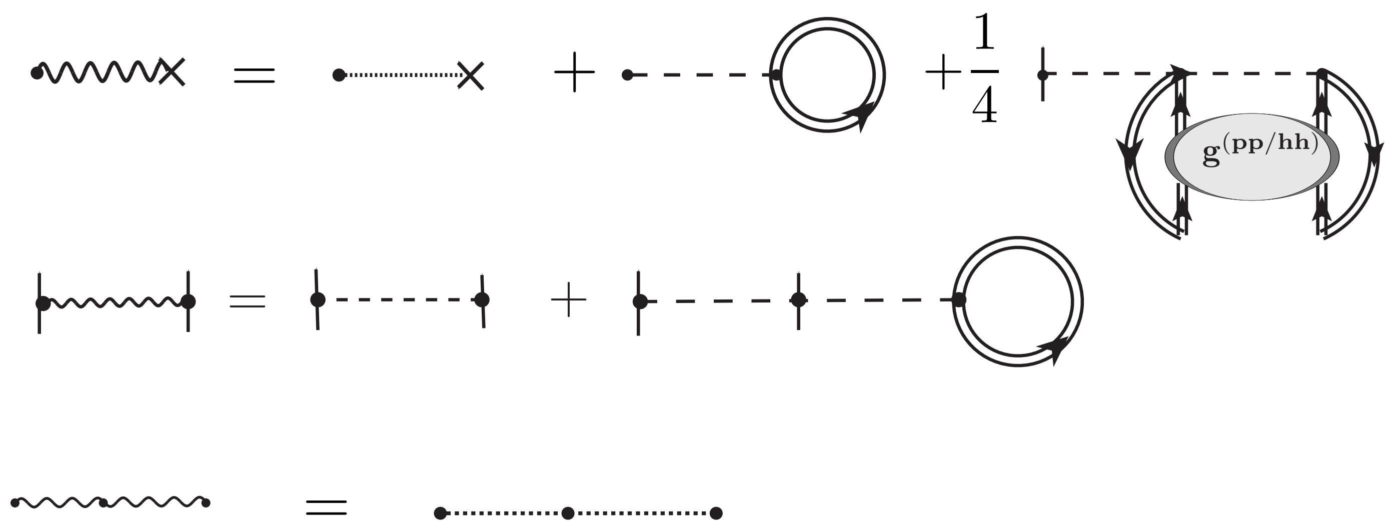


- Using *fully correlated density matrices* (BEYOND a normal ordering...)

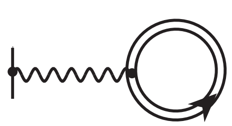
Elements of Green Function theory

- 3NF can enter the diagrams in three different ways

  - Defining 1- and 2-body effective interaction and use only *irreducible* diagrams

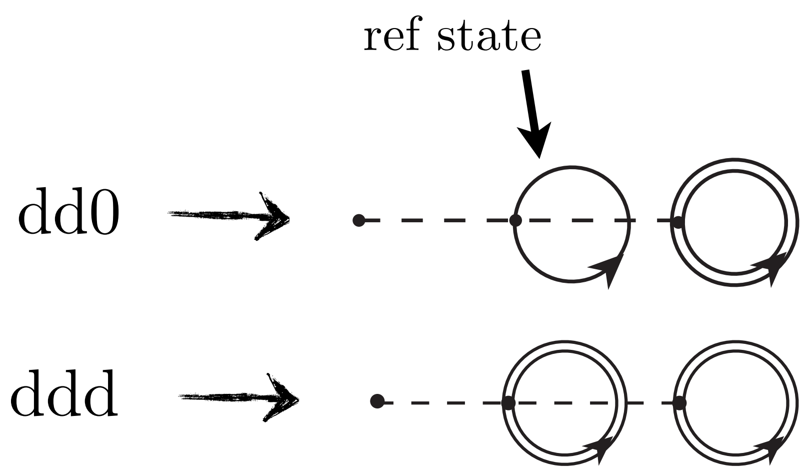


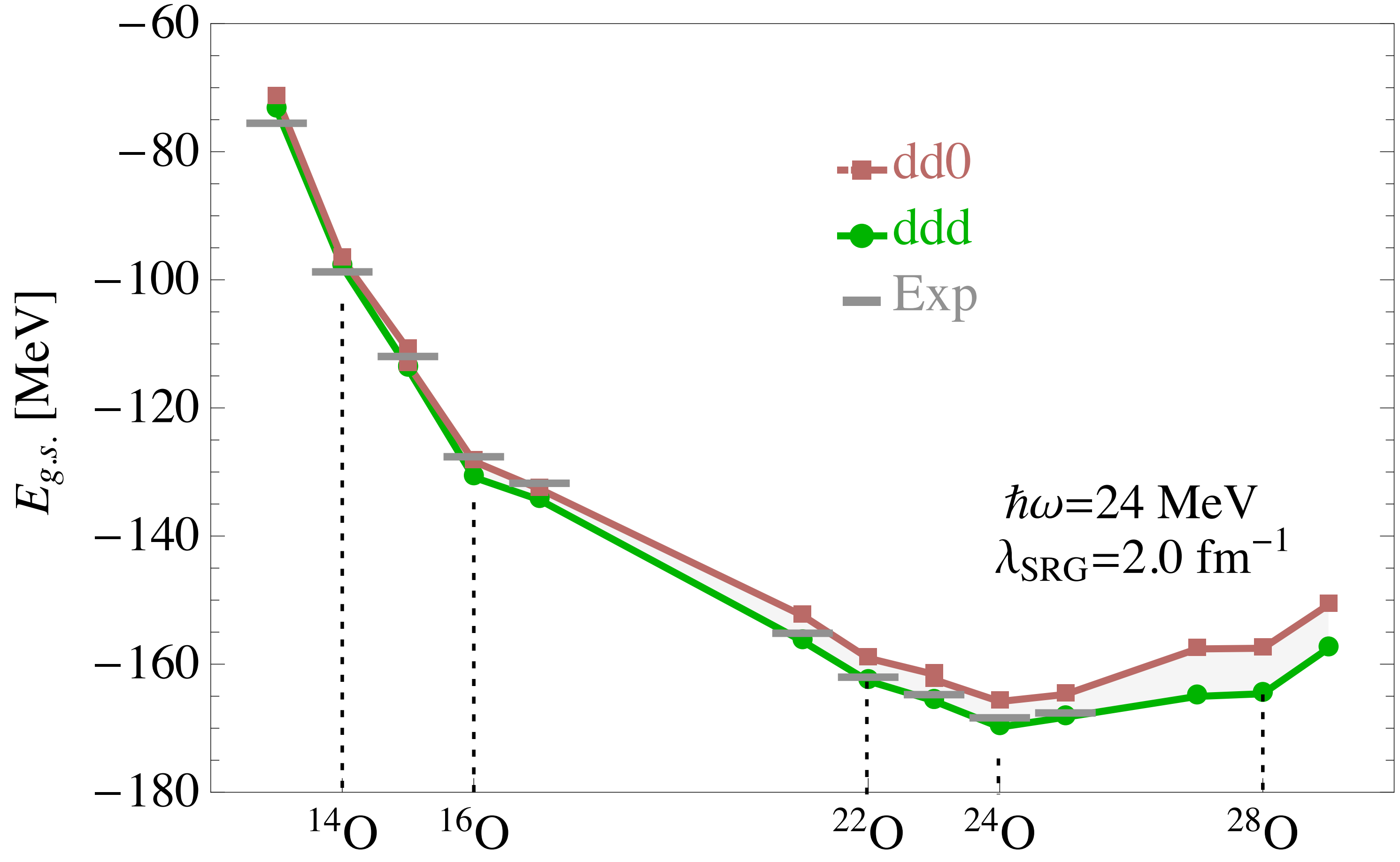
  - Beware that defining



would double-count the 1-body term

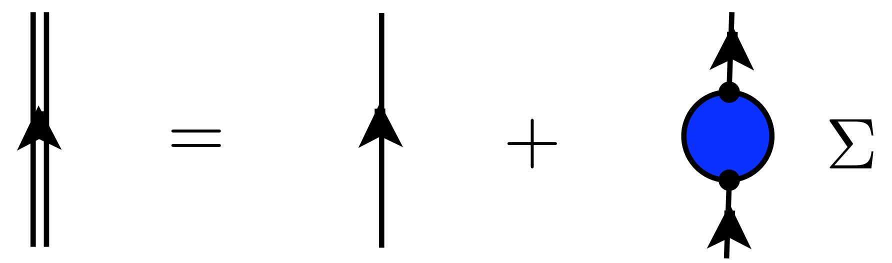
- Two different apprx.





Elements of Green Function theory

- Reducible Self-Energy



- Dyson equation (to be solved iteratively)

$$g_{\alpha\alpha'}(t-t') = g^0_{\alpha\alpha'}(t-t') + g^0_{\alpha\alpha'}(t-t_1)\Sigma^\star_{\alpha'\beta'}(t_1,t_2)g_{\beta'\beta}(t_2-t')$$

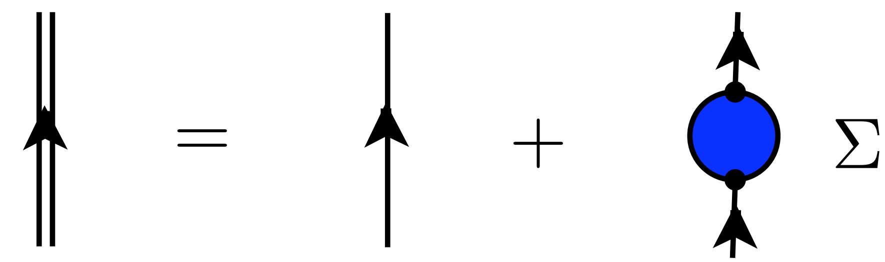
"empty" green function

the contents
(dynamical correlation)

"full" or *dressed*
green function

Elements of Green Function theory

- Reducible Self-Energy



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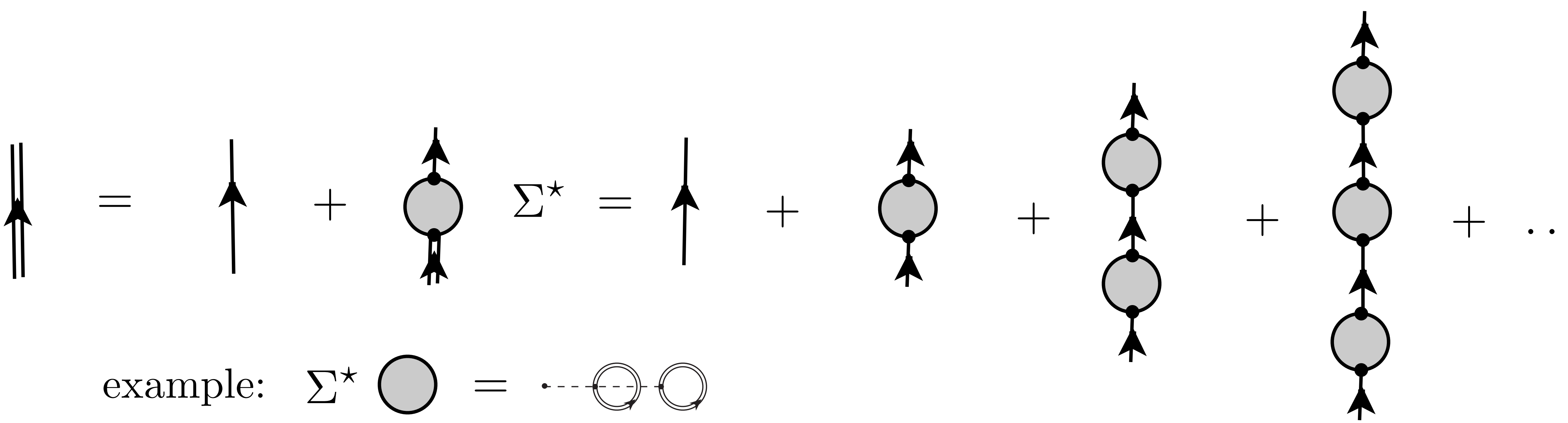
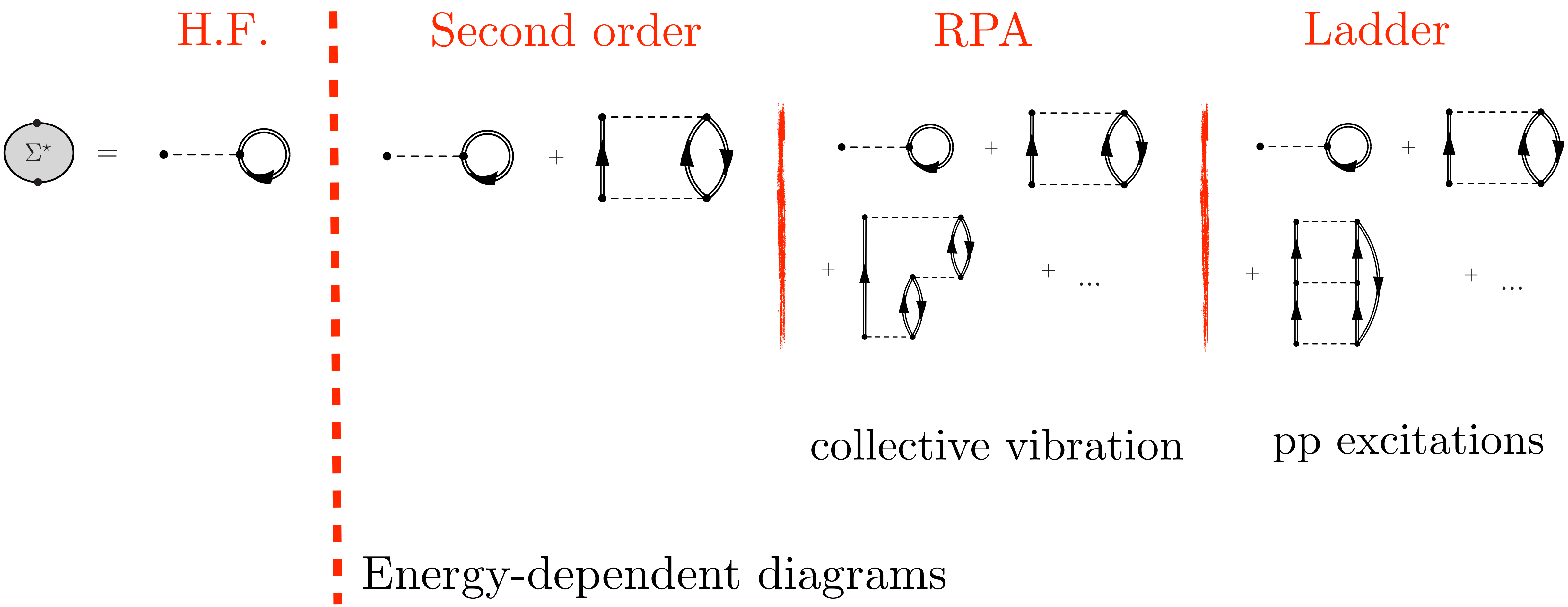


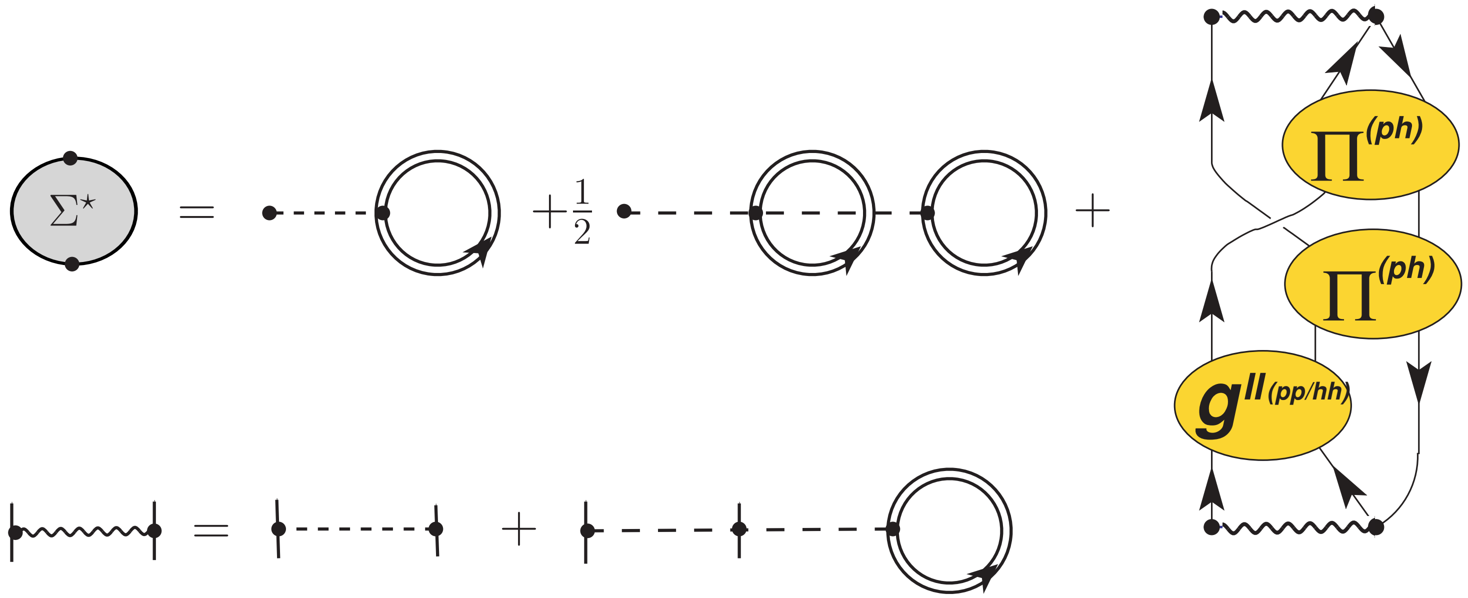
example: $\Sigma^{\star}$

- Approximation for the Σ^*



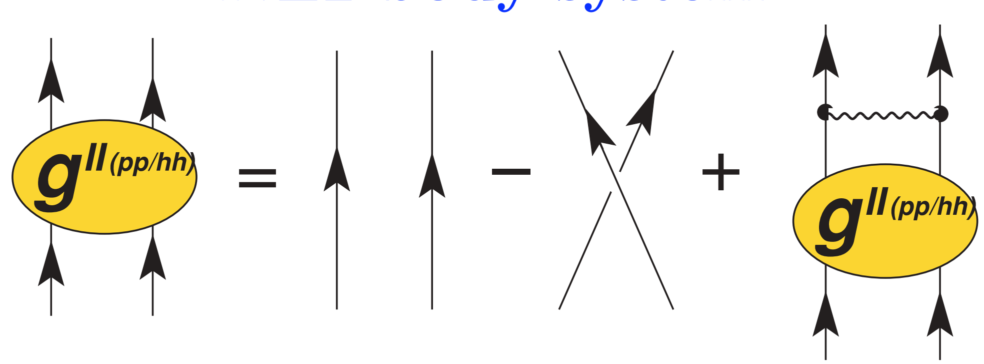
Elements of Green Function theory

- FTDA approach (Dickhoff & Barbieri 2004) extended to 3B sector

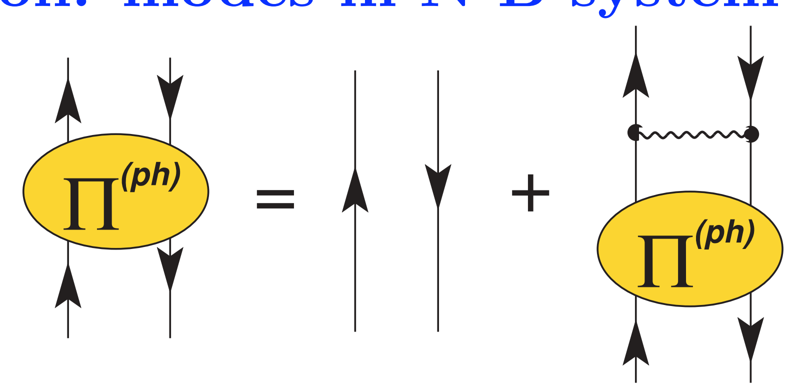


The Σ^* is intimately related to the spectrum of

N±2 body system **coll. modes in N-B system**



and



Accuracy of many-body truncation in FTDA approach

TABLE I. FRPA results for a set of small molecules in a cc-pVDZ basis set. The ground-state energy E_0 is given in hartree, the ionization energy I in electronvolt, equilibrium bond distances are in Angstrom, and the equilibrium angles in degrees. FRPA and FTDA refer to the calculations after the first iteration, while FRPA(c) and FTDA(c) refer to the calculations where consistency at the Hartree-Fock level was applied. The calculated data are compared to the coupled-cluster method at the level of CCSD(T) and to experimental data or exact calculations taken from Ref. [27]. The FCI energies were calculated at the FRPA(c) geometry.

Molecule		FTDA	FTDA(c)	FRPA	FRPA(c)	CCSD(T)	FCI	Expt.
H_2								
	E_0	−1.170	−1.161	−1.170	−1.161	−1.164	−1.164	−1.175
	r_{H-H}	0.769	0.757	0.770	0.757	0.761		0.741
	I	16.16	16.03	16.16	16.03	16.12		16.08
HF								
	E_0	−100.175	−100.224	−100.173	−100.228	−100.228	−100.231	
	r_{H-F}	0.904	0.916	0.897	0.913	0.920		0.917
	I	15.70	15.70	15.56	15.54	15.42		16.12
HCl								
	E_0	−460.295	−460.256	−460.293	−460.255	−460.254		
	r_{H-Cl}	1.314	1.297	1.314	1.293	1.290		1.275
	I	12.44	12.24	12.44	12.24	12.26		
BF								
	E_0	−124.331	−124.365	−124.332	−124.368	−124.380		
	r_{B-F}	1.285	1.284	1.305	1.285	1.295		1.267
	I	11.35	10.75	11.73	10.94	11.01		
BeH_2								
	E_0	−15.855	−15.831	−15.856	−15.832	−15.835	−15.836	
	r_{Be-H}	1.374	1.337	1.383	1.337	1.339		1.340
	I	11.89	11.78	11.84	11.76	11.89		

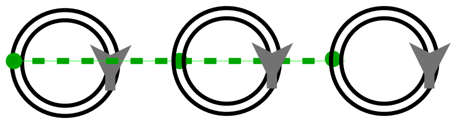
M. Degroote, D. Van Neck and C. Barbieri, Phys. Rev. A **83**, 042517 (2011)

Elements of Green Function theory

- Binding energy from Kultun Sum-Rule (extended)

$$\langle H \rangle = \langle T \rangle + \langle V \rangle + \langle W \rangle = \sum_{\alpha\beta} \frac{1}{4\pi i} \int_{C\uparrow} d\omega \left[\, T_{\alpha\beta} + \omega\, \delta_{\alpha\beta} \,\right] g_{\alpha\beta}(\omega) - \frac{1}{2} \langle W \rangle$$

$$\langle W \rangle \approx \frac{1}{6}$$



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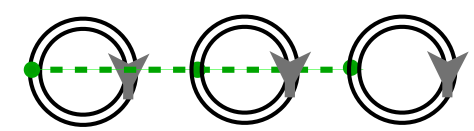
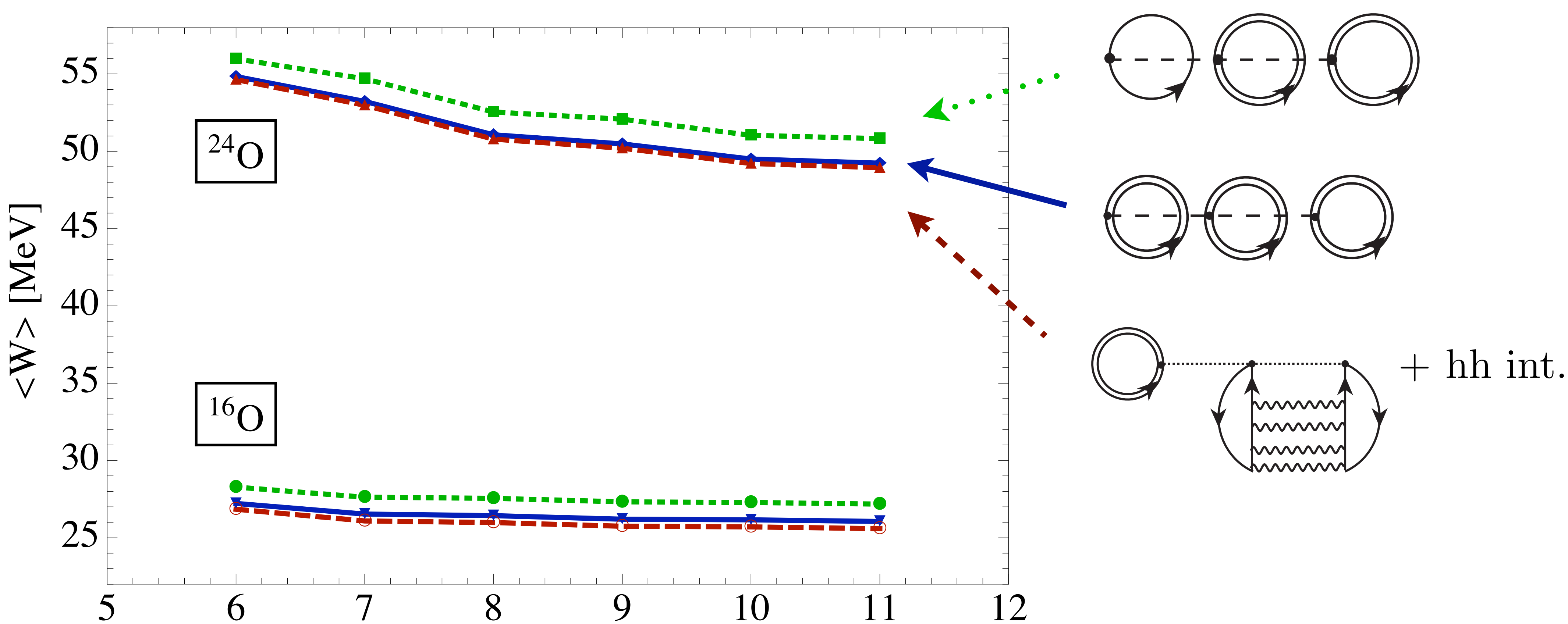
$\langle W \rangle \approx \frac{1}{6}$ 

- Different approximations for $\langle W \rangle$



Results

Two and Three-Body interactions

- [ ] We use χPT potential evolved through SRG

$$\widetilde{H} = U^{\dagger}(\lambda) H\, U(\lambda) = \widetilde{T}(\lambda) + \widetilde{V}^{2N}(\lambda) + \widetilde{W}^{3N}(\lambda) + \ldots$$

- [x] Universal low-k physics unchanged
- [x] Decoupling *low*-k and *high*-k
- [x] λ quenching SF $\sim 5\%$

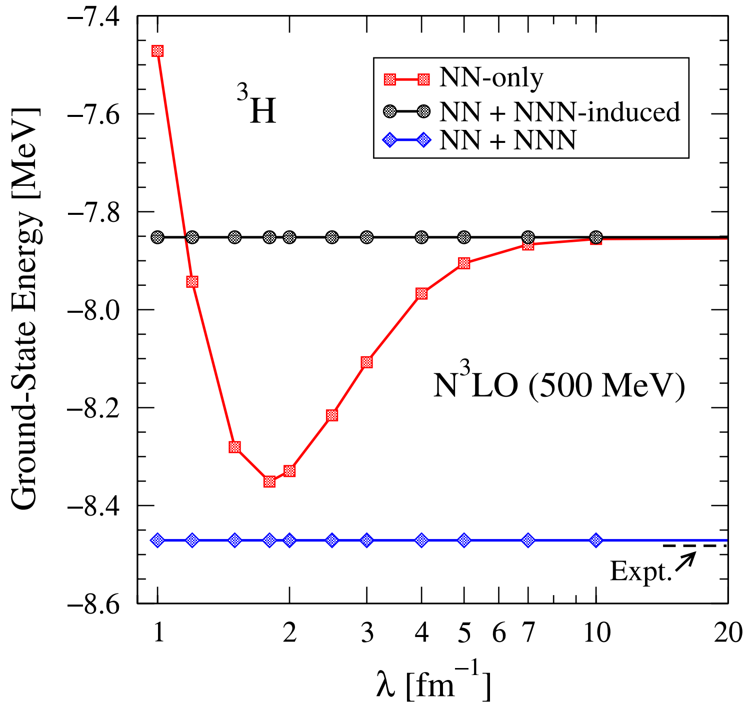


FIG. 1 (color online). Ground-state energy of ^{3}H as a function of the SRG evolution parameter, λ. See Table I for the nomenclature of the curves.

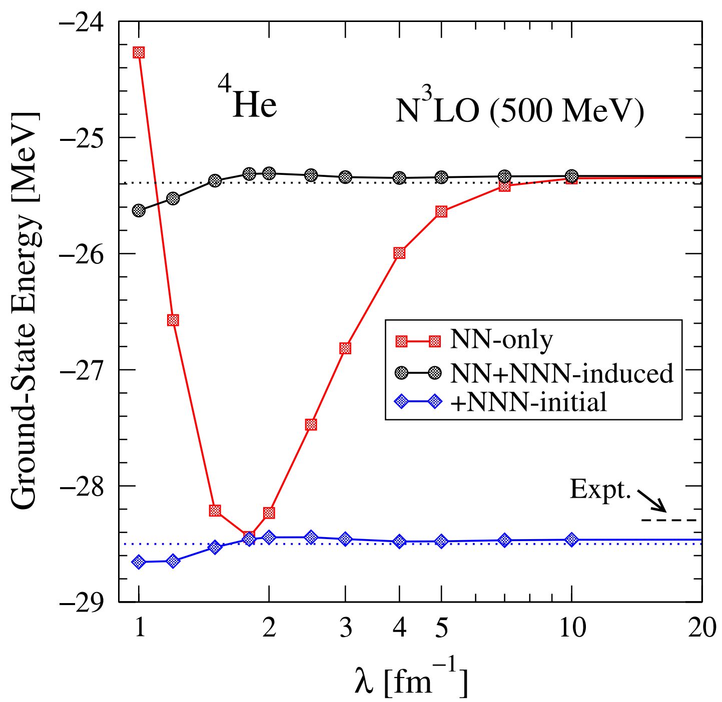


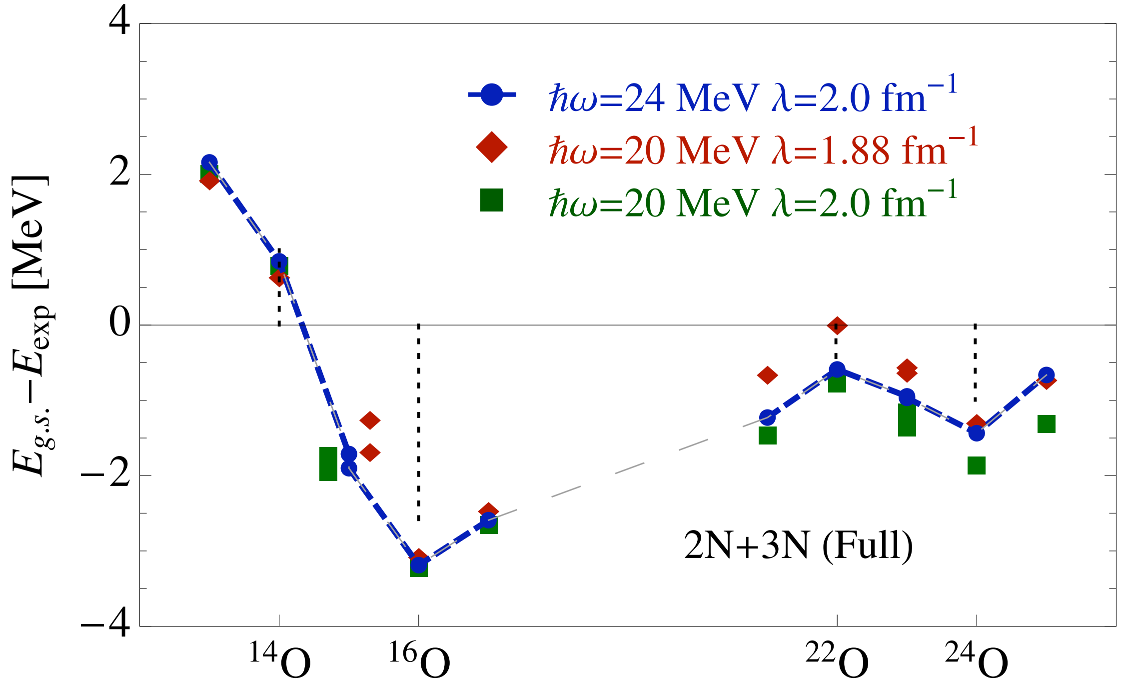
FIG. 2 (color online). Ground-state energy of ^{4}He as a function of the SRG evolution parameter, λ. See Table I for the nomenclature of the curves.

E.D. Jurgenson et al, PRL **103**,082501 (2009)

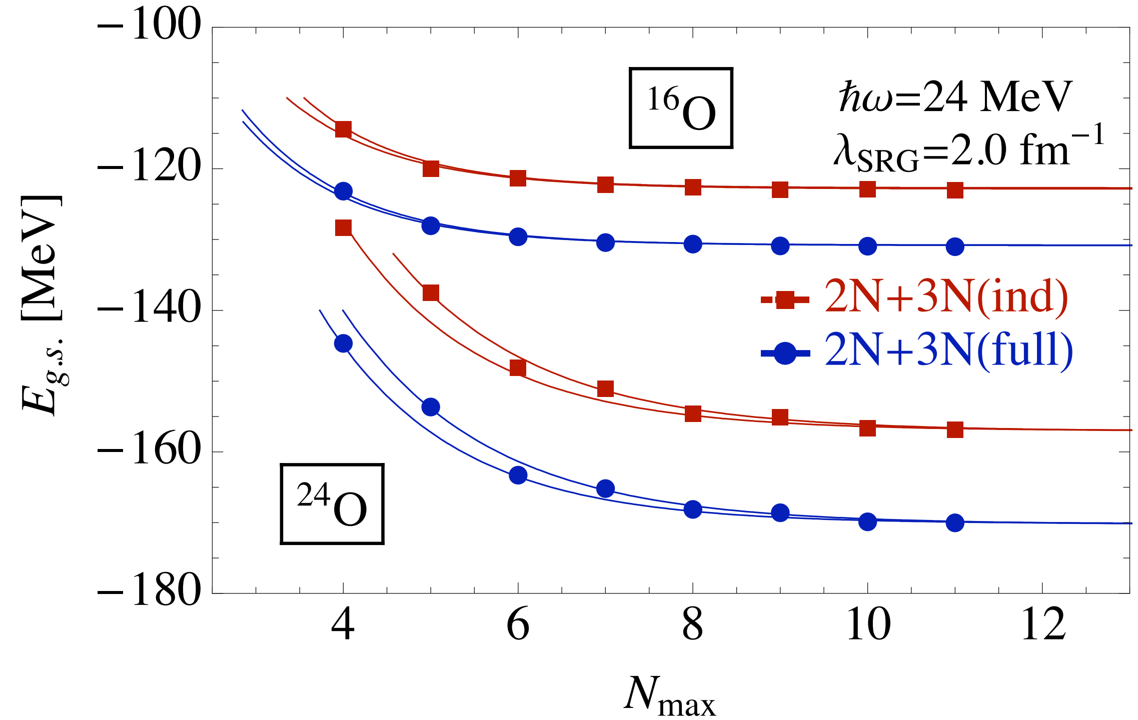
Results

- Error extimate

Distance from E_{exp}



Convergence



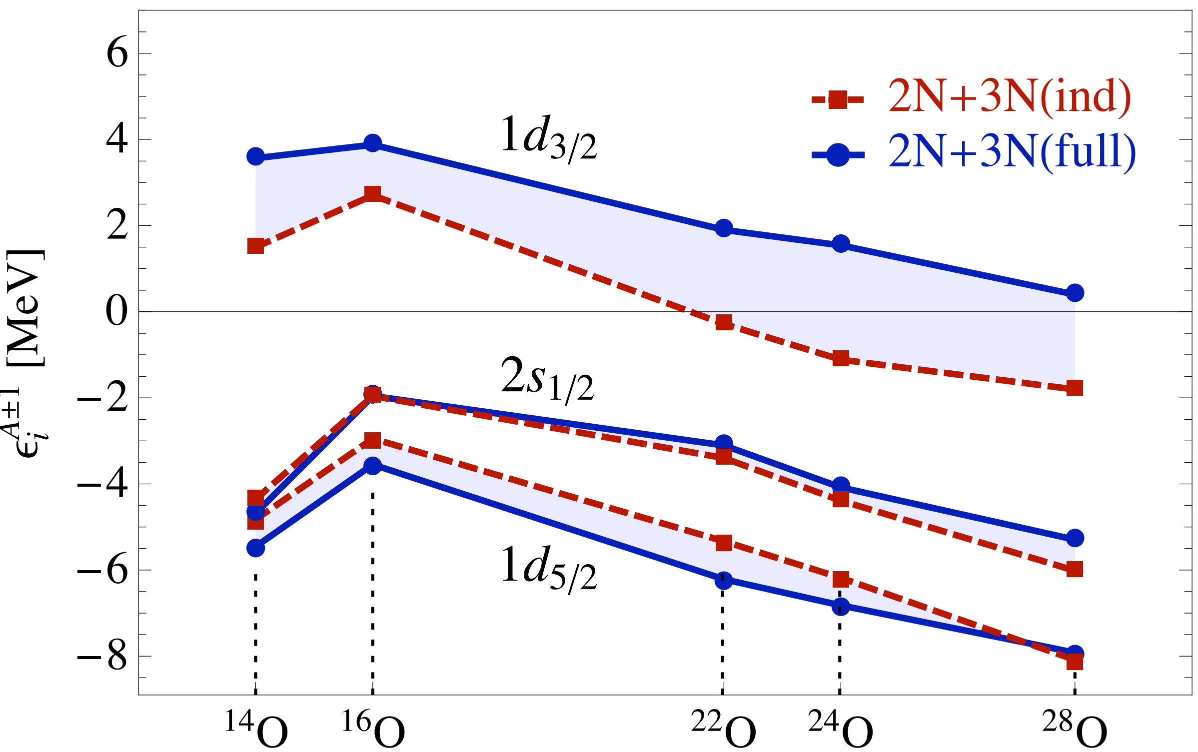
- ☑ C.M. correction included $\quad E^{A\pm1} = \pm\varepsilon_0^{A\pm1}[\widetilde{H}(A\pm1)] + E_0^A[\widetilde{H}(A\pm1)]$

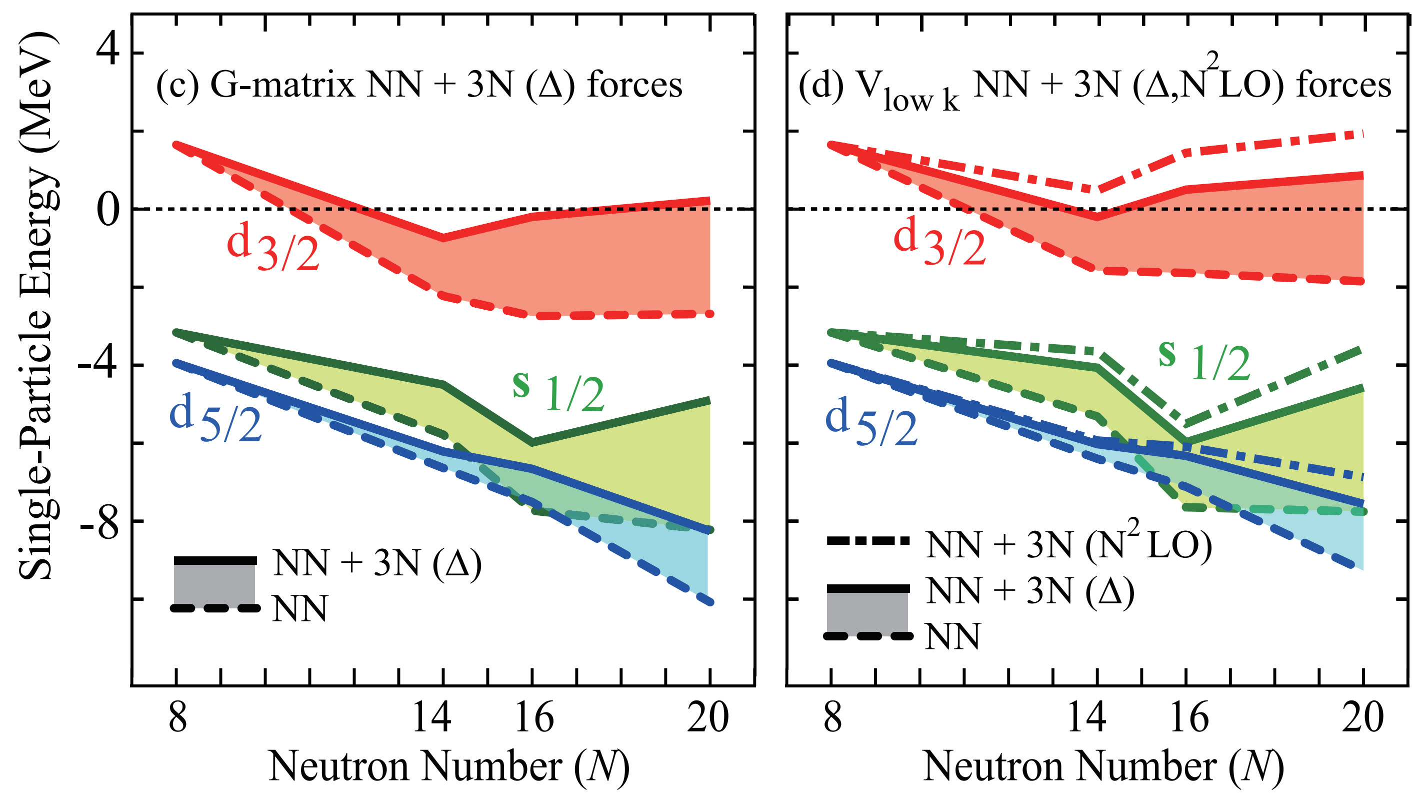
- ☑ Separate fits differs by 100 KeV,within 600 KeV of $N_{max} = 11$ result

- One-particle addition/removal energy

Ab-initio

Semi-phenomenological 3BF





AC, C. Barbieri & P. Navrátil, arXiv:1303.4900

T. Otsuka et al, PRL **105**,032501 (2010)

Results

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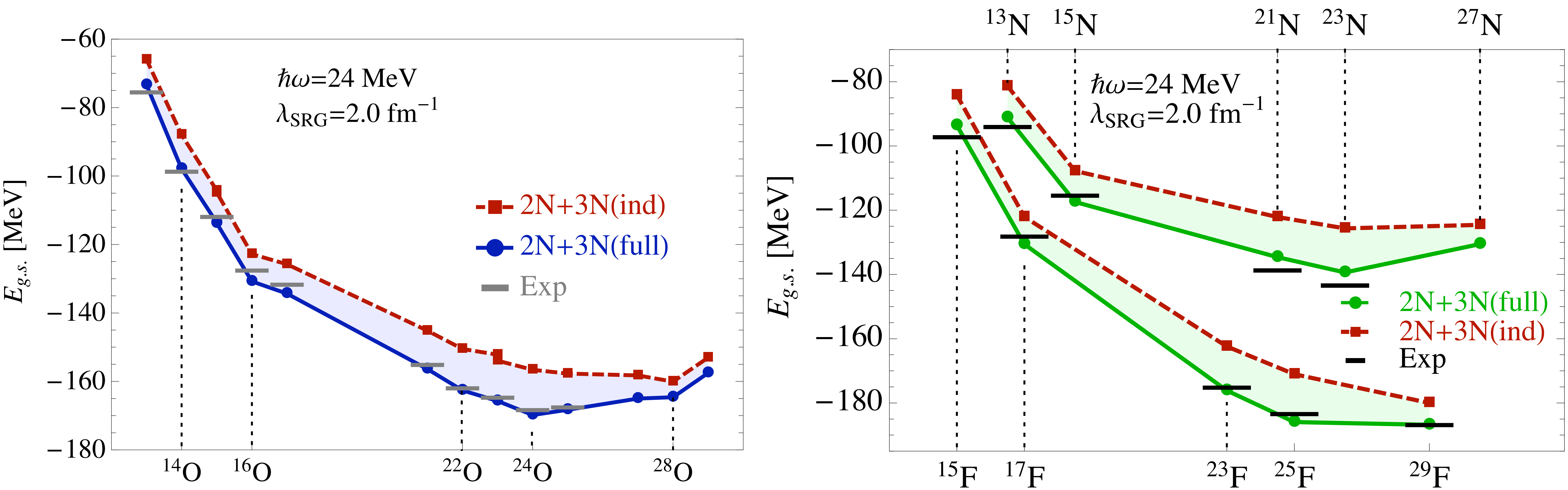
- Driplines around ^{24}O

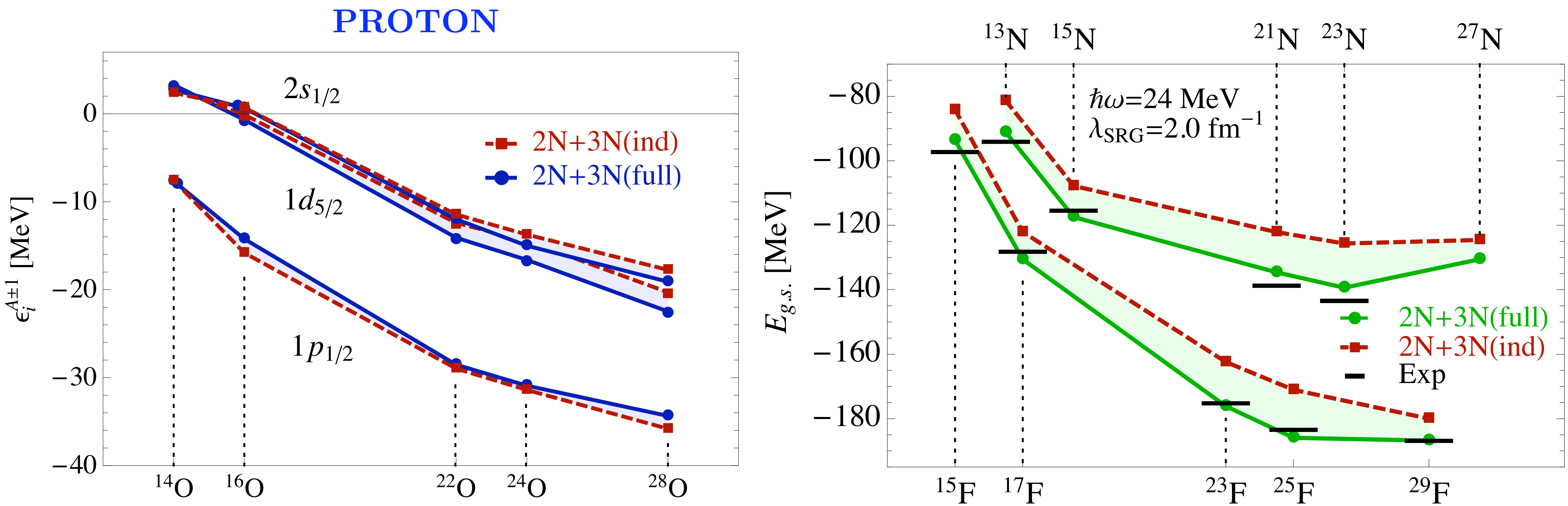


AC, C. Barbieri & P. Navrátil, arXiv:1303.4900

- ☑ Repulsive effects by filling $d_{3/2}$ shell is observed in ^{27}N, ^{28}O, ^{29}F
- ☑ The inclusion of an extra proton in ^{29}F provides enough binding energy to keep it bound

Results

Driplines around ^{24}O



AC, C. Barbieri & P. Navrátil, arXiv:1303.4900

- Repulsive effects by filling $d_{3/2}$ shell is observed in ^{27}N, ^{28}O, ^{29}F
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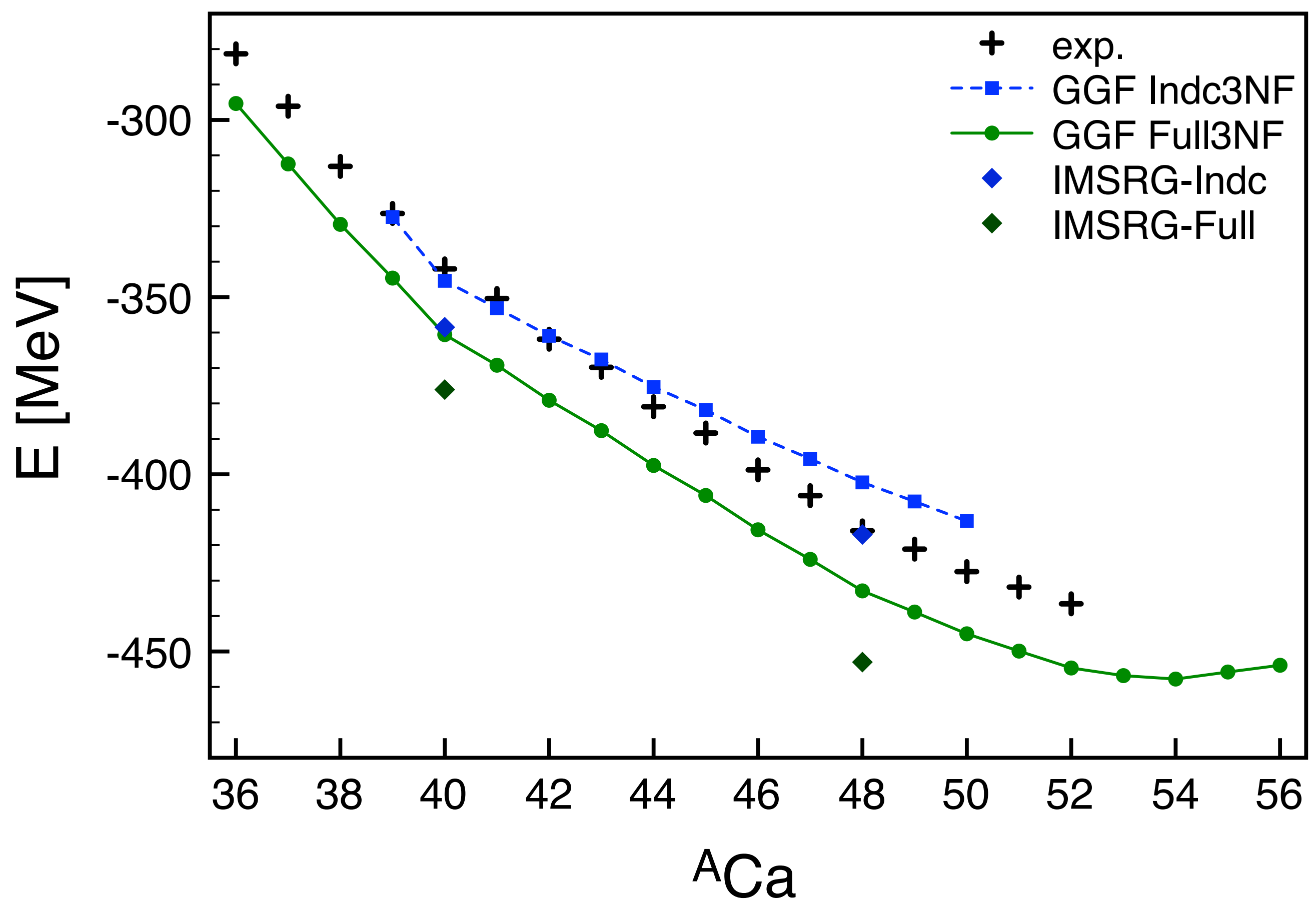
Gorkov+3NF

- 3BF in Gorkov's formalism you will see more tomorrow…



V. Somá, C. Barbieri, T. Duguet, AC, P. Navratil, in progress

Conclusions

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- Self Consistent Green function is a microscopic "ab initio" method applicable to medium mass nuclei and it is link to several (experimentally accessible) information

- The inclusion of three-body forces lead to a *significant* increase of the predictive power of SCGF. In particular it well reproduces *energies*:

  - ☑ Ground-state energies
  - ☑ Neutron drip line

Thank you for the attention!!

- This approach can be naturally extended to include many other corrections (like Coupled Cluster amplitude). Moreover the extension to *open-shell* nuclei is underway