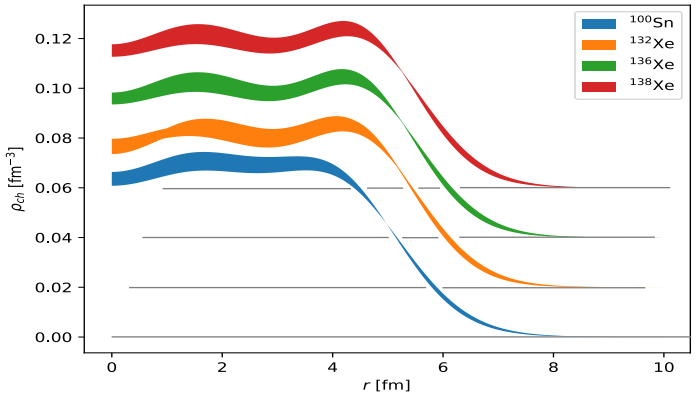
UNIVERSITÀ DEGLI STUDI DI MILANO
DIPARTIMENTO DI FISICA

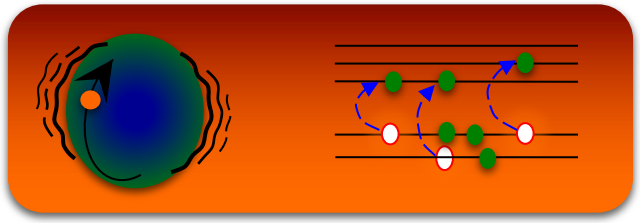
UNIVERSITY OF SURREY

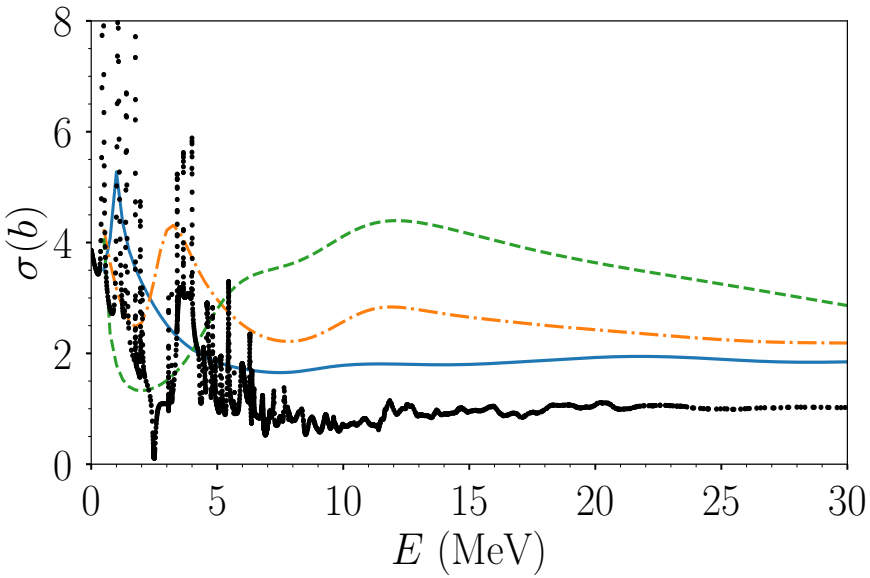
Self-consistent Green's function and other propagator-based approaches to the fermionic many-body problem

Carlo Barbieri — Università degli studi di Milano

1 February 2021







第9回国際レクチャーシリーズ(The 9th International Lecture Series)

Many-Body Green's Functions

Tentative schedule:

Lecture 1: Definitions of Many-body Green's functions (MBGFs), relation to experiment

Lecture 2: - Diagramatic expansion, Dyson eq. etc.. :
- ADC(n) formalism – how to solve it
- PV coupling (Faddeev RPA)

Lecture 3: Gorkov formalism (pairing and particle number breaking)
Many-body forces
Handling short-range repulsion

Some emphasis on the most recent computational methods

Seminar: Applications to Nuclear Physics

Many-Body Green's Functions

Many-body Green's functions (MBGF) are a set of techniques that originated in quantum field theory but have then found wide applications to the many-body problem.

In this case, the focus are complex systems such as crystals, molecules, or atomic nuclei.

Development of formalism: late 1950s/ 1960s → imported from quantum field theory

1970s – today → applications and technical developments…

Many-Body Green's Functions

Many-body Green's functions are a VAST formalism. They have a wide range of applications and contain a lot of information that is accessible from experiments.

Here we want to give an introduction:

- Teach the basic definitions and results
- Make connection with experimental quantities → gives insight into physics
- Discuss some specific application to many-bodies

Many-Body Green's Functions

- Green's functions
- Propagators
- Correlation functions

} names for the same objects

- Many-body Green's functions ← Green's functions applied to the MB problem

- Self-consistent Green's functions (SCGF) ← a particular approach to calculate GFs

Many-Body Green's Functions

Books on many-body Green's Functions:

- A. L. Fetter and J. D. Walecka, *Quantum Theory of Many-Particle Physics,* (McGraw-Hill, New York, 1971)
- A. A. Abrikosov, L. P. Gorkov and I. E. Dzyaloshinski, *Methods of Quantum Field Theory in Statistical Physics* (Dover, New York, 1975)

- W. H. Dickhoff and D. Van Neck, *Many-Body Theory Exposed!*, 2nd ed. (World Scientific, Singapore, 2007)

- R. D. Mattuck, *A Guide to Feynmnan Diagrams in the Many-Body Problem*, (McGraw-Hill, 1976) [reprinted by Dover, 1992]
- J. P. Blaizot and G. Ripka, *Quantum Theory of Finite Systems,* (MIT Press, Cambridge MA, 1986)
- J. W. Negele and H. Orland, *Quantum Many-Particle Systems,* (Benjamin, Redwood City CA, 1988)
- …

Many-Body Green's Functions

Recent reviews:

- F. Aryasetiawan and O. Gunnarsson, Rep. Prog. Phys. **61**, 237 (1998), arXiv:cond-mat/9712013. → GW method
- G. Onida, L. Reining and A. Rubio, Rev. Mod. Phys. **74**, 601 (2002). → comparison of TDDTF and GF
- H. Müther and A. Polls, Prog. Part. Nucl. Phys. **45**, 243 (2000). → Applications to
- C.B. and W. H. Dickhoff, Prog. Part. Nucl. Phys. **52**, 377 (2004). nuclear physics

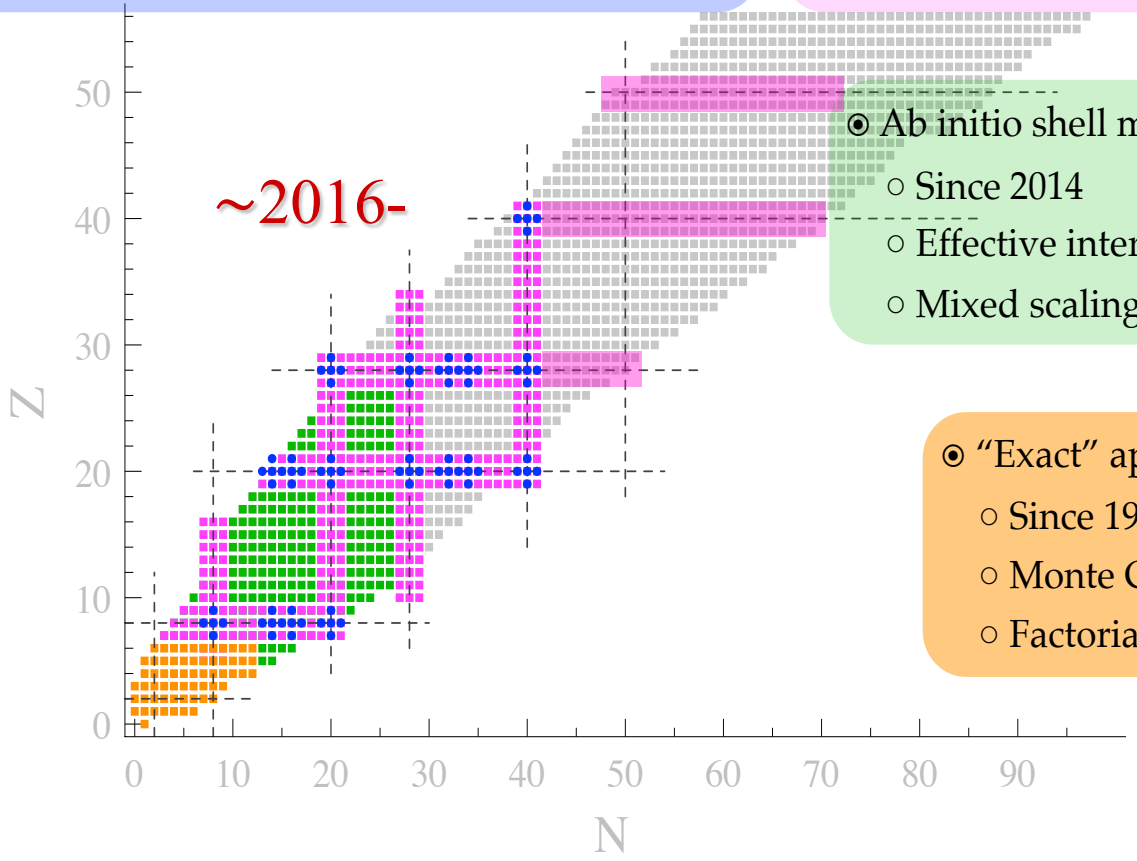
(Some) classic papers on formalism:

- G. Baym and L. P. Kadanoff, Phys. Rev. **124**, 287 (1961).
- G. Baym, Phys. Rev. **127**, 1391 (1962).
- L. Hedin, Phys. Rev. **139**, A796 (1965).
- J. Schirmer et al., Phys. Rev. A26, 2395 (1982); Phys. Rev. A28, 1237 (1983)

Reach of ab initio methods across the nuclear chart

- Approximate approaches for closed-shell nuclei
  - Since 2000's
  - SCGF, CC, IMSRG
  - Polynomial scaling

- Approximate approaches for open-shells
  - Since 2010's
  - GGF, BCC, MR-IMSRG
  - Polynomial scaling



- Ab initio shell model
  - Since 2014
  - Effective interaction via CC/IMSRG
  - Mixed scaling

- "Exact" approaches
  - Since 1980's
  - Monte Carlo, CI, …
  - Factorial scaling

Slide, courtesy of V. Somà

Key developments in *SCGF*:

Dyson ADC(2), ADC(3)
Schirmer 1982

Dyson ADC(4), ADC(5)
Schirmer 1983 (formalism)

Particle-vibration coupling, FRPA(3)
CB 2000, 2007

Gorkov ADC(2): open shells!
Somà 2011, 2013

3-nucleon forces basic formalism
Carbone, Cipollone 2013

3NFs in Dyson ADC(3)
Raimondi 2018

Gorkov ADC(3) and higher orders (automatic)
Raimoindi, Arthuis 2019

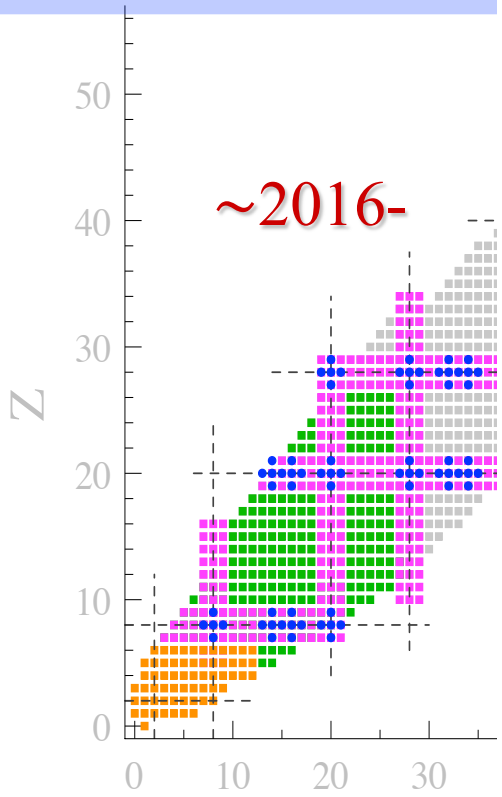
Deformation
???

Symmetry restoration
???

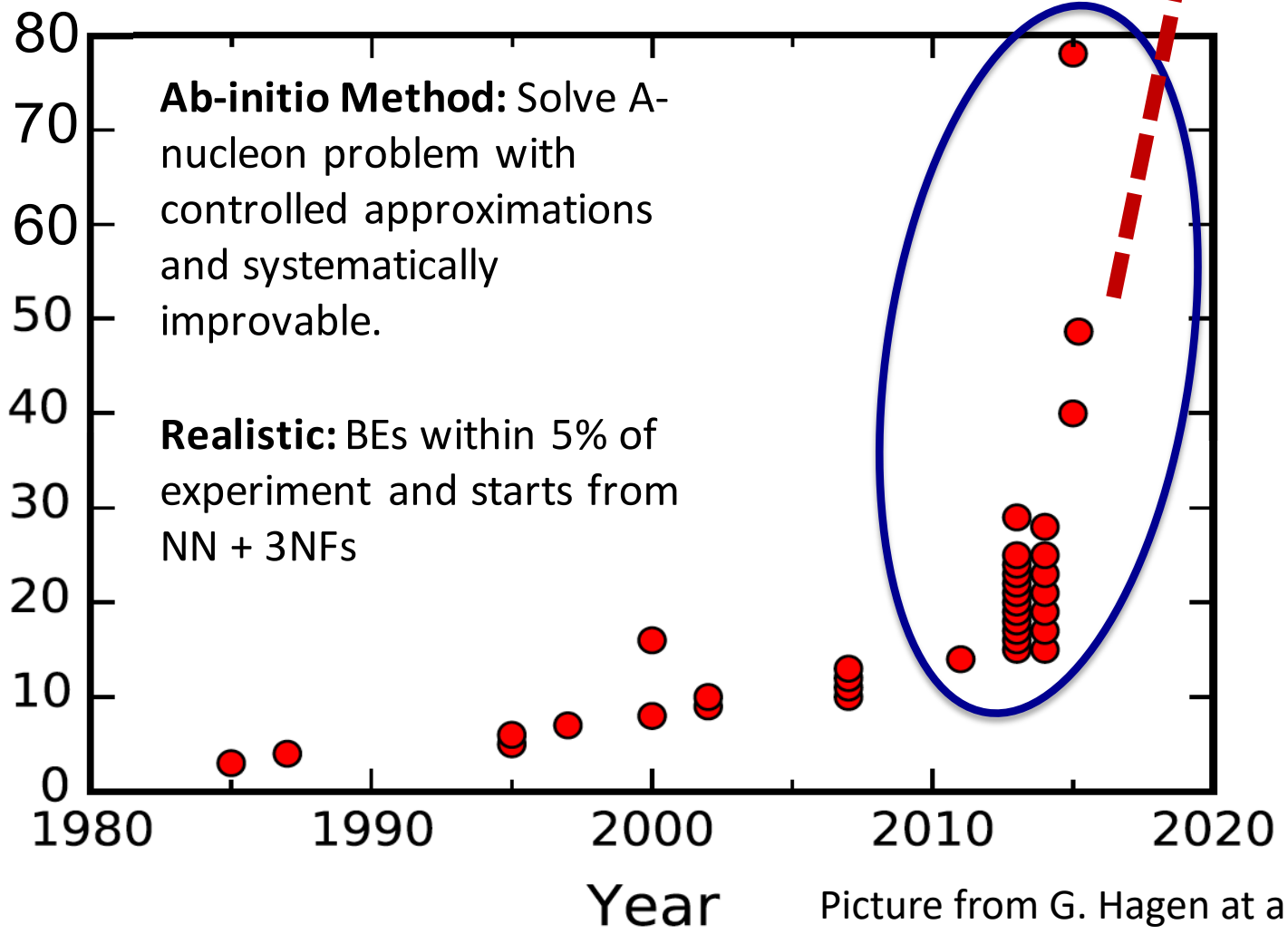
Reach of ab initio methods across the nuclear chart

- Approximate approaches for closed-shell nuclei
  - Since 2000's
  - SCGF, CC, IMSRG
  - Polynomial scaling

- Approximate approaches for open-shells
  - Since 2010's



Slide, courtesy of V. Somà



Picture from G. Hagen at al., Nature (2016)

$^{132-138}$Xe

P. Arthuis, CB, et al., Phys. Rev. Lett. **125**, 182501 (2020).

Key developments in *SCGF*:

Dyson ADC(2), ADC(3)

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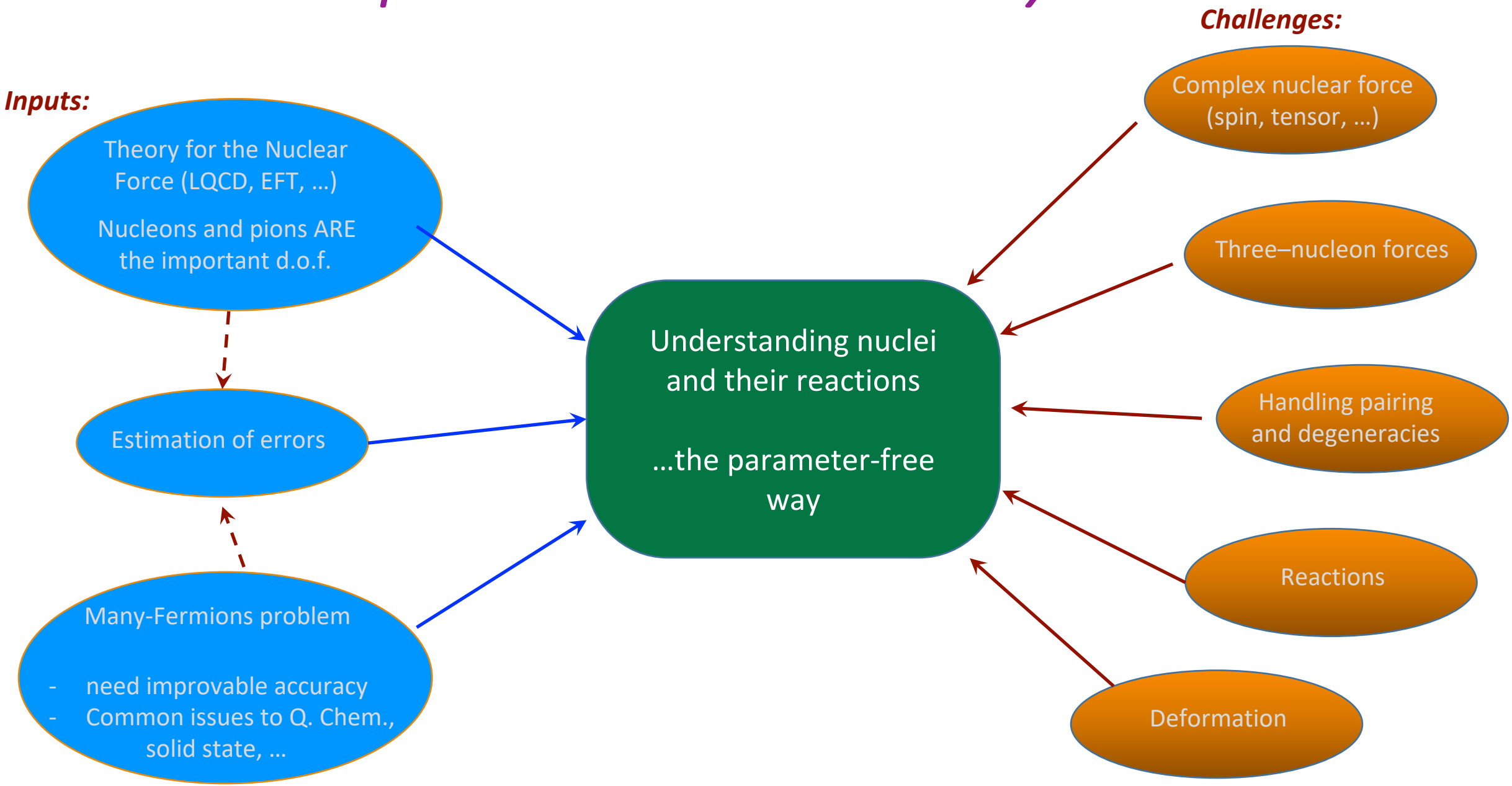
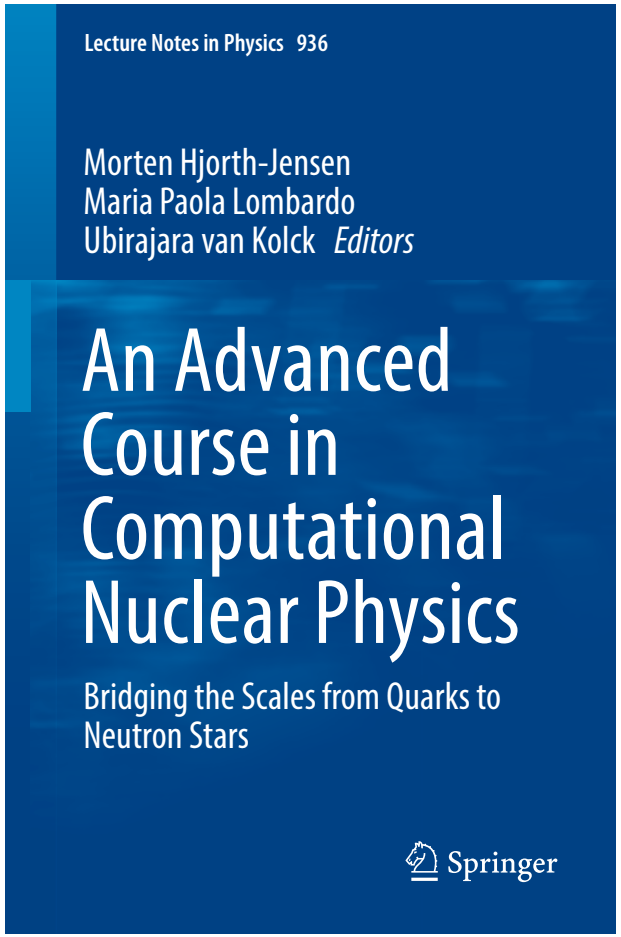
er orders (automatic)

The ab initio problem in Nuclear Physics



Ab-initio Nuclear Computation & BcDor code

Self-consistent Green's function formalism and methods for Nuclear Physics

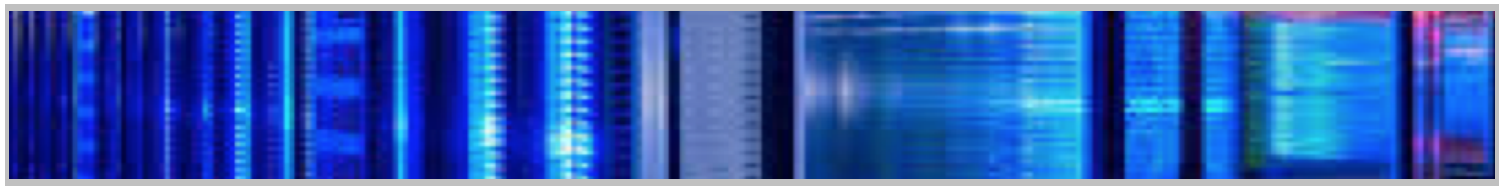


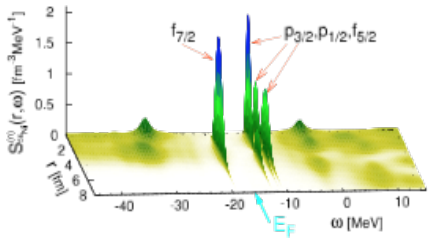
CB and A. Carbone,
chapter 11 of
Lecture Notes in Physics 936 (2017)

http://personal.ph.surrey.ac.uk/~cb0023/bcdor/

https://github.com/craolus/BoccaDorata-public

Computational Many-Body Physics





Download

Documentation

Welcome

From here you can download a public version of my self-consistent Green's function (SCGF) code for nuclear physics. This is a code in J-coupled scheme that allows the calculation of the single particle propagators (a.k.a. one-body Green's functions) and other many-body properties of spherical nuclei.

This version allows to:

- Perform Hartree-Fock calculations.
- Calculate the the correlation energy at second order in perturbation theory (MBPT2).
- Solve the Dyson equation for propagators (self consistently) up to second order in the self-energy.
- Solve coupled cluster CCD (doubles only!) equations.

When using this code you are kindly invited to follow the creative commons license agreement, as detailed at the weblinks below. In particular, we kindly ask you to refer to the publications that led the development of this software.

Relevant references (which can also help in using this code) are:

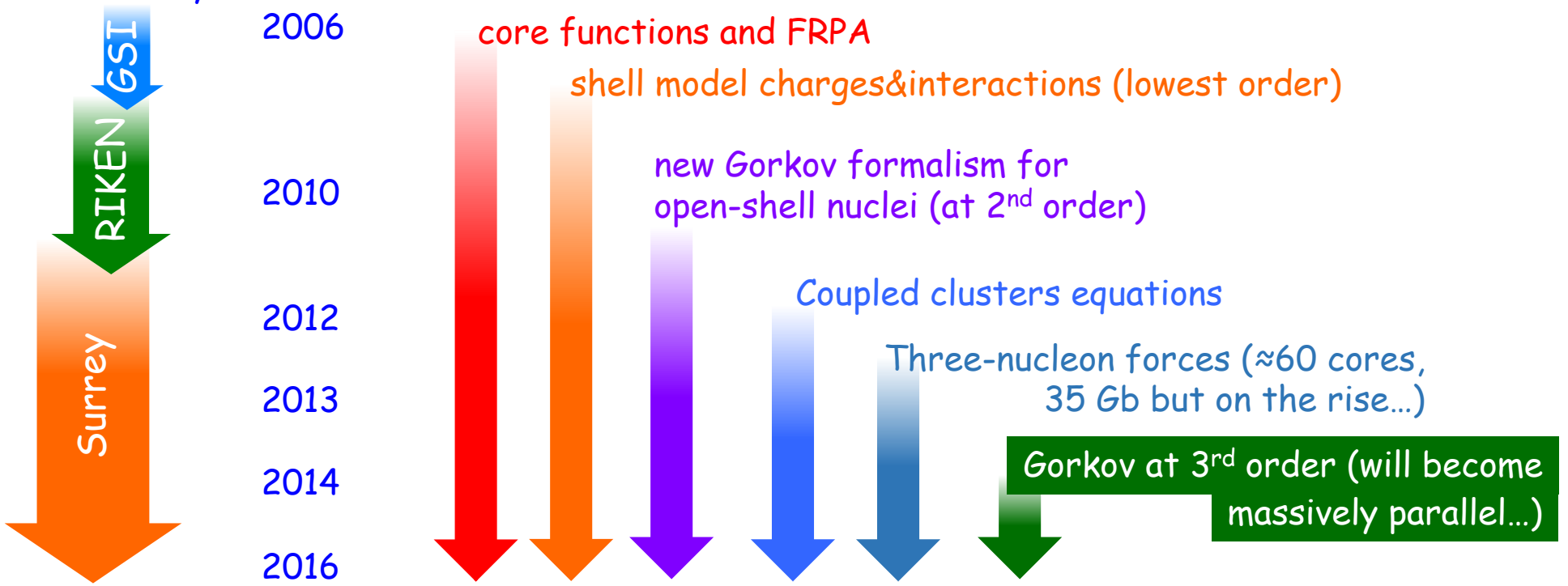
Prog. Part. Nucl. Phys. 52, p. 377 (2004),
Phys. Rev. A76, 052503 (2007),
Phys. Rev. C79, 064313 (2009),
Phys. Rev. C89, 024323 (2014)

Ab-initio Nuclear Computation & BcDor code

BoccaDorata code:
(*C. Barbieri* 2006-16
V. Somà 2010-15
A. Cipollone 2011-14)

- Provides a *C++ class library* for handling many-body propagators (≈40,000 lines, MPI&OpenMP based).
- Allows to solve for nuclear spectral functions, many-body propagators, RPA responses, coupled cluster equations and effective interaction/charges for the shell model.

Code history:



Propagating a free particle

Consider a free particle with Hamiltonian

$h_1 = t + U(r)$

the eigenstates and egienenergies are $h_1|\phi_n\rangle = \varepsilon_n|\phi_n\rangle$

The time evolution is

$$i\hbar\frac{d}{dt}|\psi(t)\rangle = h_1|\psi(t)\rangle \rightarrow |\psi(t)\rangle = e^{-ih_1 t/\hbar}|\psi_{tr}\rangle$$

$$\langle \mathbf{r}|\psi(t)\rangle = \langle \mathbf{r}|e^{-ih_1 t/\hbar}|\psi_{tr}\rangle = \int d\mathbf{r}'\langle \mathbf{r}|e^{-ih_1 t/\hbar}|\mathbf{r}'\rangle\langle \mathbf{r}'|\psi_{tr}\rangle$$

with:

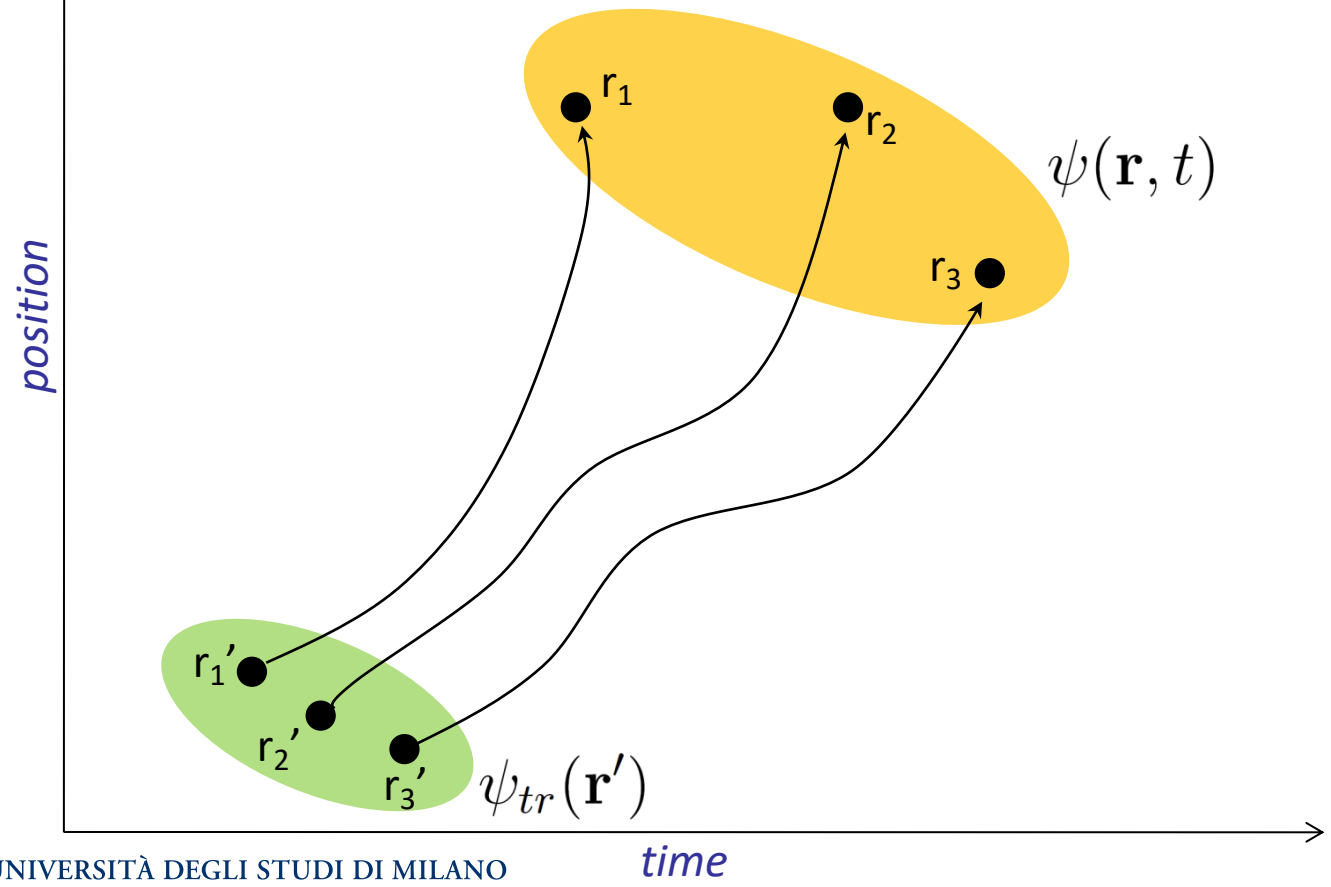
$\langle \mathbf{r}|\psi_{tr}\rangle$ wave fnct. at t=0

$\langle \mathbf{r}|\psi(t)\rangle$ wave fnct. at time t

Propagating a free particle

Green's function (=propagator) for a free particle:

$$G(\mathbf{r},\mathbf{r}';t) \equiv \langle \mathbf{r}| e^{-ih_1 t/\hbar} |\mathbf{r}'\rangle$$



$$\langle \mathbf{r}|\psi(t)\rangle = \int d\mathbf{r}' G(\mathbf{r},\mathbf{r}';t)\psi_{tr}(\mathbf{r}')$$

Propagating a free particle

Green's function (=propagator) for a free particle:

$$G(\mathbf{r},\mathbf{r}';t) \equiv \langle \mathbf{r}|e^{-ih_1 t/\hbar}|\mathbf{r}'\rangle$$

$$= \sum_n \underbrace{\langle \mathbf{r}|\phi_n\rangle e^{-i\varepsilon_n t/\hbar}\langle \phi_n|\mathbf{r}'\rangle}$$

Fourier transform
of the eigenspectrum*!*

$\langle \mathbf{r}|\phi_n\rangle$ → states

ε_n → energies

The spectrum of the Hamiltonian is separated by the FT because the time evolution is driven by H: $e^{-iH(t-t_0)/\hbar}$

Definitions of Green's functions

- Take a generic the Hamiltonian H and its static Schrödinger equation

$$H = H_0 + V$$

$$H\,|\Psi_n^N\rangle \;=\; E_n^N\,|\Psi_n^N\rangle$$

- We evolve in time the field operators instead of the wave function by using the Heisenberg picture

$$\psi_s^\dagger(\mathbf{r},t) = e^{iHt/\hbar}\;\psi_s^\dagger(\mathbf{r})\;e^{-iHt/\hbar}$$

$$\psi_s(\mathbf{r},t) = e^{iHt/\hbar}\;\psi_s(\mathbf{r})\;e^{-iHt/\hbar}$$

- (→ creation/annihilation of a particle in $\vec{r}$ at time t)

Definitions of Green's functions

- The one body propagator (≡Green's function) associated to the ground state is defined as $|\Psi_0^N\rangle$

$$g_{ss'}(\mathbf{r},t;\mathbf{r}',t') = -\frac{i}{\hbar}\langle\Psi_0^N|T[\psi_s(\mathbf{r},t)\psi_{s'}^\dagger(\mathbf{r}',t')]|\Psi_0^N\rangle$$

- with the time ordering operator

$$T[\psi_s(\mathbf{r},t)\psi_{s'}^\dagger(\mathbf{r}',t')] = \begin{cases} \psi_s(\mathbf{r},t)\psi_{s'}^\dagger(\mathbf{r}',t') , & t > t' \text{ adds a particle} \\ \pm\psi_{s'}^\dagger(\mathbf{r}',t')\psi_s(\mathbf{r},t) , & t' > t \text{ removes a particle} \end{cases}$$

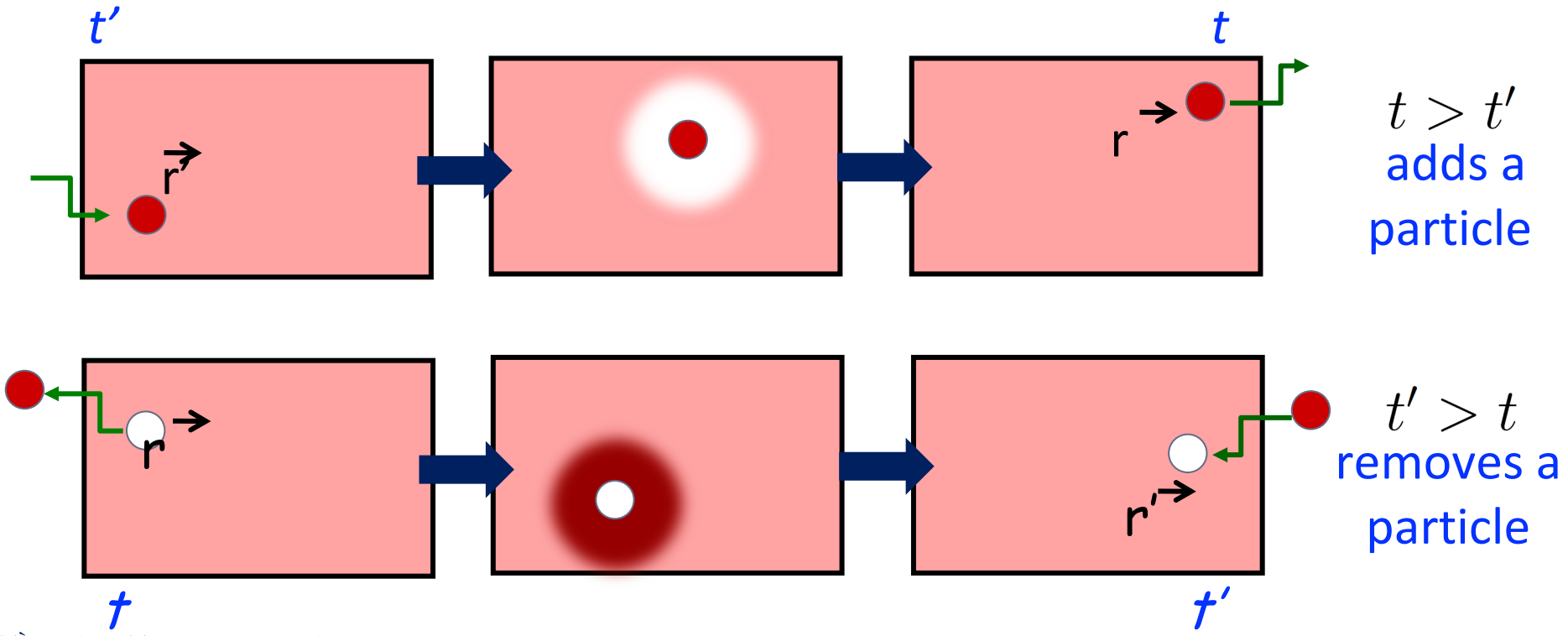
(+ for bosons,
- for fermions)

- Expand t-dep in operators: $\psi_s(\mathbf{r},t) = e^{iHt/\hbar}\,\psi_s(\mathbf{r})\,e^{-iHt/\hbar}$ →

Definitions of Green's functions

- With explicit time dependence:

$$g_{ss'}(\mathbf{r},\mathbf{r}';t-t') = -\frac{i}{\hbar}\theta(t-t')\langle\Psi_0^N|\psi_s(\mathbf{r})e^{-i(H-E_0^N)(t-t')/\hbar}\psi_{s'}^\dagger(\mathbf{r}')|\Psi_0^N\rangle$$
$$\mp\frac{i}{\hbar}\theta(t'-t)\langle\Psi_0^N|\psi_{s'}^\dagger(\mathbf{r}')e^{i(H-E_0^N)(t-t')/\hbar}\psi_s(\mathbf{r})|\Psi_0^N\rangle$$



Definitions of Green's functions

- Green's function can be defined in *any* single-particle basis (not just **r** or **k** space). So let's call {**α**} a general orthonormal basis with wave functions {$u_\alpha(\mathbf{r})$}

$$\psi^\dagger(\mathbf{r}) = \sum_\alpha c_\alpha^\dagger u_\alpha^*(\mathbf{r})$$

- The Heisenberg operators are:

$$c_\alpha^\dagger(t) = e^{iHt/\hbar}\, c_\alpha^\dagger\, e^{-iHt/\hbar}$$
$$c_\alpha(t) = e^{iHt/\hbar}\, c_\alpha\, e^{-iHt/\hbar}$$

- and

$$g_{ss'}(\mathbf{r},t;\mathbf{r}',t') = \sum_{\alpha\beta} u_\alpha(\mathbf{r},s) g_{\alpha\beta}(t,t') u_\beta^*(\mathbf{r}',s')$$

Definitions of Green's functions

- In general it is possible to define propagators for more particles and different times:

$$g_{\alpha\beta}^{2-pt}(t,t') = -\frac{i}{\hbar}\langle \Psi_0^N | T[c_\alpha(t) c_\beta^\dagger(t')] | \Psi_0^N \rangle$$

$$g_{\alpha\beta,\gamma\delta}^{4-pt}(t_1,t_2;t_1',t_2') = -\frac{i}{\hbar}\langle \Psi_0^N | T[c_\beta(t_2) c_\alpha(t_1) c_\gamma^\dagger(t_1') c_\delta^\dagger(t_2')] | \Psi_0^N \rangle$$

$$g_{\alpha\beta\gamma,\mu\nu\lambda}^{6-pt}(t_1,t_2,t_3;t_1',t_2',t_3') =$$
$$-\frac{i}{\hbar}\langle \Psi_0^N | T[c_\gamma(t_3) c_\beta(t_2) c_\alpha(t_1) c_\mu^\dagger(t_1') c_\nu^\dagger(t_2') c_\lambda^\dagger(t_3')] | \Psi_0^N \rangle$$

$$\vdots$$

Definitions of Green's functions

Graphic conventions:

$\equiv g_{\alpha\beta}(t>t')$
(quasi)particle

$\equiv g_{\alpha\beta}(t'>t)$
(quasi)hole

$$g^{4-pt}_{\alpha\beta,\gamma\delta}(t_1,t_2;t_1',t_2') = -\frac{i}{\hbar}\langle\Psi_0^N|T[c_\beta(t_2)c_\alpha(t_1)c_\gamma^\dagger(t_1')c_\delta^\dagger(t_2')]|\Psi_0^N\rangle$$

Definitions of Green's functions

Graphic conventions:

$\equiv g_{\alpha\beta}(t>t')$
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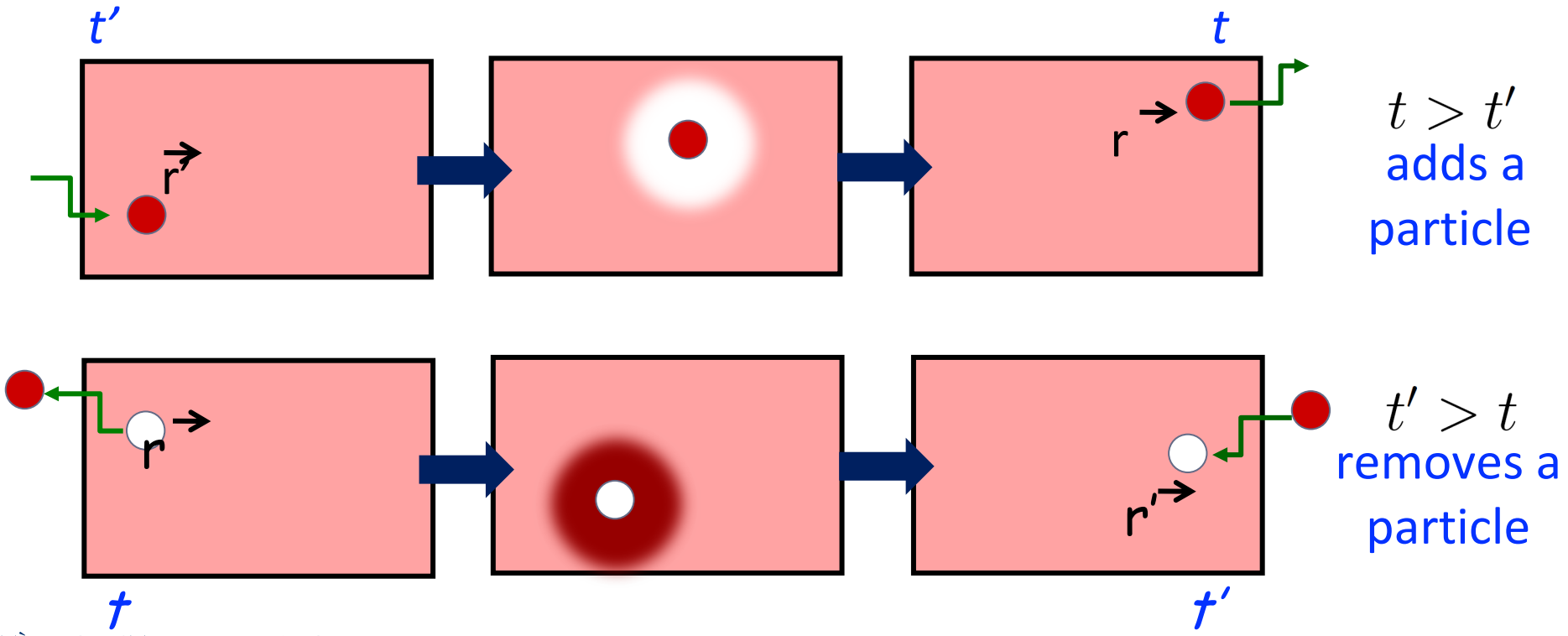
$$g^{4-pt}_{\alpha\beta,\gamma\delta}(t_1,t_2;t_1',t_2') = -\frac{i}{\hbar}\langle\Psi_0^N|T[c_\beta(t_2)c_\alpha(t_1)c_\gamma^\dagger(t_1')c_\delta^\dagger(t_2')]|\Psi_0^N\rangle$$

Definitions of Green's functions

- With explicit time dependence:

$$g_{ss'}(\mathbf{r},\mathbf{r}';t-t') = -\frac{i}{\hbar}\theta(t-t')\langle\Psi_0^N|\psi_s(\mathbf{r})e^{-i(H-E_0^N)(t-t')/\hbar}\psi_{s'}^\dagger(\mathbf{r}')|\Psi_0^N\rangle$$
$$\mp\frac{i}{\hbar}\theta(t'-t)\langle\Psi_0^N|\psi_{s'}^\dagger(\mathbf{r}')e^{i(H-E_0^N)(t-t')/\hbar}\psi_s(\mathbf{r})|\Psi_0^N\rangle$$



Lehmann representation and spectral function

- Expand on the eigenstates of N±1

$$
\begin{aligned}
g_{\alpha\beta}(t-t') &= -\frac{i}{\hbar}\theta(t-t')\langle\Psi_0^N|c_\alpha e^{-i(H-E_0^N)(t-t')/\hbar}c_\beta^\dagger|\Psi_0^N\rangle \\
&\quad \mp\frac{i}{\hbar}\theta(t'-t)\langle\Psi_0^N|c_\beta^\dagger e^{i(H-E_0^N)(t-t')/\hbar}c_\alpha|\Psi_0^N\rangle \\
&= -\frac{i}{\hbar}\theta(t-t')\sum_n\langle\Psi_0^N|c_\alpha|\Psi_n^{N+1}\rangle\langle\Psi_n^{N+1}|c_\beta^\dagger|\Psi_0^N\rangle\, e^{-i(E_n^{N+1}-E_0^N)(t-t')/\hbar} \\
&\quad \mp\frac{i}{\hbar}\theta(t'-t)\sum_k\langle\Psi_0^N|c_\beta^\dagger|\Psi_k^{N-1}\rangle\langle\Psi_k^{N-1}|c_\alpha|\Psi_0^N\rangle\, e^{i(E_k^{N-1}-E_0^N)(t-t')/\hbar}
\end{aligned}
$$

(- bosons, + fermions)

- → Fourier transform to energy representation…

$$g_{\alpha\beta}(\omega) = \int d\tau e^{i\omega\tau} g_{\alpha\beta}(\tau)$$

$$\theta(\pm\tau) = \mp \lim_{\eta\to 0^+} \frac{1}{2\pi i}\int_{-\infty}^{+\infty} d\omega \frac{e^{-i\omega\tau}}{\omega \pm i\eta}$$

Lehmann representation and spectral function

The *Lehman* representation of $g_{\alpha\beta}(\omega)$ is:

$$g_{\alpha\beta}(\omega) = \sum_n \frac{\langle \Psi_0^N | c_\alpha | \Psi_n^{N+1} \rangle \langle \Psi_n^{N+1} | c_\beta^\dagger | \Psi_0^N \rangle}{\hbar\omega - (E_n^{N+1} - E_0^N) + i\eta} \quad \leftarrow \textit{(quasi)particles}$$

$$\mp \sum_k \frac{\langle \Psi_0^N | c_\beta^\dagger | \Psi_k^{N-1} \rangle \langle \Psi_k^{N-1} | c_\alpha | \Psi_0^N \rangle}{\hbar\omega - (E_0^N - E_k^{N-1}) - i\eta} \quad \leftarrow \textit{(quasi)holes}$$

Poles → energy absorbed/released in particle transfer

Residues: $|\langle \Psi_n^{N+1} | c_\alpha^\dagger | \Psi_0^N \rangle|^2$ particle addition

$|\langle \Psi_k^{N-1} | c_\alpha | \Psi_0^N \rangle|^2$ particle ejected

Lehmann representation and spectral function

The *Lehman* representation of $g_{\alpha\beta}(\omega)$ is:

$$g_{\alpha\beta}(\omega) = \sum_n \frac{\langle \Psi_0^N | c_\alpha | \Psi_n^{N+1} \rangle \langle \Psi_n^{N+1} | c_\beta^\dagger | \Psi_0^N \rangle}{\hbar\omega - (E_n^{N+1} - E_0^N) + i\eta} \quad \leftarrow \textit{(quasi)particles}$$

$$\mp \sum_k \frac{\langle \Psi_0^N | c_\beta^\dagger | \Psi_k^{N-1} \rangle \langle \Psi_k^{N-1} | c_\alpha | \Psi_0^N \rangle}{\hbar\omega - (E_0^N - E_k^{N-1}) - i\eta} \quad \leftarrow \textit{(quasi)holes}$$

(- bosons,
+ fermions)

To extract the imaginary part:

$$\frac{1}{x \pm i\eta} = \mathcal{P}\frac{1}{x} \mp i\pi\delta(x)$$

Lehmann representation and spectral function

The spectral function is the Im part of $g_{\alpha\beta}(\omega)$

$$S_{\alpha\beta}(\omega) = S^p_{\alpha\beta}(\omega) + S^h_{\alpha\beta}(\omega)$$

$$\begin{aligned} S^p_{\alpha\beta}(\omega) &= -\frac{1}{\pi}\,\mathrm{Im}\; g^p_{\alpha\beta}(\omega) \qquad \leftarrow \textit{(quasi)particles} \\ &= \sum_n \langle \Psi_0^N | c_\alpha | \Psi_n^{N+1} \rangle \langle \Psi_n^{N+1} | c_\beta^\dagger | \Psi_0^N \rangle \; \delta\left(\hbar\omega - (E_n^{N+1} - E_0^N)\right) \end{aligned}$$

$$\begin{aligned} S^h_{\alpha\beta}(\omega) &= \frac{1}{\pi}\,\mathrm{Im}\; g^h_{\alpha\beta}(\omega) \qquad \leftarrow \textit{(quasi)holes} \\ &= \mp \sum_k \langle \Psi_0^N | c_\beta^\dagger | \Psi_k^{N-1} \rangle \langle \Psi_k^{N-1} | c_\alpha | \Psi_0^N \rangle \; \delta\left(\hbar\omega - (E_0^N - E_k^{N-1})\right) \end{aligned}$$

(- bosons,
+ fermions)

→ *Contains the same information as the Lehmann rep.*

Lehmann representation and spectral function

- $g_{\alpha\beta}(\omega)$ is fully constrained by its imaginary part:

$$g_{\alpha\beta}(\omega) = \int d\omega' \frac{S^p_{\alpha\beta}(\omega')}{\omega - \omega' + i\eta} + \int d\omega' \frac{S^h_{\alpha\beta}(\omega')}{\omega - \omega' - i\eta}$$

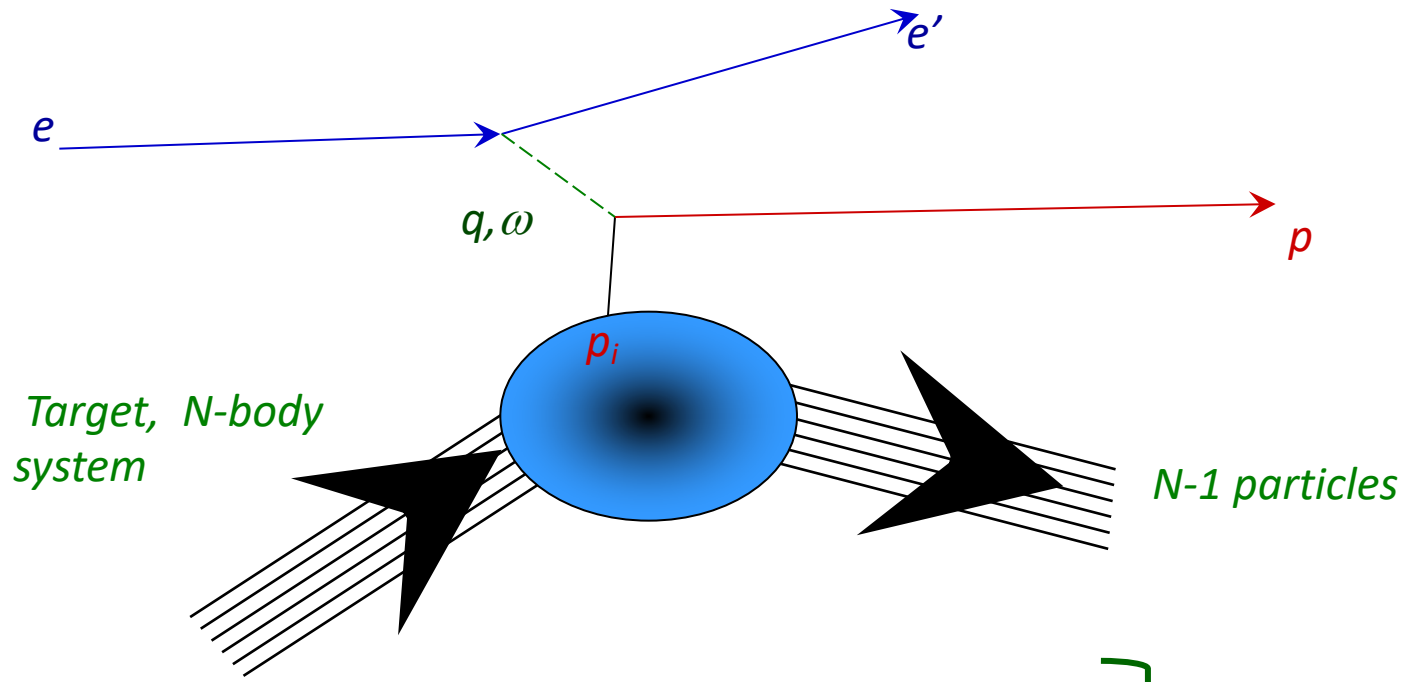
Why many-body Green's functions??

- "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

Spectroscopy via knock out reactions - basic idea

Use a probe (ANY probe) to eject the particle we are interested to:



Basic idea:

- we know, e, e' and p
- "get" *energy and momentum* of p_i: $p_i = k_e' + k_p - k_e$

$$E_i = E_e' + E_p - E_e$$

Better to choose large transferred momentum and weak probes*!!!*

Knock-out processes

- Initial state: $|\Psi_i\rangle = |\Psi_0^N\rangle$
- Final state: $|\Psi_f\rangle = a_{\boldsymbol{p}}^\dagger |\Psi_n^{N-1}\rangle$ ← particle flying out, better if interacting as little as possible with the rest of the system
- Prob $\rho(\boldsymbol{q}) = \sum_{j=1}^{N} \exp\left(i\boldsymbol{q}\cdot\boldsymbol{r}_j\right)$ ← This can be anything: it *transfers* energy, and momentum q to the system; it's the simplest model for such a probe

$$\hat{\rho}(\boldsymbol{q}) = \sum_{\boldsymbol{p},\boldsymbol{p}'} \langle \boldsymbol{p}| \exp\left(i\boldsymbol{q}\cdot\boldsymbol{r}\right)|\boldsymbol{p}'\rangle a_{\boldsymbol{p}}^\dagger a_{\boldsymbol{p}'} = \sum_{\boldsymbol{p}} a_{\boldsymbol{p}}^\dagger a_{\boldsymbol{p}-\boldsymbol{q}} \quad ; \qquad \langle \mathbf{r}|\mathbf{p}\rangle = \frac{1}{(2\pi)^{3/2}} e^{-i\mathbf{r}\mathbf{p}/\hbar}$$

Knock-out processes

$$\hat{\rho}(\boldsymbol{q}) = \sum_{\boldsymbol{p},\boldsymbol{p}'} \langle \boldsymbol{p}| \exp\left(i\boldsymbol{q}\cdot\boldsymbol{r}\right)|\boldsymbol{p}'\rangle a^{\dagger}_{\boldsymbol{p}} a_{\boldsymbol{p}'} = \sum_{\boldsymbol{p}} a^{\dagger}_{\boldsymbol{p}} a_{\boldsymbol{p}-\boldsymbol{q}}$$

- Transition matrix element:

$$\begin{aligned}
\langle \Psi_f|\hat{\rho}(\boldsymbol{q})|\Psi_i\rangle &= \sum_{\boldsymbol{p}'} \langle \Psi^{N-1}_n|a_{\boldsymbol{p}} a^{\dagger}_{\boldsymbol{p}'} a_{\boldsymbol{p}'-\boldsymbol{q}}|\Psi^{N}_0\rangle \\
&= \sum_{\boldsymbol{p}'} \langle \Psi^{N-1}_n|\delta_{\boldsymbol{p}',\boldsymbol{p}} a_{\boldsymbol{p}'-\boldsymbol{q}} + a^{\dagger}_{\boldsymbol{p}'} a_{\boldsymbol{p}'-\boldsymbol{q}} a_{\boldsymbol{p}}|\Psi^{N}_0\rangle \\
&\approx \langle \Psi^{N-1}_n|a_{\boldsymbol{p}-\boldsymbol{q}}|\Psi^{N}_0\rangle .
\end{aligned}$$

Impulse Approximation (IA) means throwing away this part. If the particle is ejected with very high momentum transfer, it is usually a good approximation

Knock-out processes

$$H_N = \sum_{i=1}^{N} \frac{\boldsymbol{p}_i^2}{2m} + \sum_{i<j=1}^{N} V(i,j) = H_{N-1} + \frac{\boldsymbol{p}_N^2}{2m} + \sum_{i=1}^{N-1} V(i,N)$$

$$|\Psi_f\rangle = a_{\boldsymbol{p}}^{\dagger} |\Psi_n^{N-1}\rangle$$

← The plane wave approximation assumes the flies out without interacting with the rest of the system. This is OK in some cases. In others, one has to worry about the distortion due to final state interactions.

Knock-out processes

- Use the Fermi Golden rule:

$$d\sigma \sim \sum_n \delta(\omega + E_i - E_f)|\langle \Psi_f|\hat{\rho}(\boldsymbol{q})|\Psi_i\rangle|^2$$

- "missing" momentu $\boldsymbol{p}_{miss} = \boldsymbol{p} - \boldsymbol{q}$
- "missing" energy $E_{miss} = \boldsymbol{p}^2/2m - \omega = E_0^N - E_n^{N-1}$

Interpreted as *energy* and *momentum* of initial particle*!!*

- In plane wave impulse approximation (PWIA):

$$d\sigma \sim \sum_n \delta(E_{miss} - E_0^N + E_n^{N-1})|\langle \Psi_n^{N-1}|a_{\boldsymbol{p}_{miss}}|\Psi_0^N\rangle|^2$$

$$d\sigma = \sigma_{probe}\ S^h(\boldsymbol{p}_{miss}, E_{miss})$$

PWIA is not always justified, but it is all OK for our display purposes: Can "see" the spectral fnct.!!!

One-hole spectral function

Overlap function:

$$\psi_k^{overlap}(\mathbf{r}) \quad = \quad \langle \Psi_k^{N-1} | \psi_s(\mathbf{r}) | \Psi_0^N \rangle$$

Spectroscopic factor:

$$S_k = \int d\mathbf{r} |\psi_k^{overlap}(\mathbf{r})|^2$$

= 1 , for free fermions
< 1 , for interacting particles (correlations!!)

$$S^h(\mathbf{p},\omega) = \sum_k \left| \langle \Psi_k^{N-1} | \psi_k(\mathbf{p}) | \Psi_0^N \rangle \right|^2 \delta\left(\hbar\omega - (E_0^N - E_k^{N-1})\right)$$

Integrate S^h over ***p*** : → spectral strength distribution

Integrate S^h over ω : → momentum distribution

Knock-out processes

So, I can "see" $S^h(\mathbf{p},\omega)$:

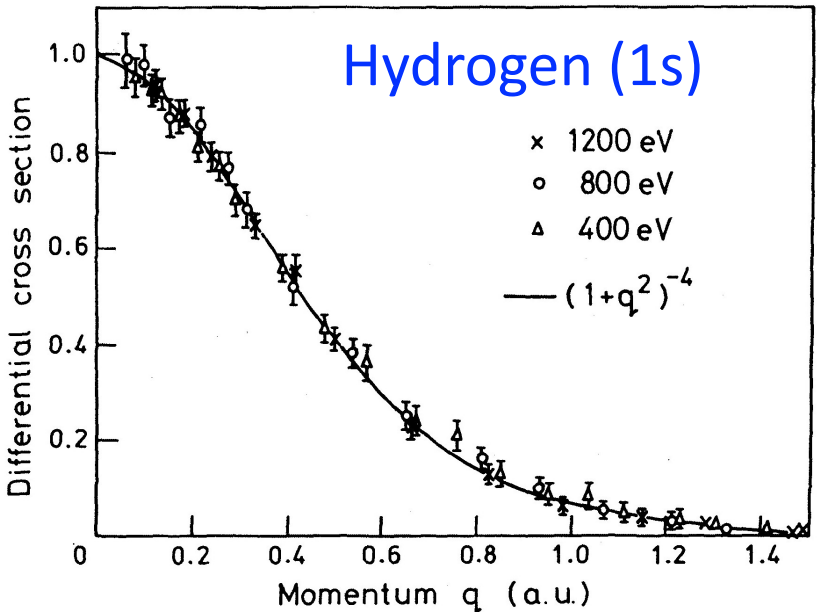
$$d\sigma = \sigma_{probe}\ S^h(\boldsymbol{p}_{miss}, E_{miss})$$

x-sec for scattering on
a free particle

PWIA is not always justified, but it is all OK for our display purposes: Can "see" the spectralfnct.!!!

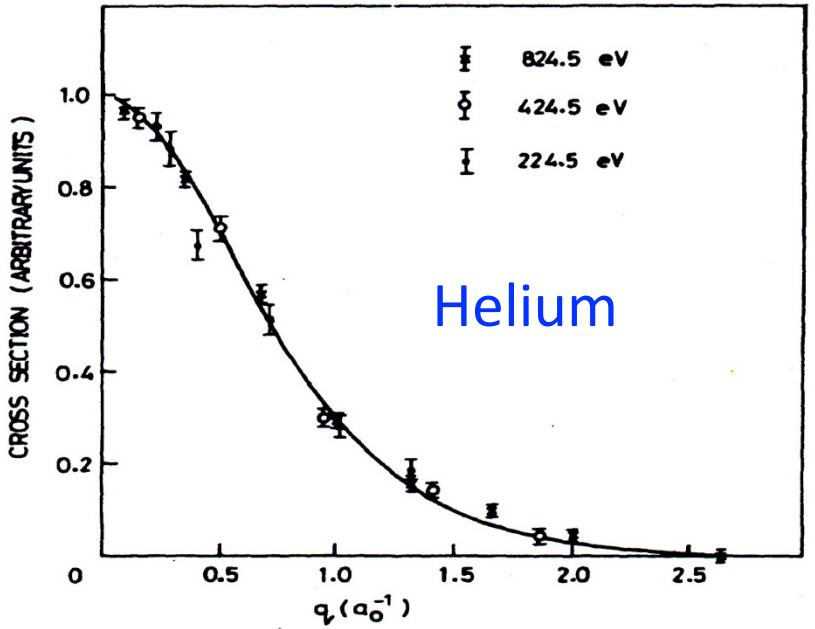
…does it really work ?!?!?!?

electron knock out in atoms by (e,2e)



$$\varphi_{1s}(q) = 2^{3/2}\pi \frac{1}{(1+q^2)^2} 3$$

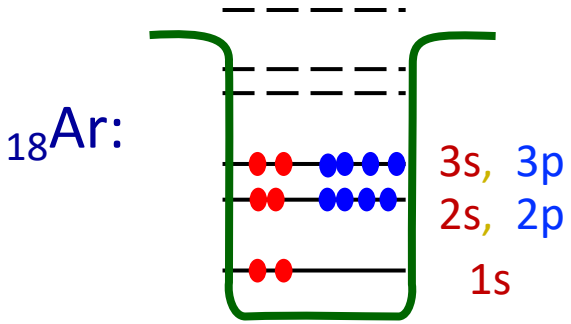
Hydrogen 1s wave function "seen" experimentally
Phys. Lett. 86A, 139 (1981)



And so on for other atoms…

Helium in Phys. Rev. A8, 2494 (1973)

electron knock out in atoms by (e,2e)



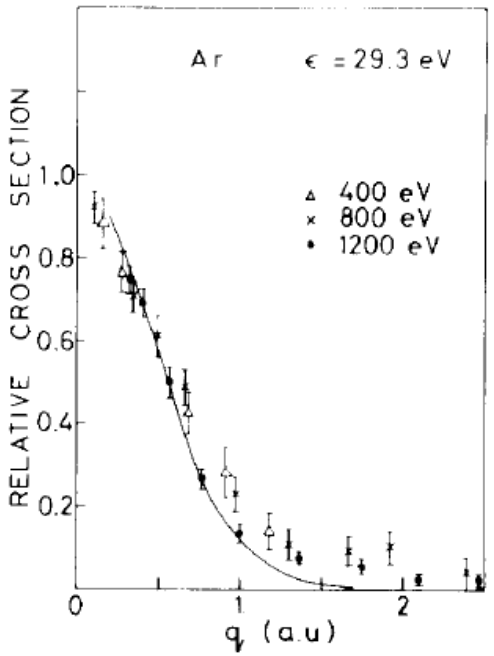


Fig. 9.3. The distribution of recoil momenta q for the 29.3 eV (3s) transition in argon at 400 eV (triangles), 800 eV (crosses)

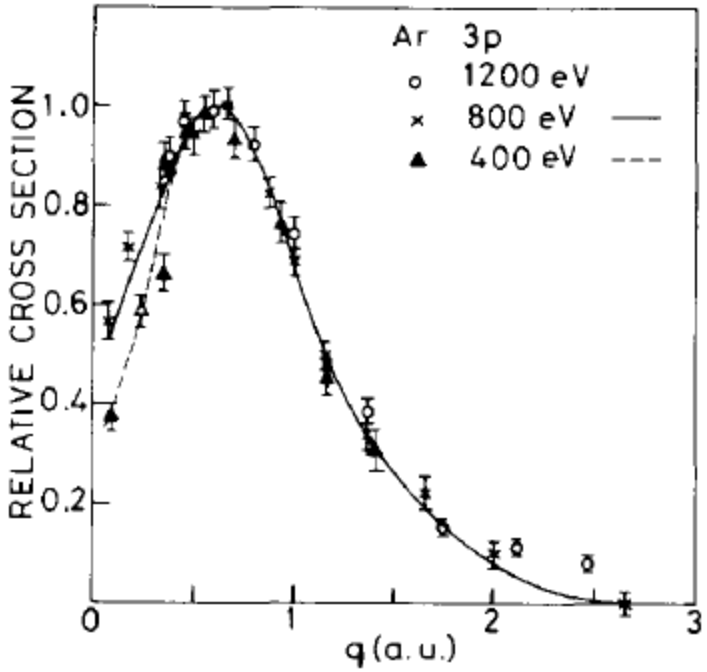
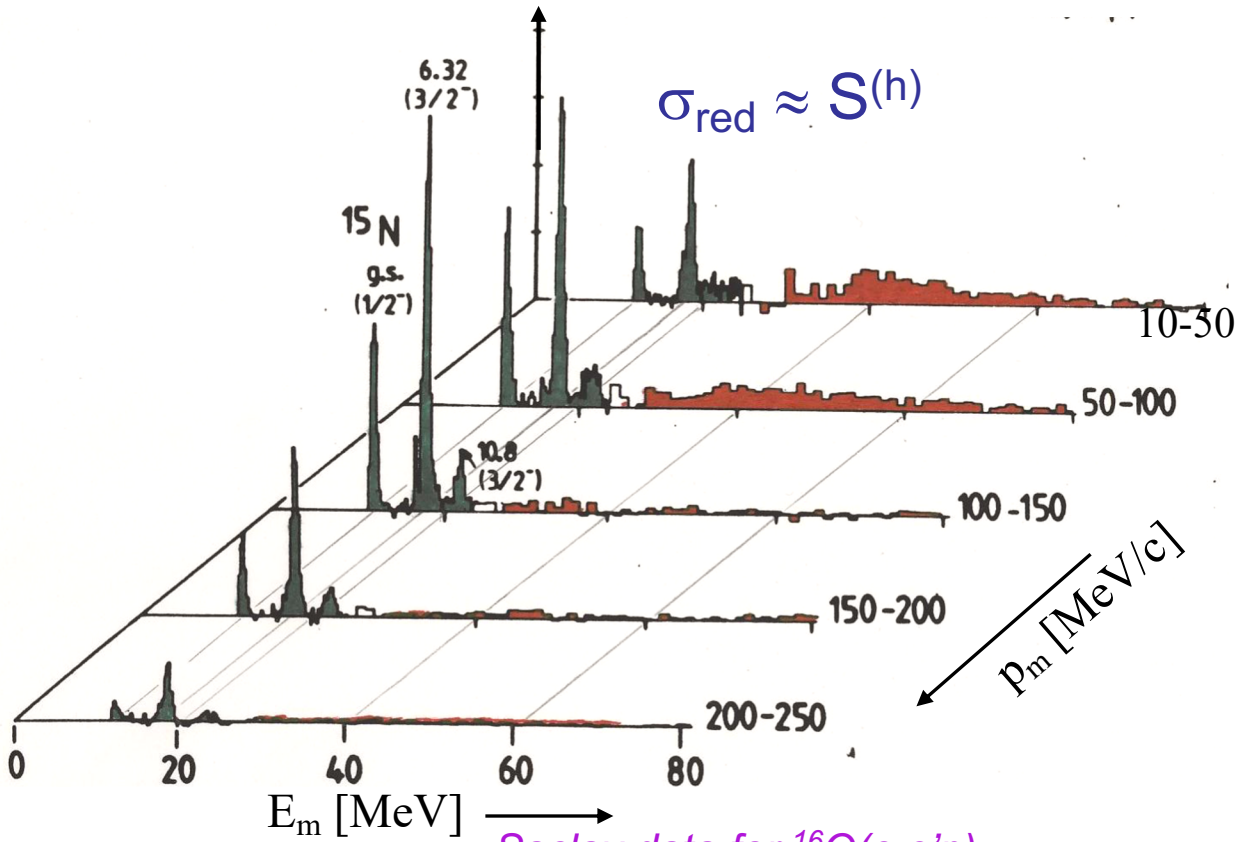


Fig. 9.2. The distribution of recoil momenta q for the argon ground state (3p) transition in the noncoplanar symmetric geometry at 400 eV (triangles), 800 eV (crosses) [46, 47] and 1200 eV (open circles) [154]. The curve is the plane wave theory using the Hartree–Fock wave function of Froese-Fischer [131].

Phys. Rep. 27, 275 (1976)

Concept of correlations

Spectral function: distribution of momentum (p_m) and energies (E_m)



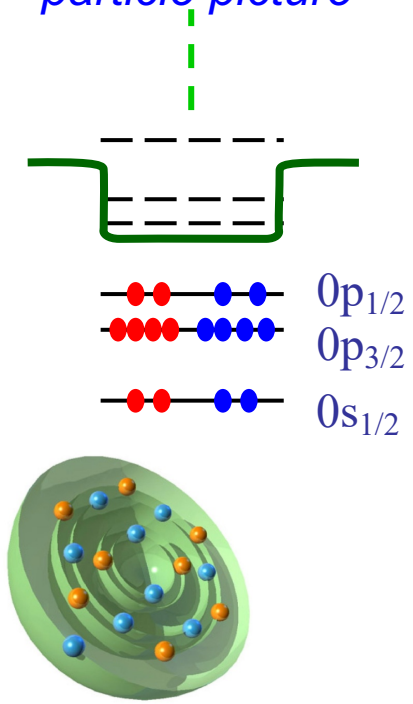
Saclay data for ^{16}O(e,e'p)

[Mougey et al., Nucl. Phys. A335, 35 (1980)]

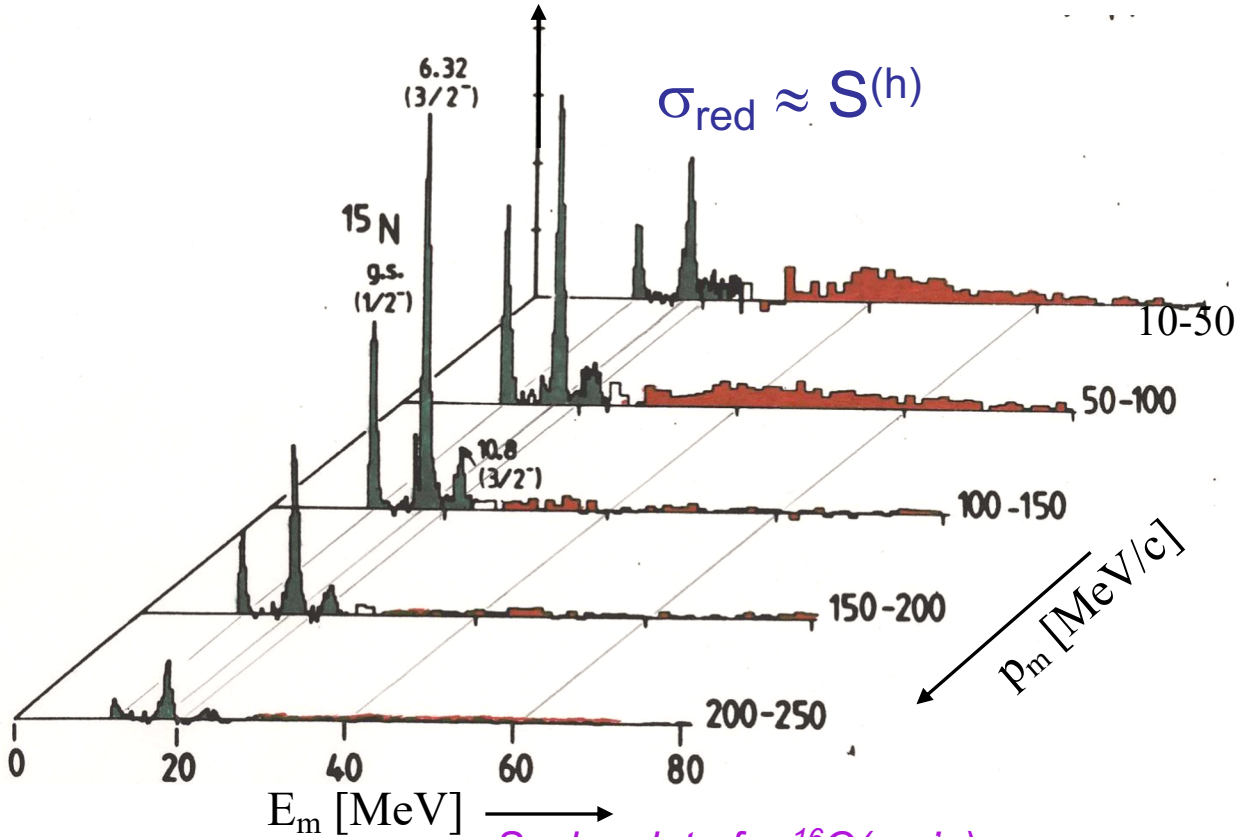
$$S^{(h)}(p_m, E_m) = \sum_n \left| \langle \Psi_n^{A-1} \mid c_{\vec{p}_m} \mid \Psi_0^A \rangle \right|^2 \delta(E_m - (E_0^A - E_n^{A-1}))$$

Concept of correlations

independent particle picture



Spectral function: distribution of momentum (p_m) and energies (E_m)



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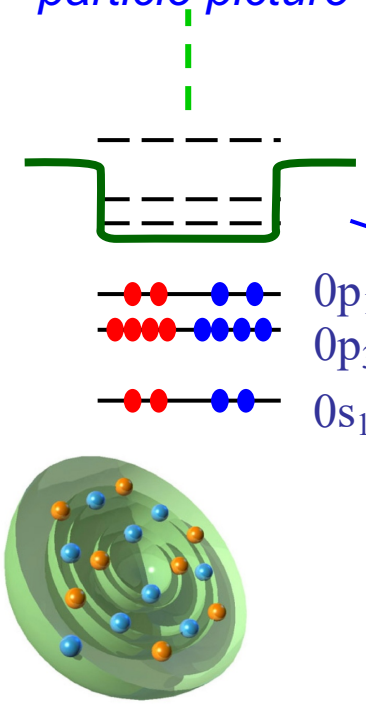
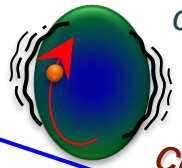
Concept of correlations

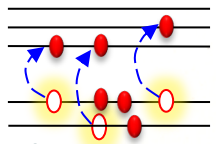
independent particle picture



Particle-vibration coupling (PV)



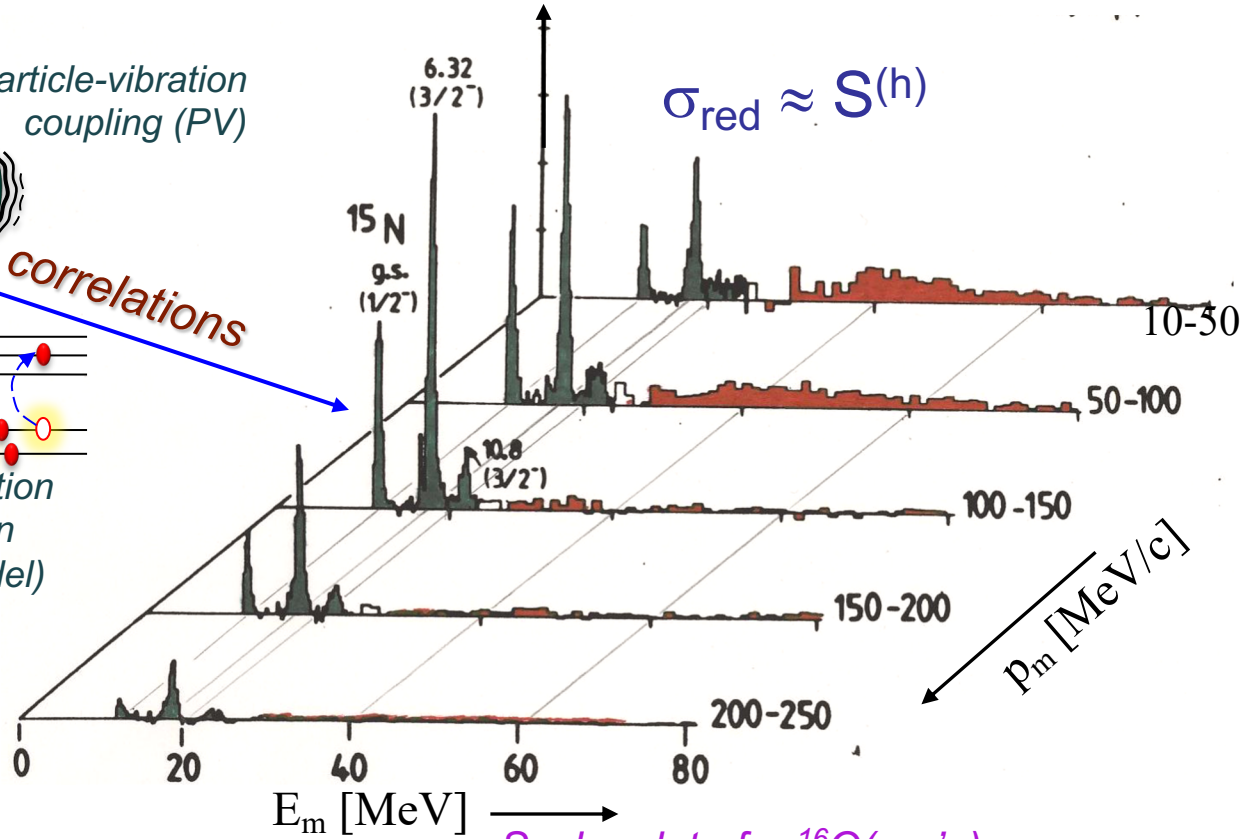
correlations



Configuration interaction (shell model)

Spectral function: distribution of momentum (p_m) and energies (E_m)

$\sigma_{red} \approx S^{(h)}$



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[Mougey et al., Nucl. Phys. A335, 35 (1980)]

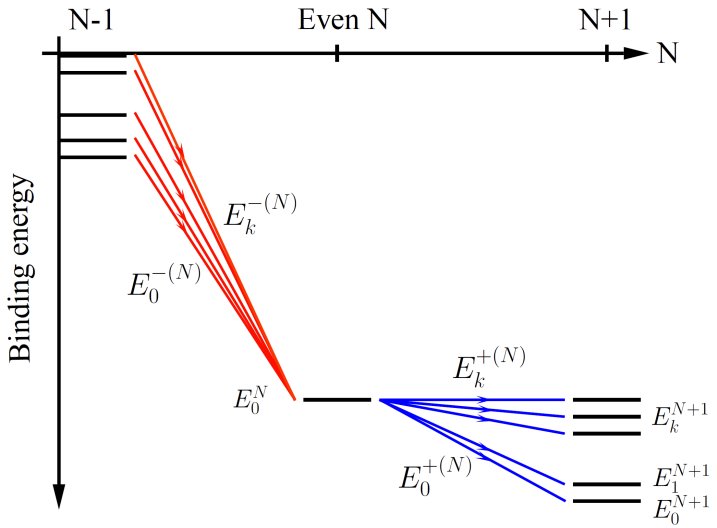
$$S^{(h)}(p_m, E_m) = \sum_n \left| \langle \Psi_n^{A-1} \mid c_{\vec{p}_m} \mid \Psi_0^A \rangle \right|^2 \delta(E_m - (E_0^A - E_n^{A-1}))$$

Green's functions in many-body theory

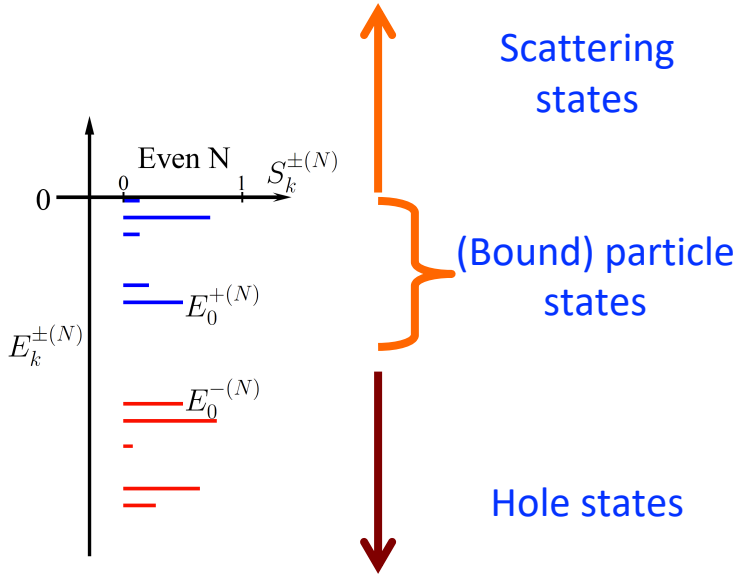
One-body Green's function (or propagator) describes the motion of quasi- particles and holes:

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

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



[pic. J. Sadoudi]



Separation energies and transfer strengths

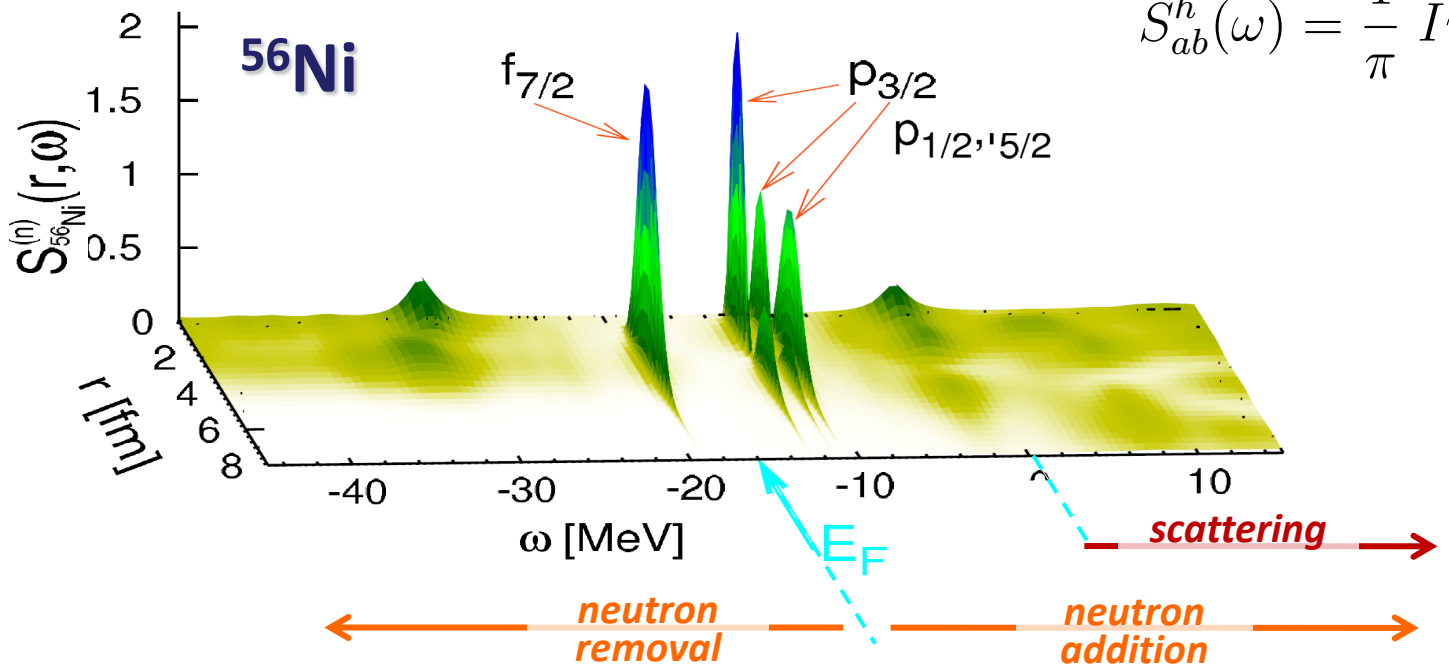
Example of spectral function ^{56}Ni

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

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

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

$$S_{ab}^h(\omega) = \frac{1}{\pi} \, Im \, g_{ab}(\omega)$$



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

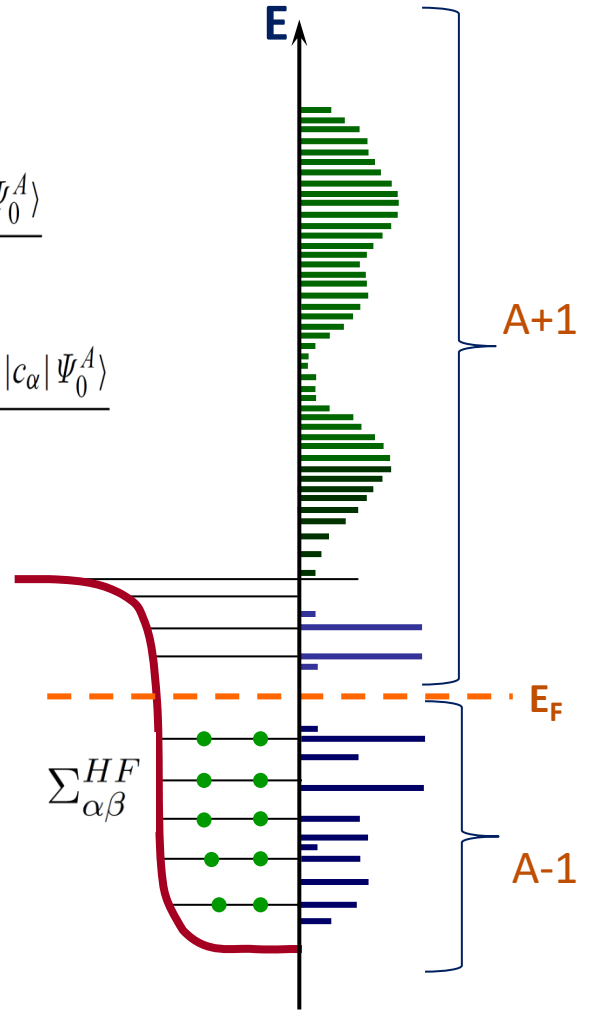
Nucleon elastic scattering

The full Lehmann representation of the single particle propagator is

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

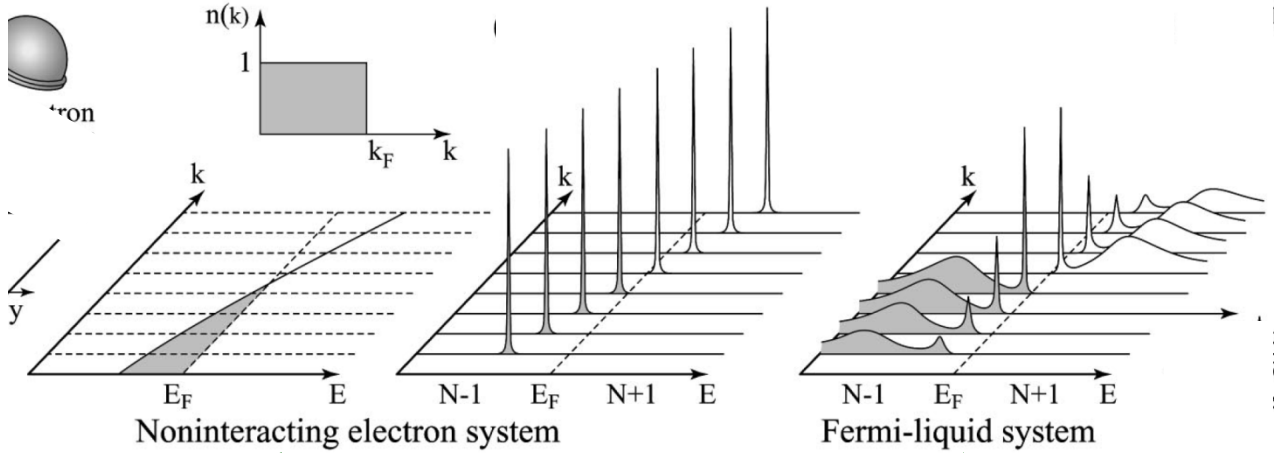
$$+ \int_{\varepsilon_T^+}^{\infty} d\varepsilon_\nu^+ \frac{\langle \Psi_0^A | c_\alpha | \Psi_\nu^{A+1} \rangle \langle \Psi_\nu^{A+1} | c_\beta^\dagger | \Psi_0^A \rangle}{\hbar\omega - \varepsilon_\nu^+ + i\eta} + \int_{-\infty}^{\varepsilon_T^-} d\varepsilon_\kappa^- \frac{\langle \Psi_0^A | c_\beta^\dagger | \Psi_\kappa^{A-1} \rangle \langle \Psi_\kappa^{A-1} | c_\alpha | \Psi_0^A \rangle}{\hbar\omega - \varepsilon_\kappa^- - i\eta}$$

→ In real systems these is always a continuum for large particle and hole energies—The one body equation for the residues is the same in both discrete and continuum spectrum



One-hole spectral function

Spectral function of infinite fermion systems



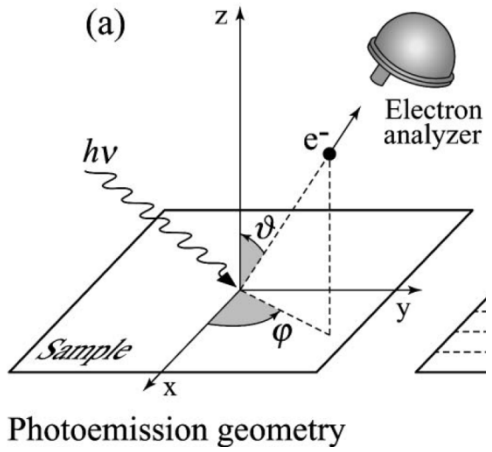
$$S(\mathbf{p},\omega) = \theta(|\mathbf{p}| - k_F)\delta\left(\hbar\omega - \frac{p^2}{2m}\right) + \theta(k_F - |\mathbf{p}|)\delta\left(\hbar\omega - \frac{p^2}{2m}\right)$$

$$S^h(\mathbf{p},\omega) = \sum_k \left|\langle\Psi_k^{N-1}|\psi_k(\mathbf{p})|\Psi_0^N\rangle\right|^2 \delta\left(\hbar\omega - (E_0^N - E_k^{N-1})\right)$$

[Picture credit: A. Damascelli, Rev. Mod. Phys. **75**, 473 (2003)]

Angle Resolved Photon Emission Spectroscopy (ARPES)

An ARPES setup – spectroscopy at the Fermi surface



Photoemission geometry

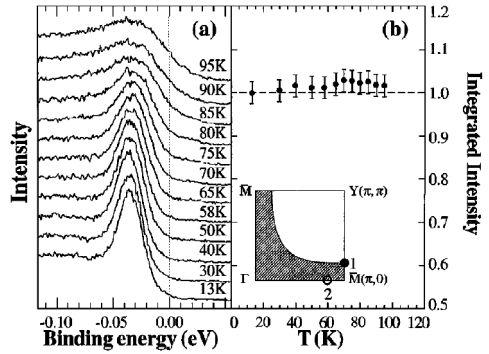


FIG. 4. Temperature dependence of the photoemission data from $Bi_2Sr_2CaCu_2O_{8+\delta}$ (T_c=87 K): (a) ARPES spectra measured at $\mathbf{k}=\mathbf{k}_F$ (point 1 in the Brillouin-zone sketch); (b) integrated intensity. From Randeria *et al.*, 1995.

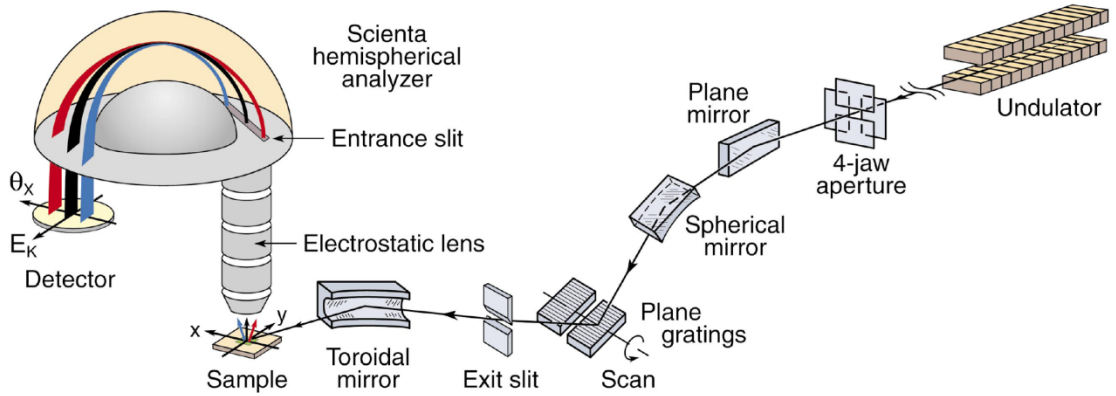


FIG. 6. Generic beamline equipped with a plane grating monochromator and a Scienta electron spectrometer (Color).

- Incoming beam of real photons
- Measure the emitted electron
- From angle and energy recover the momentum of the ejected particle + separation energy

[Pictures credit: A. Damascelli, et. al, Rev. Mod. Phys. 75, 473 (2003)]

Angle Resolved Photon Emission Spectroscopy (ARPES)

An ARPES setup – spectroscopy at the Fermi surface

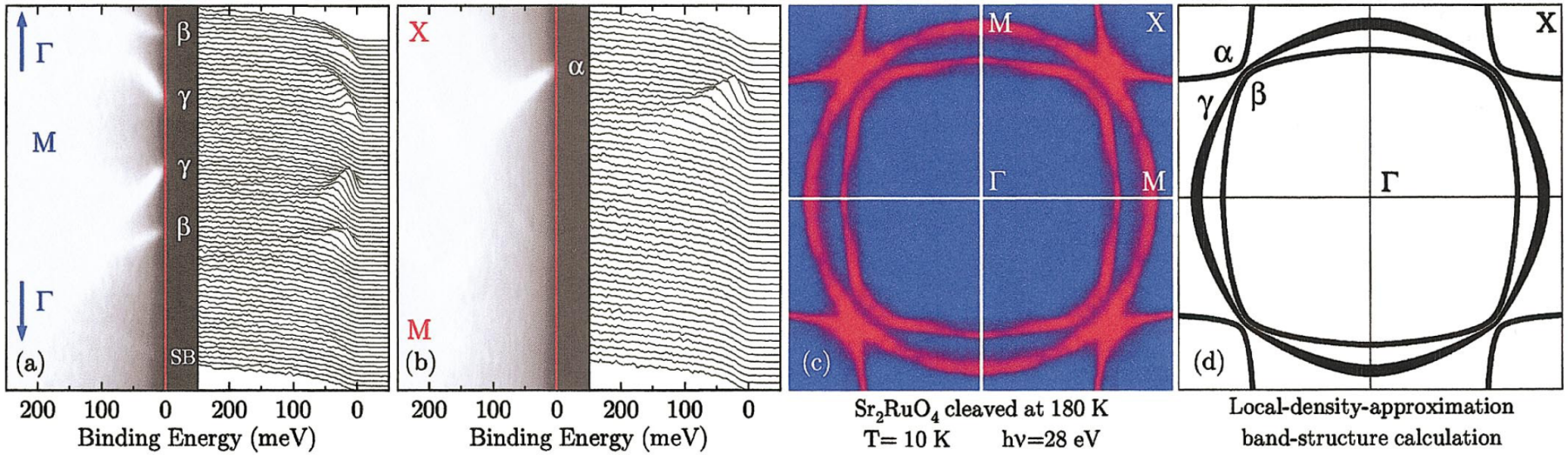


FIG. 9. Photoemission results from Sr_2RuO_4: ARPES spectra and corresponding intensity plot along (a) Γ-*M* and (b) *M*-*X*; (c) measured Fermi surface; (d) calculated Fermi surface (Mazin and Singh, 1997). From Damascelli *et al.*, 2000 (Color).

→ can "see" the Fermi surface*!!*

[Rev. Mod. Phys. 75, 473 (2003)]

Observables and physics quantities of interest

Various forms of the 1-body Green's function

$$g_{\alpha\beta}(t-t') = -\frac{i}{\hbar}\theta(t-t')\langle\Psi_0^N|c_\alpha e^{-i(H-E_0^N)(t-t')/\hbar}c_\beta^\dagger|\Psi_0^N\rangle \mp \frac{i}{\hbar}\theta(t'-t)\langle\Psi_0^N|c_\beta^\dagger e^{i(H-E_0^N)(t-t')/\hbar}c_\alpha|\Psi_0^N\rangle$$

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

$$S_{\alpha\beta}^p(\omega) = -\frac{1}{\pi}\,\mathrm{Im}\; g_{\alpha\beta}^p(\omega) \qquad \leftarrow \textit{(quasi)particles}$$

$$= \sum_n \langle\Psi_0^N|c_\alpha|\Psi_n^{N+1}\rangle\langle\Psi_n^{N+1}|c_\beta^\dagger|\Psi_0^N\rangle\;\delta\left(\hbar\omega-(E_n^{N+1}-E_0^N)\right)$$

$$S_{\alpha\beta}^h(\omega) = \frac{1}{\pi}\,\mathrm{Im}\; g_{\alpha\beta}^h(\omega) \qquad \leftarrow \textit{(quasi)holes}$$

$$= \mp\sum_k \langle\Psi_0^N|c_\beta^\dagger|\Psi_k^{N-1}\rangle\langle\Psi_k^{N-1}|c_\alpha|\Psi_0^N\rangle\;\delta\left(\hbar\omega-(E_0^N-E_k^{N-1})\right)$$

(- bosons,
+ fermions)

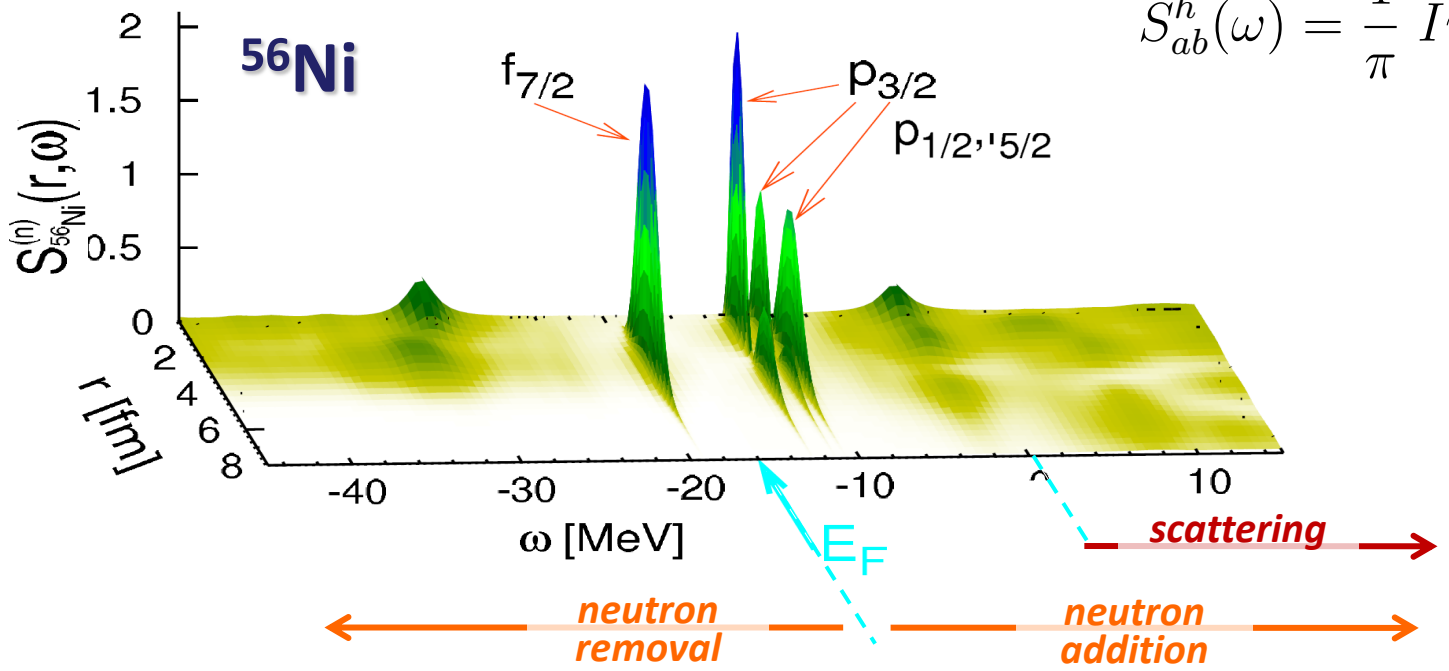
Example of spectral function ^{56}Ni

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

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

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

$$S_{ab}^h(\omega) = \frac{1}{\pi} \, Im \, g_{ab}(\omega)$$



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

Expectation values

- Take the Hamiltonian, $$H = \sum_{\alpha\beta} t_{\alpha\beta}\, c^\dagger_\alpha c_\beta + \sum_{\alpha\beta\gamma\delta} v_{\alpha\beta\gamma\delta}\, c^\dagger_\alpha c^\dagger_\beta c_\delta c_\gamma$$
- (or any 1- and 2-body operators). The g.s. expectation values are:

$$\langle \Psi^N_0 | H | \Psi^N_0 \rangle = \sum_{\alpha\beta} t_{\alpha\beta} \langle \Psi^N_0 | c^\dagger_\alpha c_\beta | \Psi^N_0 \rangle + \frac{1}{4} \sum_{\alpha\beta\gamma\delta} v_{\alpha\beta\gamma\delta} \langle \Psi^N_0 | c^\dagger_\alpha c^\dagger_\beta c_\delta c_\gamma | \Psi^N_0 \rangle$$

$$= \sum_{\alpha\beta} t_{\alpha\beta} \rho_{\beta\alpha} + \frac{1}{4} \sum_{\alpha\beta\gamma\delta} v_{\alpha\beta,\gamma\delta} \Gamma_{\gamma\delta,\alpha\beta}$$

one-body density matrix

two-body density matrix

$$\rho_{\alpha\beta} = \langle \Psi^N_0 | c^\dagger_\beta c_\alpha | \Psi^N_0 \rangle = \pm i\hbar \lim_{t' \to t^+} g_{\alpha\beta}(t, t') = \mp \int d\omega\, S^h_{\alpha\beta}(\omega)$$

$$\Gamma_{\alpha\beta,\gamma\delta} = \langle \Psi^N | c^\dagger_\gamma c^\dagger_\delta c_\beta c_\alpha | \Psi^N \rangle = -\frac{1}{4} \int d\omega S^{hh}_{\alpha\beta,\gamma\delta}(\omega)$$

Total Energy – Koltun rum rule

- The time evolution of a Heisenberg operator is: $$i\hbar \frac{d}{dt} c_\alpha(t) = e^{iHt/\hbar} \left[c_\alpha, H\right] e^{-iHt/\hbar}$$

- with: $$H = \sum_{\alpha\beta} t_{\alpha\beta}\, c^\dagger_\alpha c_\beta + \sum_{\alpha\beta\gamma\delta} v_{\alpha\beta\gamma\delta}\, c^\dagger_\alpha c^\dagger_\beta c_\delta c_\gamma$$

- Hence:

It is exaxct for 1- and 2-body interactions only!!!
(3-body forces require a correction)

Migdal-Galitski-Koltun sum rule:

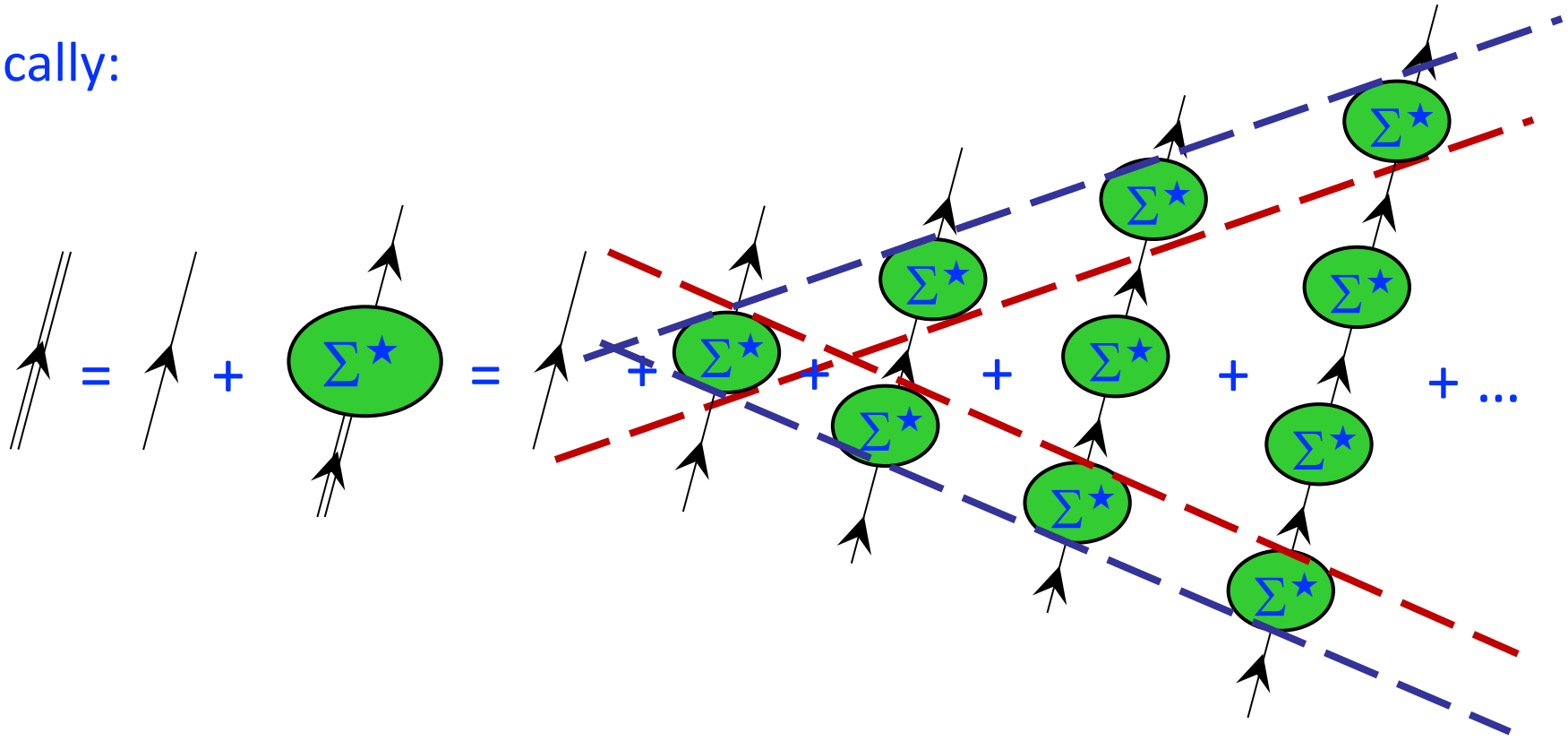
$$\langle H\rangle = \langle U\rangle + \langle V\rangle = \pm i\hbar \frac{1}{2} \lim_{t'\to t^+} \sum_{\alpha\beta} \left\{ \delta_{\alpha\beta} \frac{\partial}{\partial t} + t_{\alpha\beta} \right\} g_{\beta\alpha}(t-t')$$

$$= \mp \frac{1}{2} \sum_{\alpha\beta} \int d\omega \, \left\{\delta_{\alpha\beta}\omega + t_{\alpha\beta}\right\} S^h_{\beta\alpha}(\omega)$$

Dyson equation

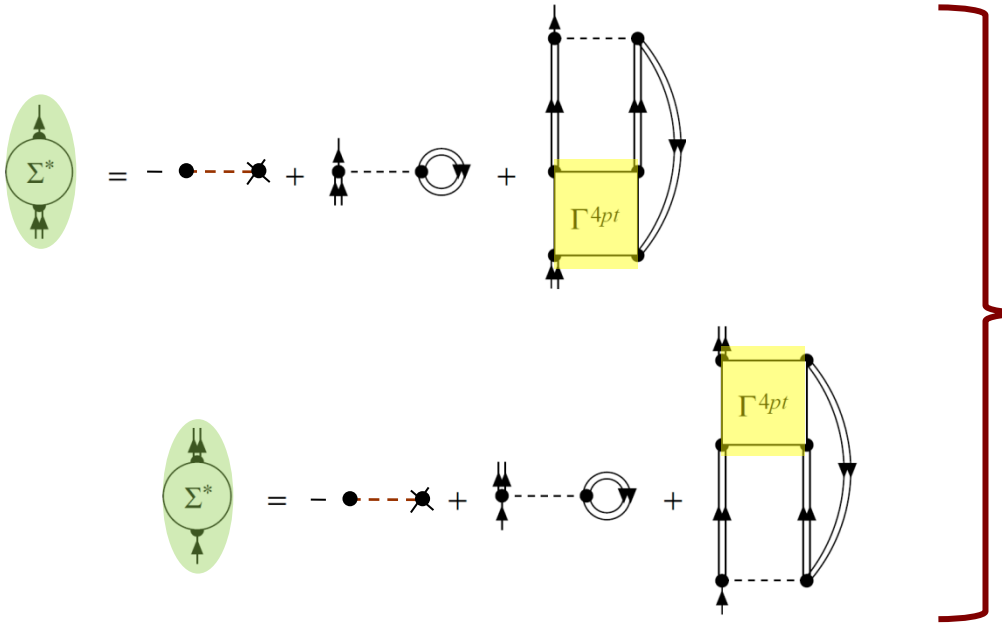
$$g_{\alpha\beta}(t-t') \;=\; g^{(0)}_{\alpha\beta}(t-t') \;+\; g^{(0)}_{\alpha\gamma}(t-t_\gamma)\,\Sigma^{\star}_{\gamma\delta}(t_\gamma,t_\delta)\,g_{\delta\beta}(t_\gamma-t')$$

- Diagrammatically:

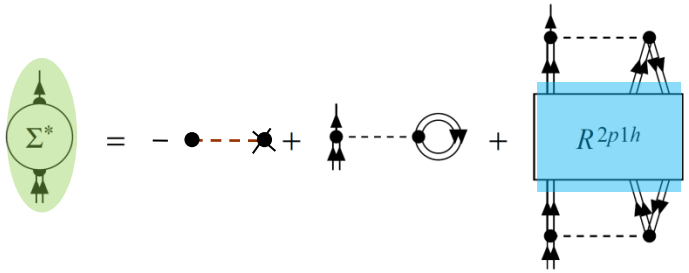


Dyson equation

Different forms for the self-energy



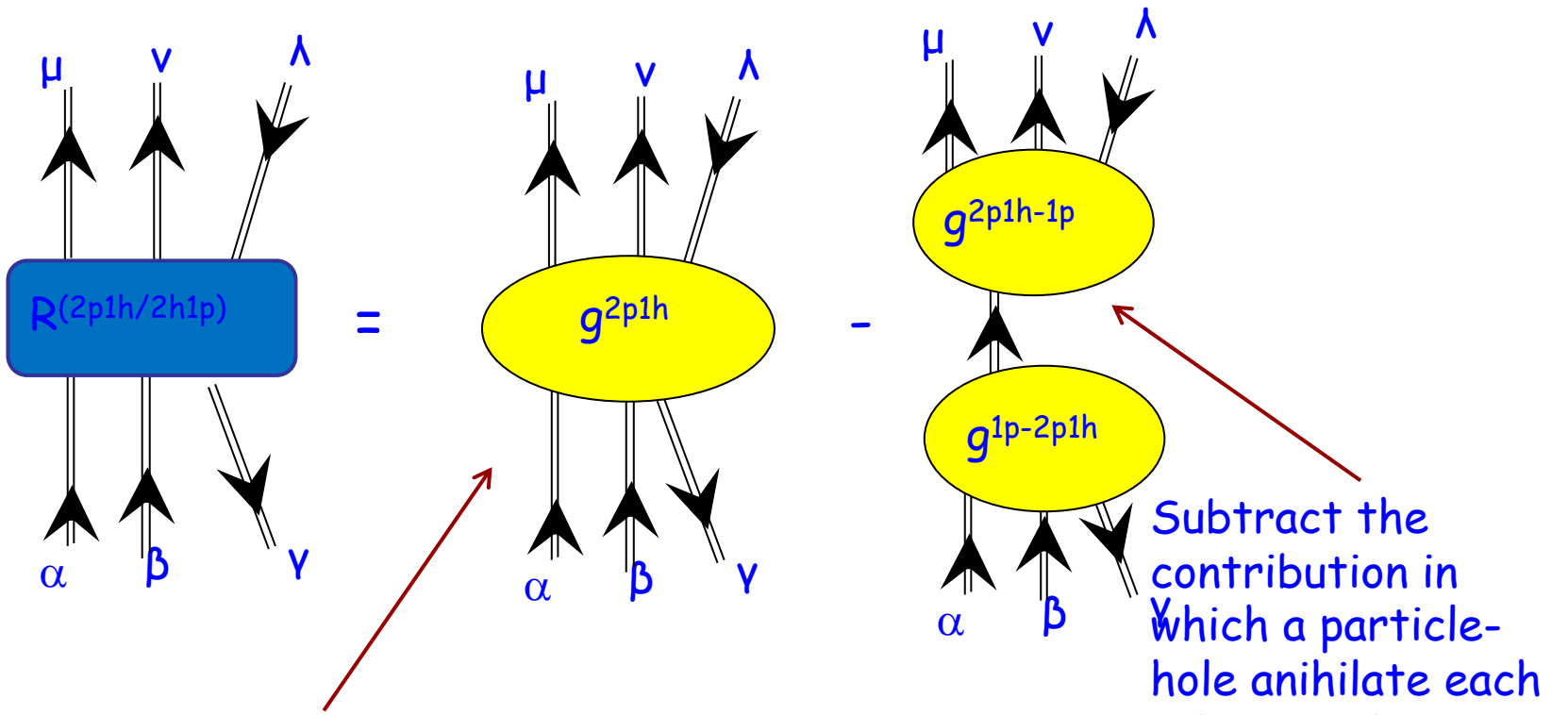
← if $\Gamma^{4\text{-pt}}$ is approximated in such a way that these two are equivalent, then conservation laws are fulfilled.
←The exact $\Gamma^{4\text{-pt}}$ depends of 4 times variables



← R^{2p1h} is specialized to two-times only!

Irreducible 2p1h/2h1p propagator

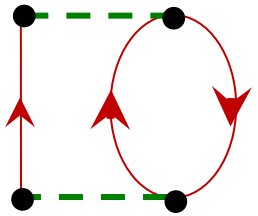
Graphic representation of the 2p1h/2h1p irreducible propagator R(ω):



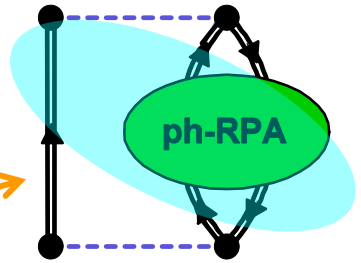
Approximations for the Self-energy

Diagrams of some common approximations for the self- energy:

- 2nd

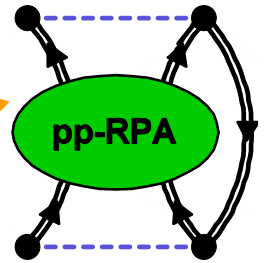


- ph "rings"



GW approach; particle-vibration coupling

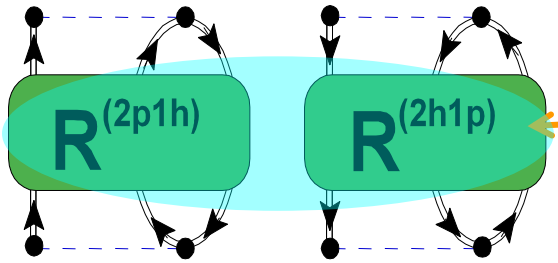
- pp "ladders"



Pairing-like effects; Used for nuclear matter

Keep in mind that in certain cases these two interfere and should not be used separately from each other…

- R^{2p1h}



This is the most complete, including both pp and ph correlations and their interference

Approaches to compute the irreducible self-energy:

- Use PT ➔ Feynman diagram expansion

- Equation of Motion method
  ➔ Leads to important concepts:
    - self consistency
    - all-order summations
    - conservation theorems

- Algebraic diagrammatic constructions ADC(3)
  ➔ typically the working approach
  for most finite systems

Dyson equation

- The reducible self-energy sums $\Sigma^{\star}_{\alpha\beta}$ll orders,

$$\Sigma_{\alpha\beta}(t,t') = \Sigma^{\star}_{\alpha\beta}(t,t') + \Sigma^{\star}_{\alpha\gamma}(t,t_\gamma)\, g^{(0)}_{\gamma\delta}(t_\gamma,t_\delta)\; \Sigma_{\delta\beta}(t_\gamma - t')$$

- Then:

$$g_{\alpha\beta}(t-t') = g^{(0)}_{\alpha\beta}(t-t') + g^{(0)}_{\alpha\gamma}(t-t_\gamma)\, \Sigma_{\gamma\delta}(t_\gamma,t_\delta)\, g^{(0)}_{\delta\beta}(t_\gamma - t')$$

Conservation laws

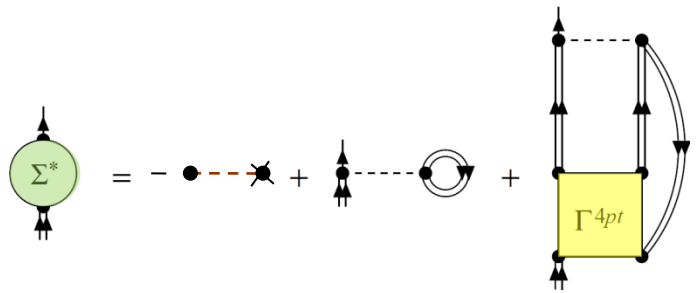
- Macroscopic quantities can be calculated from the single particle propagator:

- $\langle N(t)\rangle = -i\hbar \sum_{\alpha} g_{\alpha\alpha}(t,t^{+})$ particle number
- $\langle \mathbf{P}(t)\rangle = -i\hbar \sum_{\alpha\beta} \langle \alpha|\mathbf{p}|\beta\rangle g_{\beta\alpha}(t,t^{+})$ tot. momentum
- $\langle \mathbf{J}(t)\rangle = -i\hbar \sum_{\alpha\beta} \langle \alpha|\mathbf{r}\times\mathbf{p}|\beta\rangle g_{\beta\alpha}(t,t^{+})$ angular momentum
- $\langle E(t)\rangle = -i\hbar \frac{1}{2} \sum_{\alpha\beta} \left\{ \delta_{\alpha\beta}\frac{\partial}{\partial t} + t_{\alpha\beta} \right\} g_{\beta\alpha}(t,t^{+})$ energy

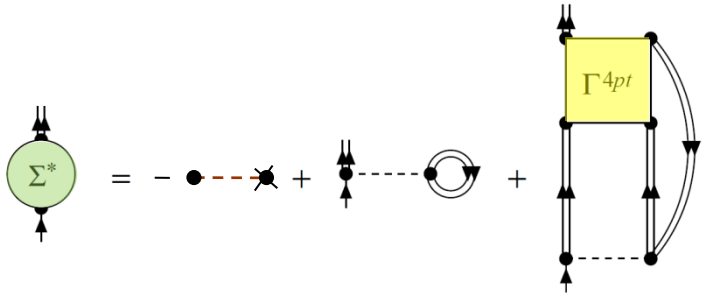
Conservation laws

- There exist two-different forms of the Dyson equation:

$$g_{\alpha\beta}(t-t') = g^{(0)}_{\alpha\beta}(t-t') + g^{(0)}_{\alpha\gamma}(t-t_\gamma)\,\Sigma^{A,\star}_{\gamma\delta}(t_\gamma,t_\delta)\,g_{\delta\beta}(t_\gamma-t')$$



$$g_{\alpha\beta}(t-t') = g^{(0)}_{\alpha\beta}(t-t') + g_{\alpha\gamma}(t-t_\gamma)\,\Sigma^{B,\star}_{\gamma\delta}(t_\gamma,t_\delta)\,g^{(0)}_{\delta\beta}(t_\gamma-t')$$



- ➔ One usually chooses an approximation for Γ and then builds an approximation of $\Sigma^{\star}_{\alpha\beta}$ *!!!!*

- Theorem (Baym, Kadanoff 1961):

- Assume that the propagator $g_{\alpha\beta}(t\text{-}t')$ solves both forms of the Dyson equation (that means $\Sigma^{A,\star}_{\alpha\beta} = \Sigma^{B,\star}_{\alpha\beta}$ and $\Gamma_{\alpha\beta,\gamma\delta} = \Gamma_{\beta\alpha,\delta\gamma}$. Then <N>, <P>, <L> and <E> calculated with $g_{\alpha\beta}(t\text{-}t')$ are all conserved:

$$\frac{d\langle N(t)\rangle}{dt} = 0 \qquad \frac{d\langle \mathbf{P}(t)\rangle}{dt} = 0 \qquad \frac{d\langle \mathbf{J}(t)\rangle}{dt} = 0 \qquad \frac{d\langle E(t)\rangle}{dt} = 0$$

[G. Baym and L. P. Kadanoff, Phys. Rev. **124**, 287 (1961)

Adiabatic theorem and perturbations

Assume that the Hamiltonian splits in two parts, one component (H_0) can be solved exactly but not the full Hamiltonian:

$$H = H_0 + H_1$$

If the second part (H_1) is small, we can treat it as a small correction→ *perturbation theory*.

The complete propagator requires the Heisenberg evolution for the full H:

$$g_{\alpha\beta}(t,t') = -\frac{i}{\hbar}\langle \Psi_0^N | T[c_\alpha(t) c_\beta^\dagger(t')] | \Psi_0^N \rangle, \qquad c_\alpha(t) = e^{iHt/\hbar}\, c_\alpha\, e^{-iHt/\hbar}$$

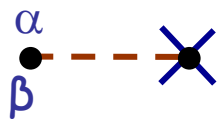
but we can handle only H_0 . Thus, evolve operators according to H_0 and compensate for the missing H_1 part ( ) evolving the wave function → This is the Interaction (or Dirac) picture.

Feynman diagram rules

Graphic conventions:

$$i\hbar g_{\alpha\beta}(t-t') = \quad = i\hbar g_{\alpha\beta}(\omega)$$

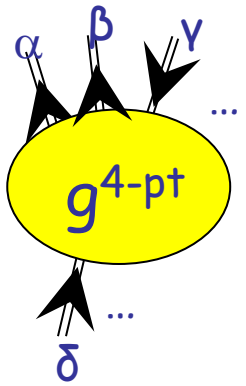
$$\frac{-i}{\hbar}u_{\alpha\beta}\ , \quad \frac{-i}{\hbar}t_{\alpha\beta} =$$



$$i\hbar g^{(0)}_{\alpha\beta}(t-t') = \quad = i\hbar g^{(0)}_{\alpha\beta}(\omega)$$

$$\frac{-i}{\hbar}v_{\alpha\beta,\gamma\delta} =$$

$$i\hbar g_{\alpha\beta\gamma\ldots;\delta\ldots}(t_\alpha, t_\beta, \ldots; t_\delta) = \quad = i\hbar g_{\alpha\beta\gamma\ldots;\delta\ldots}(\omega_\alpha, \omega_\beta, \ldots; \omega_\delta)$$



Feynman diagram rules

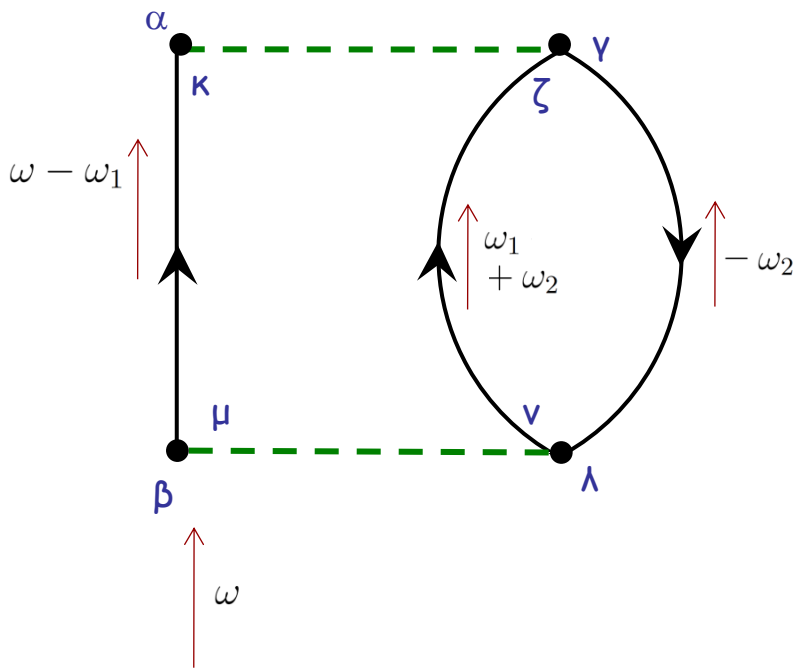
Rules in *frequency* representation

1. Write all connected and topologically equivalent diagrams—and only those.
2. At every propagator line one must associate an energy going in the direction of the arrow (energy must be conserved at each vertex)
3. Each single line w/ an arrow, contributes $i\hbar\, g^{(0)}_{\alpha\beta}(\omega)$ running from β to α (**ω** gets a **–** sign if it goes against the arrow)
4. Each closed circle contributes a density matrix $\rho_{\alpha\beta}$ (no $i\hbar$ factor!)
5. Each two-body interaction line contributes $-\frac{i}{\hbar}\, v_{\alpha\beta,\gamma\delta}$
6. Each external field line contributes $-\frac{i}{\hbar}\, u_{\alpha\beta}$
7. An extra **-1** for each closed circuit (density matrix loops excluded)
8. Sum (integrate) over all coordinate and integrate over all independent frequencies (with a **1/2π** factor for each integration)
9. IF $v_{\alpha\beta,\gamma\delta}$ are *antisymmtrized* matrix elements, and extra factor **½** is required for each pair of equivalent lines.
10. Add final factor $-\frac{i}{\hbar}$ is to get G(t-t`) .

Example of using Feynman diagram rules

Calculating the *second order* self-energy:

$$\Sigma^{2nd}_{\alpha\beta}(\omega) = i\hbar\,(i\hbar)^3\left(\frac{-i}{\hbar}\right)^2\frac{(-1)^2}{2}v_{\alpha\gamma,\kappa\zeta}v_{\mu\nu,\beta\lambda}\int\frac{d\omega_1}{2\pi}\int\frac{d\omega_2}{2\pi}g_{\kappa\mu}(\omega-\omega_1)g_{\zeta\nu}(\omega_1+\omega_2)g_{\lambda\gamma}(\omega_2)$$



Repeated greek indices are implicitly summed

Example of using Feynman diagram rules

Calculating the *second order* self-energy:

$$x_i \equiv \hbar\omega_i$$

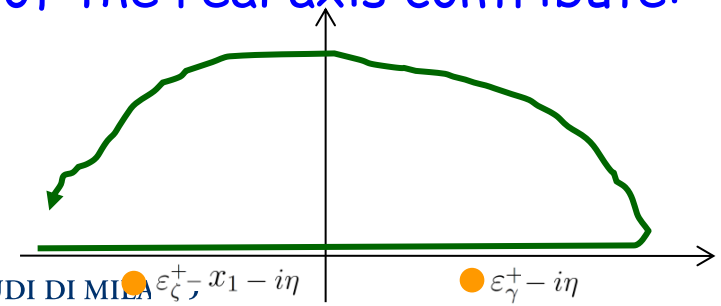
$$\Sigma^{2nd}_{\alpha\beta}(\omega) = i\hbar\,(i\hbar)^3\left(\frac{-i}{\hbar}\right)^2\frac{(-1)^2}{2}v_{\alpha\gamma,\kappa\zeta}v_{\mu\nu,\beta\lambda}\int\frac{d\omega_1}{2\pi}\int\frac{d\omega_2}{2\pi}g_{\kappa\mu}(\omega-\omega_1)g_{\zeta\nu}(\omega_1+\omega_2)g_{\lambda\gamma}(\omega_2)$$

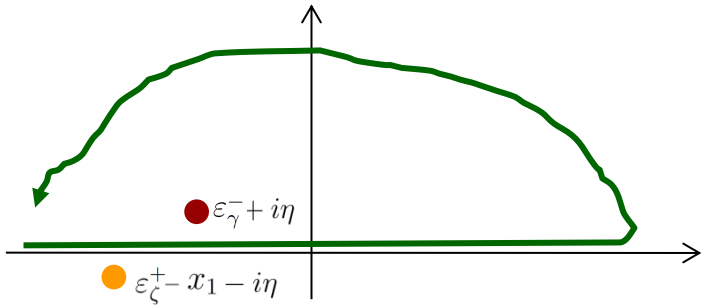
$$= -\frac{1}{2}v_{\alpha\gamma,\kappa\zeta}v_{\mu\nu,\beta\lambda}\int\frac{dx_1}{2\pi i}\int\frac{dx_2}{2\pi i}g_{\kappa\mu}(\omega-\omega_1)g_{\zeta\nu}(\omega_1+\omega_2)g_{\lambda\gamma}(\omega_2)$$

$$= -\frac{1}{2}v_{\alpha\gamma,\kappa\zeta}v_{\mu\nu,\beta\lambda}\int\frac{dx_1}{2\pi i}g_{\kappa\mu}(\omega-\omega_1)\int\frac{dx_2}{2\pi i}$$

$$\times\delta_{\zeta\nu}\left\{\underset{x_2\downarrow}{\frac{\delta_{\zeta\notin F}}{x_1+x_2-\varepsilon^+_\zeta+i\eta}}+\underset{x_2\uparrow}{\frac{\delta_{\zeta\in F}}{x_1+x_2-\varepsilon^-_\zeta-i\eta}}\right\}\left\{\underset{x_2\downarrow}{\frac{\delta_{\gamma\notin F}}{x_2-\varepsilon^+_\gamma+i\eta}}+\underset{x_2\uparrow}{\frac{\delta_{\gamma\in F}}{x_2-\varepsilon^-_\gamma-i\eta}}\right\}$$

Using the Cauchy theorem, only term with at least one pole on each side of the real axis contribute:





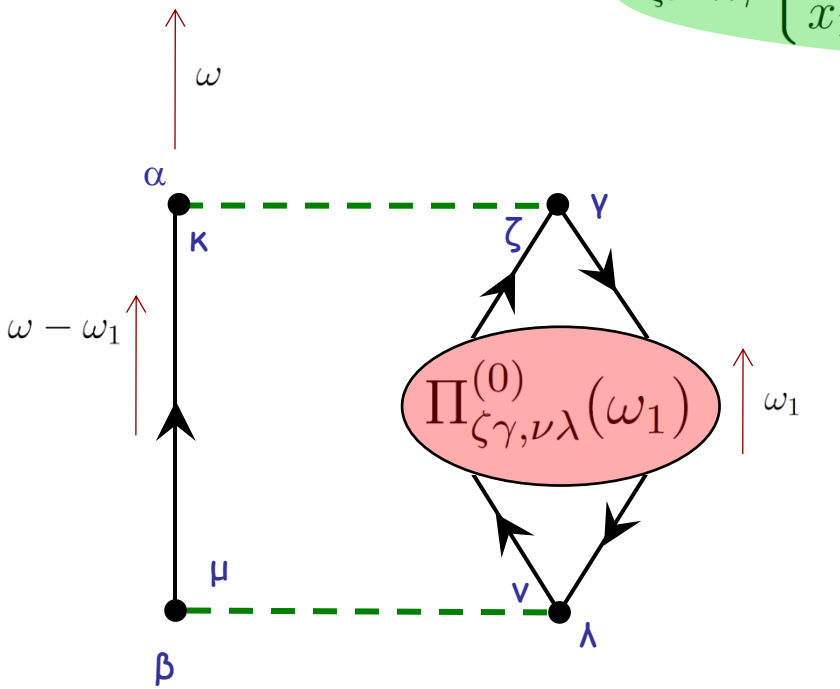
Example of using Feynman diagram rules

Calculating the *second order* self-energy:

$$x_i \equiv \hbar\omega_i$$

$$\Sigma^{2nd}_{\alpha\beta}(\omega) = -\frac{1}{2} v_{\alpha\gamma,\kappa\zeta} v_{\mu\nu,\beta\lambda} \int \frac{dx_1}{2\pi i} g_{\kappa\mu}(\omega - \omega_1)$$

$$\delta_{\zeta\nu}\delta_{\lambda\gamma} \left\{ \frac{\delta_{\zeta\notin F}\,\delta_{\gamma\in F}}{x_1 - (\varepsilon^+_\zeta - \varepsilon^-_\gamma) + i\eta} - \frac{\delta_{\zeta\in F}\,\delta_{\gamma\notin F}}{x_1 + (\varepsilon^+_\gamma - \varepsilon^-_\zeta) - i\eta} \right\}$$



$\Pi^{(0)}_{\zeta\gamma,\nu\lambda}(\omega_1)$

Example of using Feynman diagram rules

Calculating the *second order* self-energy:

$$x_i \equiv \hbar\omega_i$$

$$\Sigma^{2nd}_{\alpha\beta}(\omega) = -\frac{1}{2} v_{\alpha\gamma,\kappa\zeta} v_{\mu\nu,\beta\lambda} \int \frac{dx_1}{2\pi i} g_{\kappa\mu}(\omega - \omega_1)$$

$$\delta_{\zeta\nu}\delta_{\lambda\gamma} \left\{ \frac{\delta_{\zeta\notin F}\,\delta_{\gamma\in F}}{x_1 - (\varepsilon^+_\zeta - \varepsilon^-_\gamma) + i\eta} - \frac{\delta_{\zeta\in F}\,\delta_{\gamma\notin F}}{x_1 + (\varepsilon^+_\gamma - \varepsilon^-_\zeta) - i\eta} \right\}$$

$$= -\frac{1}{2}\delta_{\kappa\mu}\delta_{\zeta\nu}\delta_{\lambda\gamma} v_{\alpha\gamma,\kappa\zeta} v_{\mu\nu,\beta\lambda} \int \frac{dx_1}{2\pi i} \left\{ \frac{\delta_{\kappa\notin F}}{\hbar\omega - x_1 - \varepsilon^+_\kappa + i\eta} + \frac{\delta_{\kappa\in F}}{\hbar\omega - x_1 - \varepsilon^-_\kappa - i\eta} \right\}$$

(x_1 ↑ in the first denominator, x_1 ↓ in the second)

$$\times \left\{ \frac{\delta_{\zeta\notin F}\,\delta_{\gamma\in F}}{x_1 - (\varepsilon^+_\zeta - \varepsilon^-_\gamma) + i\eta} - \frac{\delta_{\zeta\in F}\,\delta_{\gamma\notin F}}{x_1 + (\varepsilon^+_\gamma - \varepsilon^-_\zeta) - i\eta} \right\}$$

(x_1 ↓ in the first denominator, x_1 ↑ in the second)

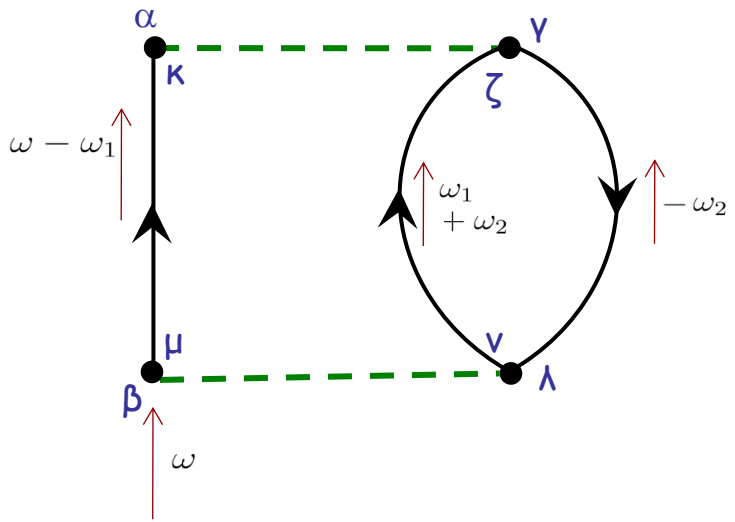
$$\Sigma^{2nd}_{\alpha\beta}(\omega) = \frac{1}{2} v_{\alpha\lambda,\mu\nu} \left\{ \frac{\delta_{\mu\notin F}\,\delta_{\nu\notin F}\,\delta_{\lambda\in F}}{\hbar\omega - (\varepsilon^+_\mu + \varepsilon^+_\nu - \varepsilon^-_\lambda) + i\eta} + \frac{\delta_{\mu\in F}\,\delta_{\nu\in F}\,\delta_{\lambda\notin F}}{\hbar\omega - (\varepsilon^-_\mu + \varepsilon^-_\nu - \varepsilon^+_\lambda) - i\eta} \right\} v_{\mu\nu,\beta\lambda}$$

Repeated greek indices are implicitly summed

Example of using Feynman diagram rules

Calculating the *second order* self-energy:

$$\Sigma^{2nd}_{\alpha\beta}(\omega) = i\hbar\,(i\hbar)^3\left(\frac{-i}{\hbar}\right)^2\frac{(-1)^2}{2}v_{\alpha\gamma,\kappa\zeta}v_{\mu\nu,\beta\lambda}\int\frac{d\omega_1}{2\pi}\int\frac{d\omega_2}{2\pi}g_{\kappa\mu}(\omega-\omega_1)g_{\zeta\nu}(\omega_1+\omega_2)g_{\lambda\gamma}(\omega_2)$$



$$\Sigma^{2nd}_{\alpha\beta}(\omega) = \frac{1}{2}v_{\alpha\lambda,\mu\nu}\left\{\frac{\delta_{\mu\notin F}\,\delta_{\nu\notin F}\,\delta_{\lambda\in F}}{\hbar\omega-(\varepsilon^+_\mu+\varepsilon^+_\nu-\varepsilon^-_\lambda)+i\eta}+\frac{\delta_{\mu\in F}\,\delta_{\nu\in F}\,\delta_{\lambda\notin F}}{\hbar\omega-(\varepsilon^-_\mu+\varepsilon^-_\nu-\varepsilon^+_\lambda)-i\eta}\right\}v_{\mu\nu,\beta\lambda}$$

Algebraic Diagrammatic Construction method at order *n* - ADC(*n*)

See J. Schirmer and collaborators.:

Phys. Rev. A**26**, 2395 (1982)

Phys. Rev. A**28**, 1237 (1983)

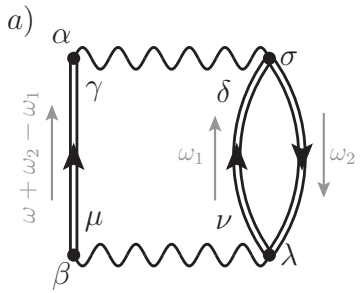
Prescription: write all the possible Feynman diagrams up to order **n** , then add minimal corrections and all-order summations to guarantee the correct spectral representation of the self energy.

CB and A. Carbone, ***chapter 11*** of Lecture Notes in Physics **936** (2017)

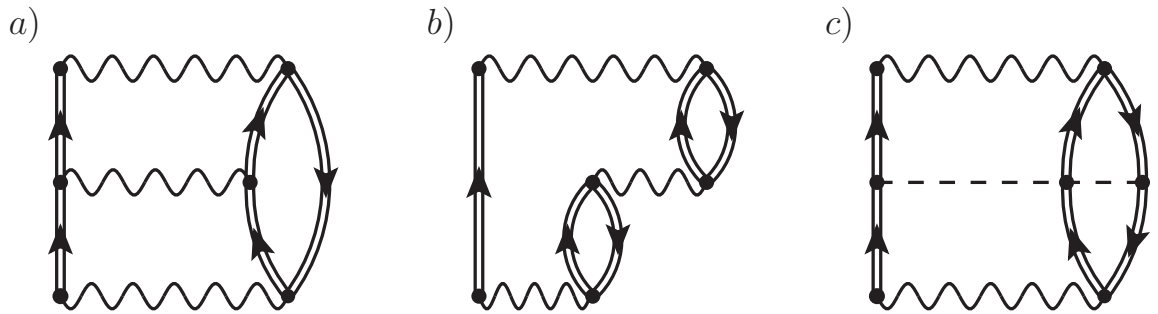
1st order

Simple Hartree-Fock,
or mean-field approach

2nd order



3rd order



Working eqs. for ADC(2) / ext-ADC(2) / ADC(3)

We consider a generic *reference propagator* that is used to expand the self-energy:

$$g^{(ref)}_{\alpha\beta}(\omega) = \sum_n \frac{(\mathcal{X}^n_\alpha)^* \mathcal{X}^n_\beta}{\omega - \varepsilon^+_n + i\eta} + \sum_k \frac{\mathcal{Y}^k_\alpha (\mathcal{Y}^k_\beta)^*}{\omega - \varepsilon^-_k - i\eta}$$

with

$$\begin{cases} \mathcal{X}^n_\alpha \equiv \langle \Psi^{A+1}_n | a^\dagger_\alpha | \Psi^A_0 \rangle \\ \varepsilon^+_n \equiv E^{A+1}_n - E^A_0 \\ E^{A+1}_n |\Psi^{A+1}_n\rangle = H^{(ref)} |\Psi^{A+1}_n\rangle \end{cases} \qquad \begin{cases} \mathcal{Y}^k_\alpha \equiv \langle \Psi^{A-1}_k | a_\alpha | \Psi^A_0 \rangle \\ \varepsilon^-_k \equiv E^A_0 - E^{A-1}_k \\ E^{A-1}_k |\Psi^{A-1}_k\rangle = H^{(ref)} |\Psi^{A-1}_k\rangle \end{cases}$$

In general, this could be and unperturbed propagator (for which $H^{(ref)}=H_0$, $\mathcal{X}^n_\alpha = \delta_{n,\alpha}\delta_{n\in F}$, etc...), an *Hartree-Fock propagator* or even fully dressed propagator.

Working eqs. for ADC(2) / ext-ADC(2) / ADC(3)

The most general form of the irreducible self-energy is:

$$\Sigma^{\star}_{\alpha,\beta}(\omega) = \Sigma^{\infty}_{\alpha,\beta} + \sum_{i\,j} \mathbf{M}^{\dagger}_{\alpha i} \left[\frac{1}{\omega - (\mathbf{E}^{fw} + \mathbf{C}) + i\eta} \right]_{i\,j} \mathbf{M}_{j\beta}$$

$$+ \sum_{r\,p} \mathbf{N}^{\dagger}_{\alpha r} \left[\frac{1}{\omega - (\mathbf{E}^{bk} + \mathbf{D}) - i\eta} \right]_{r\,p} \mathbf{N}_{p\beta}$$

where:

$i,\ j \longrightarrow$ label $\quad 2p1h,\quad 3p2h,\quad 4p3h,\ \ldots \qquad$ excitations

$r,\ p \longrightarrow$ label $\quad 2h1p,\quad 3h2p,\ \ldots \qquad$ excitations

Working eqs. for ADC(2) / ext-ADC(2) / ADC(3)

The Dyson eq. is the solved by diagonalizing

$$\varepsilon^{\pm} \begin{pmatrix} \vec{Z}^{\pm} \\ \vec{W} \\ \\ \vec{U} \end{pmatrix} = \left(\begin{array}{c|c|c} H_0 + \mathbf{\Sigma}^{\infty} & \mathbf{M}^{\dagger} & \mathbf{N}^{\dagger} \\ \hline \mathbf{M} & \mathrm{diag}(\mathbf{E}^{fw}) + \mathbf{C} & \\ \hline \mathbf{N} & & \mathrm{diag}(\mathbf{E}^{bk}) + \mathbf{D} \end{array}\right) \begin{pmatrix} \vec{Z}^{\pm} \\ \vec{W} \\ \\ \vec{U} \end{pmatrix}$$

with the normalization condition

$$(\vec{Z}^{\pm})^{\dagger}\, \vec{Z}^{\pm} \;+\; \vec{W}^{\dagger}\, \vec{W} \;+\; \vec{U}^{\dagger}\, \vec{U} = 1$$

One then identifies: $(\vec{Z}^{+n})_{\alpha} \;\rightarrow\; \mathcal{X}^{n}_{\alpha}$ that yield the new propagator and

$$(\vec{Z}^{-k})_{\alpha} \;\rightarrow\; \mathcal{Y}^{k}_{\alpha}$$

Working eqs. for ADC(2)

The dressed 1st and 2nd order diagrams are:

$$\Sigma^{\infty}_{\alpha\beta} = \quad = -U_{\alpha\beta} + \Sigma^{cHF}_{\alpha\beta}$$

$$\Sigma^{cHF}_{\alpha\beta} = \int_{C\uparrow} \frac{\mathrm{d}\omega}{2\pi i}\, v_{\alpha\gamma,\beta\delta}\, g^{(ref)}_{\delta\gamma}(\omega) = \sum_k v_{\alpha\gamma,\beta\delta}\, \mathcal{Y}^k_\delta (\mathcal{Y}^k_\gamma)^*$$

and

$$\Sigma^{(2)}_{\alpha\beta}(\omega) = \quad + \frac{1}{2}\sum_{n_1,n_2,k} \frac{v_{\alpha\lambda,\mu\nu}\,(\mathcal{X}^{n_1}_\mu \mathcal{X}^{n_2}_\nu \mathcal{Y}^k_\lambda)^*\, \mathcal{X}^{n_1}_{\mu'} \mathcal{X}^{n_2}_{\nu'} \mathcal{Y}^k_{\lambda'}\, v_{\mu'\nu',\beta\lambda'}}{\omega - (\varepsilon^+_{n_1} + \varepsilon^+_{n_2} - \varepsilon^-_k) + i\eta}$$

Goldstone diagrams

$$+\frac{1}{2}\sum_{k_1,k_2,n} \frac{v_{\alpha\lambda,\mu\nu}\, \mathcal{Y}^{k_1}_\mu \mathcal{Y}^{k_2}_\nu \mathcal{X}^n_\lambda\, (\mathcal{Y}^{k_1}_{\mu'} \mathcal{Y}^{k_2}_{\nu'} \mathcal{X}^n_{\lambda'})^*\, v_{\mu'\nu',\beta\lambda'}}{\omega - (\varepsilon^-_{k_1} + \varepsilon^-_{k_2} - \varepsilon^+_n) + i\eta}$$

Repeated greek indices are implicitly summed

Working eqs. for ADC(2)

From the previous diagrams, one extracts the matrix elements that define ADC(2):

$$(\mathbf{H}_0 + \boldsymbol{\Sigma}^{\infty})_{\alpha\beta} = (\mathbf{T} + \mathbf{U})_{\alpha\beta} + (-\mathbf{U} + \boldsymbol{\Sigma}^{cHF})_{\alpha\beta}$$
$$= t_{\alpha\beta} + \sum_k v_{\alpha\gamma,\beta\delta}\, \mathcal{Y}^k_\delta (\mathcal{Y}^k_\gamma)^*$$

$$\mathbf{M}_{(n_1,n_2,k),\alpha} = \frac{1}{\sqrt{2}} \mathcal{X}^{n_1}_\mu \mathcal{X}^{n_2}_\nu \mathcal{Y}^k_\lambda\, v_{\mu\nu,\alpha\lambda} \qquad \mathbf{N}_{(k_1,k_2,n),\alpha} = \frac{1}{\sqrt{2}} (\mathcal{Y}^{k_1}_\mu \mathcal{Y}^{k_2}_\nu \mathcal{X}^n_\lambda)^*\, v_{\mu\nu,\alpha\lambda}$$

$$\mathbf{E}^{fw}_{n_1,n_2,k} = \varepsilon^+_{n_1} + \varepsilon^+_{n_2} - \varepsilon^-_k \qquad \mathbf{E}^{bk}_{k_1,k_2,n} = \varepsilon^-_{k_1} + \varepsilon^-_{k_2} - \varepsilon^-_n$$

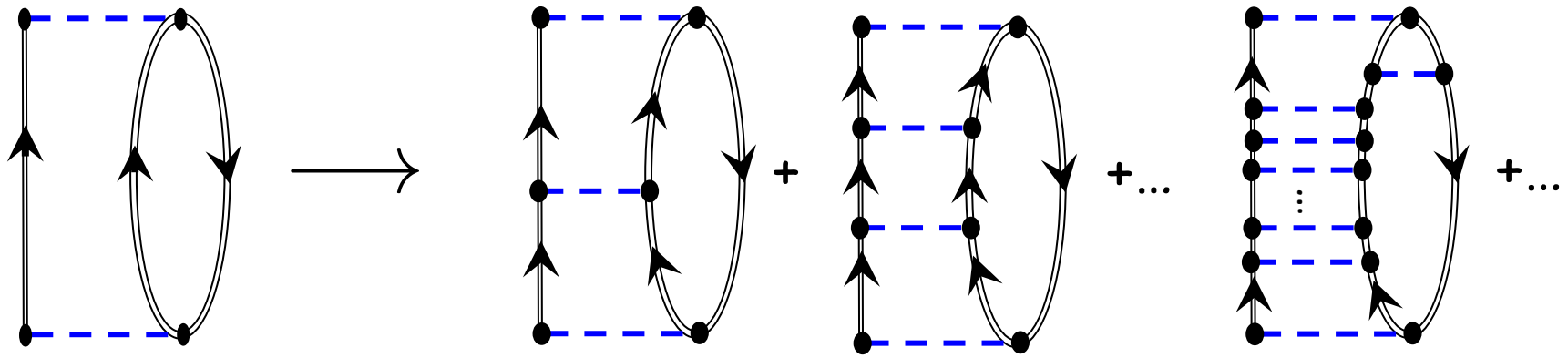
$$\mathbf{C} = 0 \qquad \mathbf{D} = 0$$

Any repeated indices are implicitly summed

Note that the auxiliary potential U (that defines the unperturbed propagator) cancels out from the Dyson equation!

Working eqs. for ext-ADC(2)

Extend the ADC(2) by inserting pp-, hh-, and ph-summations (ladders and rings):



this leads to contributions of the form:

$$\longrightarrow V\frac{1}{\omega - E_{2p1h}}V \;+\; V\frac{1}{\omega - E_{2p1h}}V\frac{1}{\omega - E_{2p1h}}V$$
$$+\; V\frac{1}{\omega - E_{2p1h}}V\frac{1}{\omega - E_{2p1h}}V\frac{1}{\omega - E_{2p1h}}V$$
$$+\; V\frac{1}{\omega - E_{2p1h}}V\frac{1}{\omega - E_{2p1h}}V\frac{1}{\omega - E_{2p1h}}V\frac{1}{\omega - E_{2p1h}}V + \ldots$$

Working eqs. for ext-ADC(2)

Expand the self-energy in the inter-particle interaction. Both the M, N matrices have leading contributions at first order in V:

$$\mathbf{M} = \mathbf{M}^1(v^1) + \mathbf{M}^2(v^2) + \mathbf{M}^3(v^3) + \dots$$

$$\mathbf{N} = \mathbf{N}^1(v^1) + \mathbf{N}^2(v^2) + \mathbf{N}^3(v^3) + \dots$$

While C and D are only at 1st order in V. This leads to contributions of the form:

$$\begin{aligned}\mathbf{M}^\dagger \frac{1}{\omega - (E + \mathbf{C})}\mathbf{M} \longrightarrow\ & \mathbf{M}^{1\dagger}\frac{1}{\omega - E}\mathbf{M}^1 \\ & + \mathbf{M}^{2\dagger}\frac{1}{\omega - E}\mathbf{M}^1 + \mathbf{M}^{1\dagger}\frac{1}{\omega - E}\mathbf{M}^2 + \mathbf{M}^{1\dagger}\frac{1}{\omega - E}\mathbf{C}\frac{1}{\omega - E}\mathbf{M}^1 \\ & + \mathbf{M}^{3\dagger}\frac{1}{\omega - E}\mathbf{M}^1 + \mathbf{M}^{2\dagger}\frac{1}{\omega - E}\mathbf{M}^2 + \mathbf{M}^{1\dagger}\frac{1}{\omega - E}\mathbf{C}\frac{1}{\omega - E}\mathbf{C}\frac{1}{\omega - E}\mathbf{M}^1 + \end{aligned}$$

➔from here one reads the minimal approximation to C needed to reproduce the 3rd order diagram. Then the full ladder and ring summation come automatically, for free!

Working eqs. for ext-ADC(2)

The matrices for the extended-ADC(2) equations are the same as for ADC(2), except for:

$$\mathbf{C}_{(n_1,n_2,k_3),(n_4,n_5,k_6)} = \frac{1}{2}\langle n_1 n_2|v|n_4 n_5\rangle\delta_{k_3,k_6} + \langle n_1 k_3|v^{ph}|n_4 k_6\rangle\delta_{n_2,n_5} + \langle n_2 k_3|v^{ph}|n_5 k_6\rangle\delta_{n_1,n_4}$$

$$\mathbf{D}_{(k_1,k_2,n_3),(k_4,k_5,n_6)} = -\frac{1}{2}\langle k_1 k_2|v|k_4 k_5\rangle\delta_{n_3,n_6} - \langle k_1 n_3|v^{ph}|k_4 n_6\rangle\delta_{k_2,k_5} - \langle k_2 n_3|v^{ph}|k_5 n_6\rangle\delta_{k_1,k_4}$$

where:

$$\langle n_1 n_2|v|n_4 n_5\rangle \equiv \mathcal{X}^{n_1}_{\gamma}\mathcal{X}^{n_2}_{\delta}\, v_{\gamma\delta,\mu\nu}\,(\mathcal{X}^{n_4}_{\mu}\mathcal{X}^{n_5}_{\nu})^*$$

$$\langle n_1 k_3|v^{ph}|n_4 k_6\rangle \equiv \mathcal{X}^{n_1}_{\alpha}\mathcal{Y}^{k_3}_{\beta}\, v_{\alpha\delta,\beta\gamma}\,(\mathcal{X}^{n_4}_{\gamma}\mathcal{Y}^{k_6}_{\delta})^*$$

$$\langle k_1 k_2|v|k_4 k_5\rangle \equiv (\mathcal{Y}^{k_1}_{\gamma}\mathcal{Y}^{k_2}_{\delta})^* v_{\gamma\delta,\mu\nu}\,\mathcal{Y}^{k_4}_{\mu}\mathcal{Y}^{k_5}_{\nu}$$

$$\langle k_1 n_3|v^{ph}|k_4 n_6\rangle \equiv (\mathcal{Y}^{k_1}_{\alpha}\mathcal{X}^{n_3}_{\beta})^* v_{\alpha\delta,\beta\gamma}\,\mathcal{Y}^{k_4}_{\gamma}\mathcal{X}^{n_6}_{\delta}$$

Any repeated indices are implicitly summed

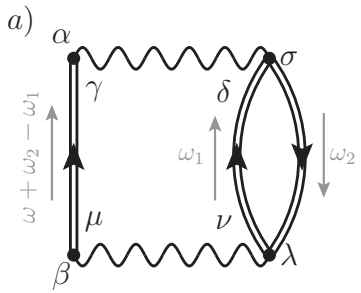
➔ The full ladder and ring summations are generated by these choices of C and D!

Working eqs. For ADC(3)

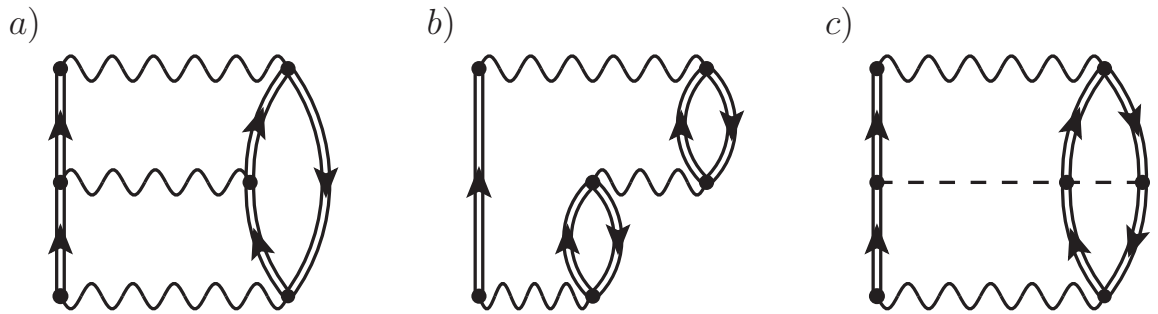
1st order

Simple Hartree-Fock,
or mean-field approach

2nd order

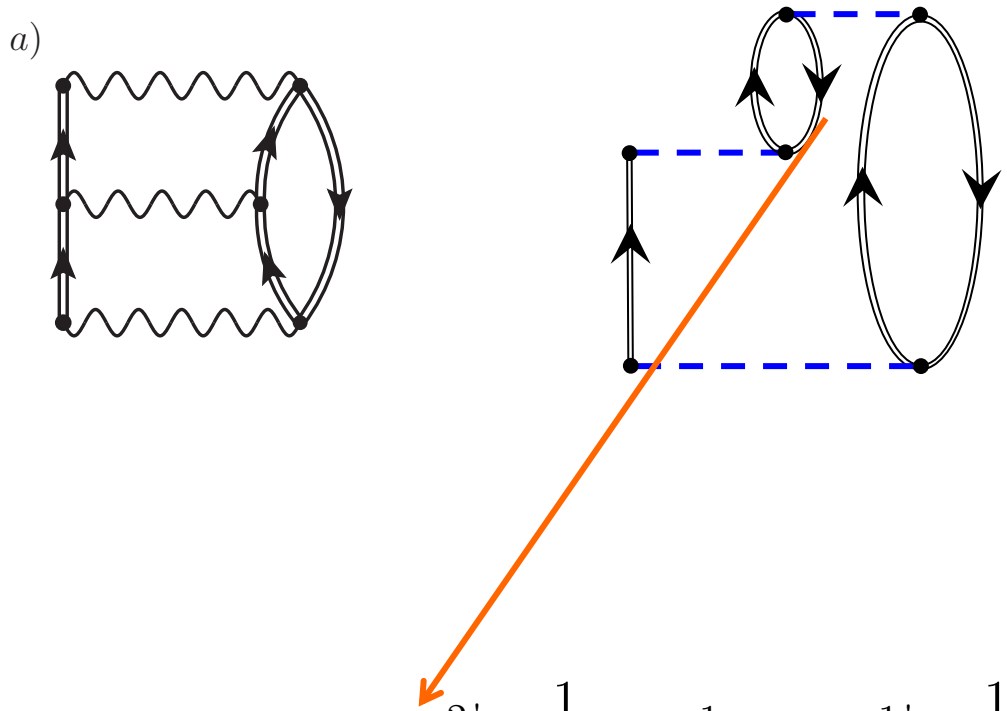


3rd order



Working eqs. For ADC(3)

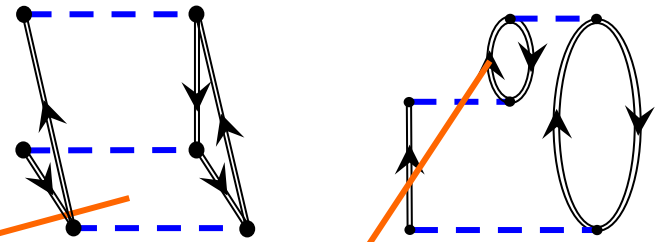
Requiring that ALL 3rd order Goldstone diagrams are included requires to also extending the coupling matrices:



$$\ldots + \mathbf{M}^{2\dagger}\frac{1}{\omega - E}\mathbf{M}^{1} + \mathbf{M}^{1\dagger}\frac{1}{\omega - E}\mathbf{C}\frac{1}{\omega - E}\mathbf{M}^{1} + \mathbf{M}^{1\dagger}\frac{1}{\omega - E}\mathbf{M}^{2} + \ldots$$

Working eqs. For ADC(3)

Requiting that ALL 3rd order Goldstone diagrams are included requires to also extending the coupling matrices:

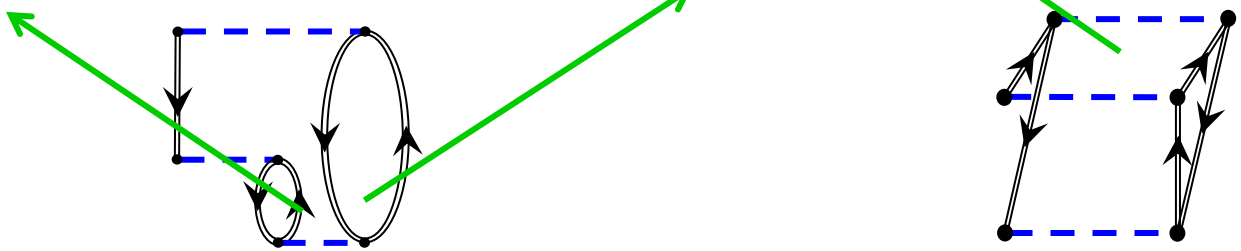


$$\sqrt{(2)}\mathbf{M}_{(n_1,n_2,k),\alpha} = \mathcal{X}^{n_1}_{\mu}\mathcal{X}^{n_2}_{\nu}\mathcal{Y}^{k}_{\lambda}\,v_{\mu\nu,\alpha\lambda} + \frac{\mathcal{X}^{n_1}_{\sigma}\mathcal{X}^{n_2}_{\rho}v_{\sigma\rho,\gamma\delta}\mathcal{Y}^{k_7}_{\gamma}\mathcal{Y}^{k_8}_{\delta}}{2(\varepsilon^{-}_{k_7}+\varepsilon^{-}_{k_8}-\varepsilon^{+}_{n_1}-\varepsilon^{+}_{n_2})}(\mathcal{Y}^{k_7}_{\mu}\mathcal{Y}^{k_8}_{\nu})^{*}\mathcal{Y}^{k}_{\lambda}\,v_{\mu\nu,\alpha\lambda}$$

$$+\frac{\mathcal{Y}^{k}_{\sigma}\mathcal{X}^{n_2}_{\rho}v_{\rho\delta,\sigma\gamma}\mathcal{Y}^{k_5}_{\gamma}\mathcal{X}^{n_6}_{\delta}}{(\varepsilon^{-}_{k}-\varepsilon^{+}_{n_2}+\varepsilon^{-}_{k_5}-\varepsilon^{+}_{n_6})}\mathcal{X}^{n_1}_{\mu}(\mathcal{Y}^{k_5}_{\nu}\mathcal{X}^{n_6}_{\lambda})^{*}\,v_{\mu\nu,\alpha\lambda} - \frac{\mathcal{Y}^{k}_{\sigma}\mathcal{X}^{n_1}_{\rho}v_{\rho\delta,\sigma\gamma}\mathcal{Y}^{k_5}_{\gamma}\mathcal{X}^{n_6}_{\delta}}{(\varepsilon^{-}_{k}-\varepsilon^{+}_{n_1}+\varepsilon^{-}_{k_5}-\varepsilon^{+}_{n_6})}\mathcal{X}^{n_2}_{\mu}(\mathcal{Y}^{k_5}_{\nu}\mathcal{X}^{n_6}_{\lambda})^{*}\,v_{\mu\nu,\alpha\lambda}$$

$$\sqrt{(2)}\mathbf{N}_{(k_1,k_2,n),\alpha} = (\mathcal{Y}^{k_1}_{\mu}\mathcal{Y}^{k_2}_{\nu}\mathcal{X}^{n}_{\lambda})^{*}\,v_{\mu\nu,\alpha\lambda} + \frac{(\mathcal{Y}^{k_1}_{\sigma}\mathcal{Y}^{k_2}_{\rho})^{*}v_{\sigma\rho,\gamma\delta}(\mathcal{X}^{n_7}_{\gamma}\mathcal{X}^{n_8}_{\delta})^{*}}{2(\varepsilon^{-}_{k_1}+\varepsilon^{-}_{k_2}-\varepsilon^{+}_{n_7}-\varepsilon^{+}_{n_8})}\mathcal{X}^{n_7}_{\mu}\mathcal{X}^{n_8}_{\nu}\mathcal{X}^{n}_{\lambda}\,v_{\mu\nu,\alpha\lambda}$$

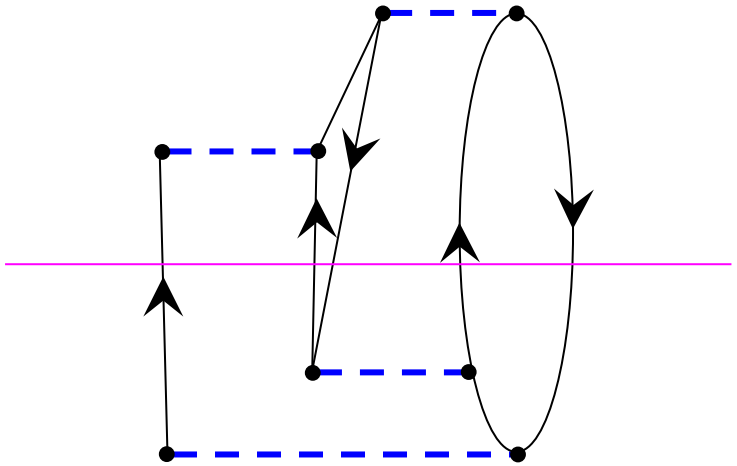
$$+\frac{(\mathcal{Y}^{k_2}_{\sigma}\mathcal{X}^{n}_{\rho})^{*}v_{\sigma\delta,\rho\gamma}(\mathcal{X}^{n_5}_{\gamma}\mathcal{Y}^{k_6}_{\delta})^{*}}{(\varepsilon^{-}_{k_2}-\varepsilon^{+}_{n}+\varepsilon^{-}_{k_6}-\varepsilon^{+}_{n_5})}(\mathcal{Y}^{k_1}_{\mu})^{*}\mathcal{X}^{n_5}_{\nu}\mathcal{Y}^{k_6}_{\lambda}\,v_{\mu\nu,\alpha\lambda} - \frac{(\mathcal{Y}^{k_1}_{\sigma}\mathcal{X}^{n}_{\rho})^{*}v_{\sigma\delta,\rho\gamma}(\mathcal{X}^{n_5}_{\gamma}\mathcal{Y}^{k_6}_{\delta})^{*}}{(\varepsilon^{-}_{k_1}-\varepsilon^{+}_{n}+\varepsilon^{-}_{k_6}-\varepsilon^{+}_{n_5})}(\mathcal{Y}^{k_2}_{\mu})^{*}\mathcal{X}^{n_5}_{\nu}\mathcal{Y}^{k_6}_{\lambda}\,v_{\mu\nu,\alpha\lambda}$$



Beyond ADC(3)...

The general strategy is: expand the self-energy in Feynman/Goldstone diagrams up to order *n* and the compare to the minimal expansion in terms of matrices C, D and M, N.

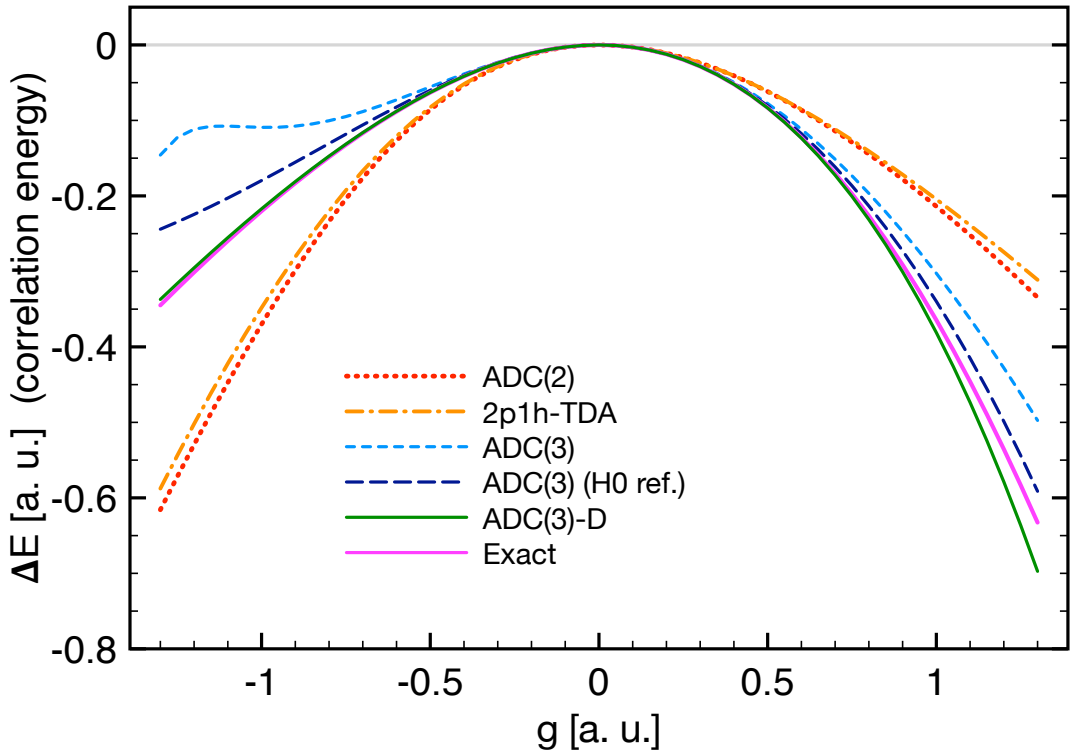
For ADC(4), also 3p2h/3h2p intermediate states appear:

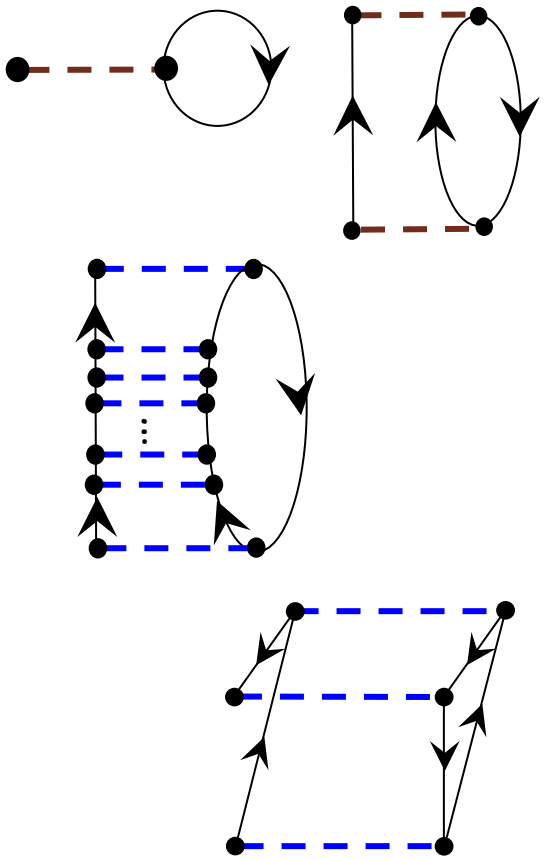


		ADC(2,3)		ADC(4,5)	
lp/lh-	2p-1h	2h-1p	3p-2h	3h-2p	...
$\varepsilon+\Sigma(\infty)$	U^{I}	U^{II}	U^{I}	U^{II}	...
	$(K+C)^{I}$		C^{I}		
		$(K+C)^{II}$		C^{II}	
			$(K+C)^{I}$		
				$(K+C)^{II}$	

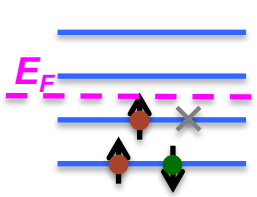
Results for the pairing model

Correlation energy for the 4-level and 4-fermions pairing model

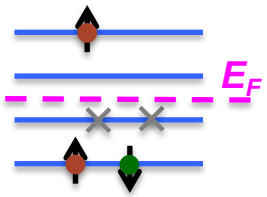




$$\langle\ \Phi_k;1h\ |H_1|\ \Phi^n_{k1,k2};2h1p\ \rangle = \langle$$



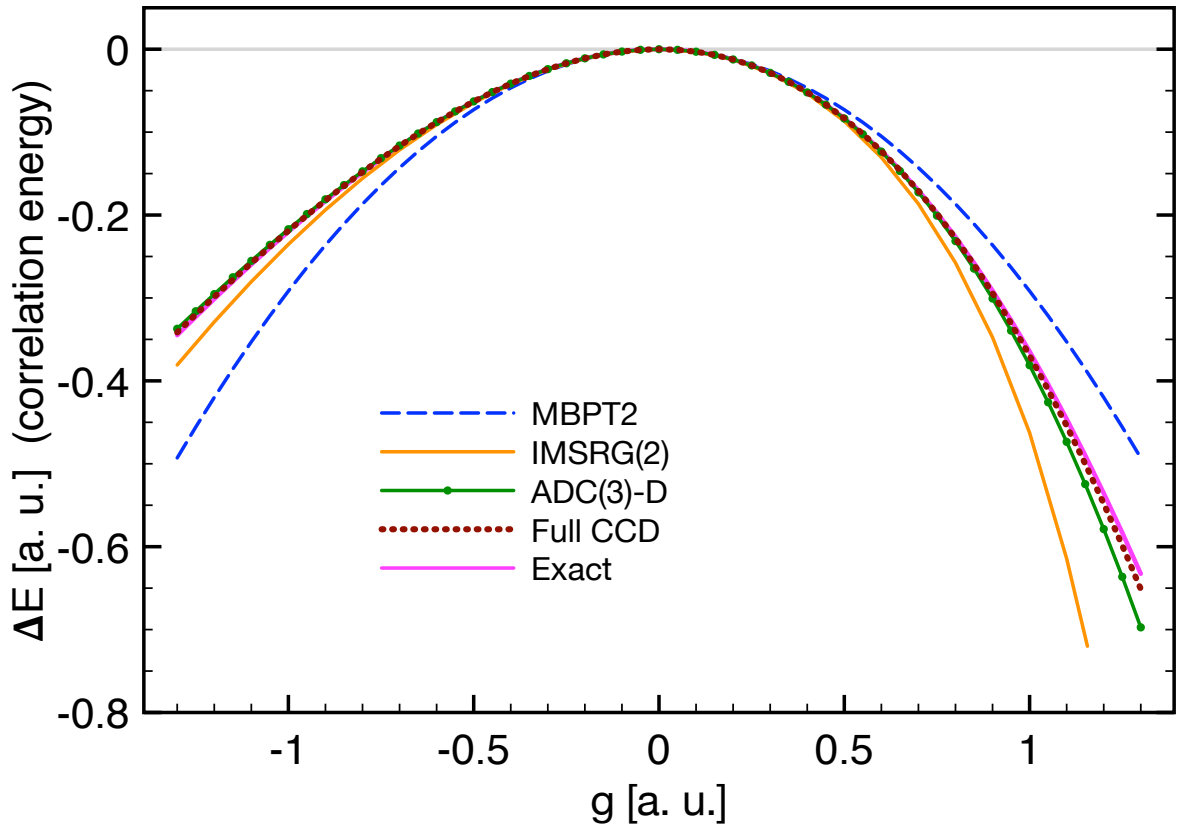
$$|\sum_{p.q} P^\dagger_p P_q|$$

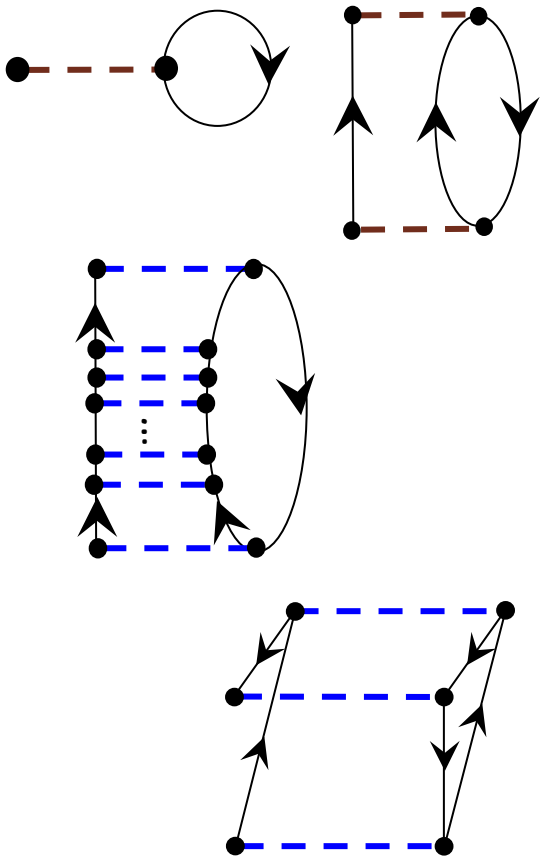


$$\rangle = 0$$

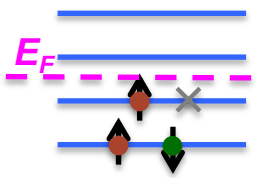
Results for the pairing model

Correlation energy for the 4-level and 4-fermions pairing model

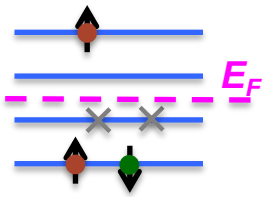




$$\langle\ \Phi_k;1h\ |H_1|\ \Phi^n_{k1,k2};2h1p\ \rangle = \langle$$



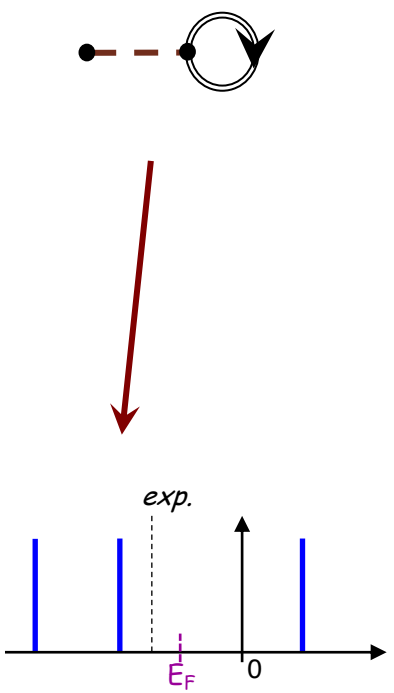
$$|\sum_{p.q} P^\dagger_p P_q|$$



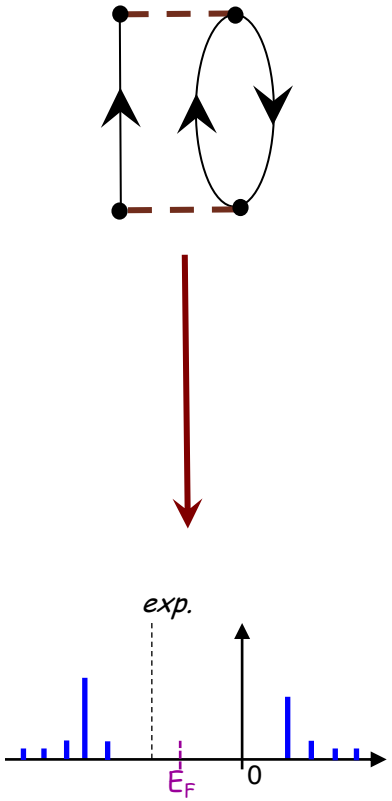
$$\rangle = 0$$

Accuracy of ADC(n) – simple atoms/molecules

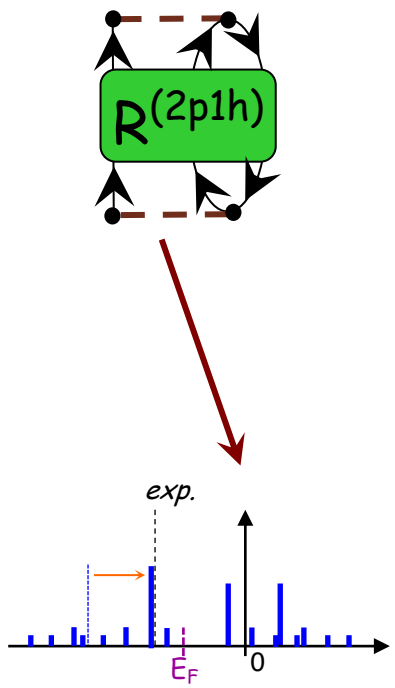
ADC(1) ≡HF



ADC(2) ≡2nd ord.



ADC(3) ≡FTDA
FRPA



98-99% of correlation energy is recovered

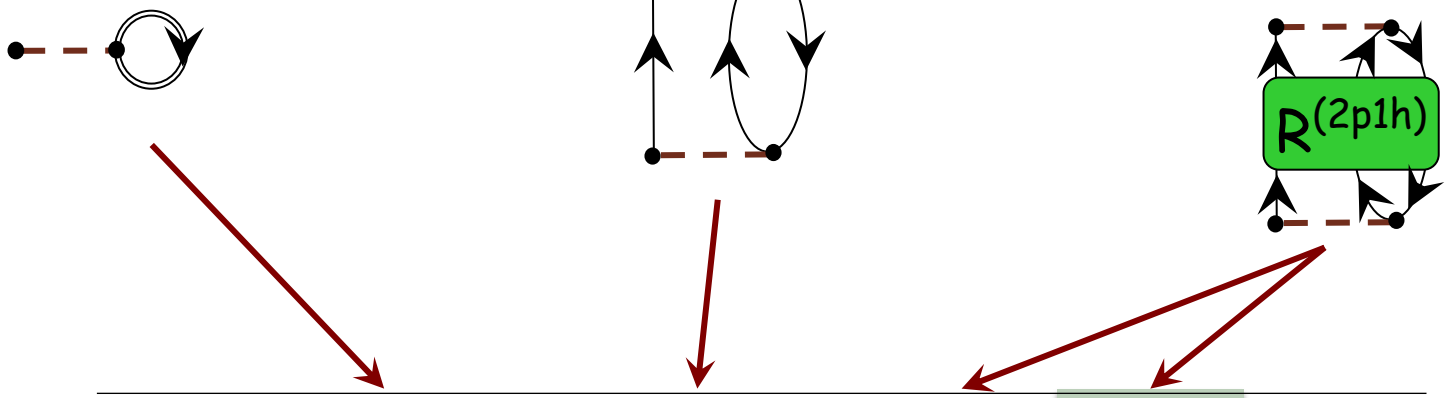
binding, eq. bond distances, → ionization energies (molecules)

Accuracy of ADC(n) – simple atoms/molecules

ADC(1) ≡HF

ADC(2) ≡2nd ord.

ADC(3) ≡FTDA
FRPA



		Hartree-Fock	Second order	FTDA	FRPA	Experiment [63,64]
He	1*s*	0.918(+14)	0.9012(−2.5)	0.9025(−1.2)	0.9008(−2.9)	0.9037
Be^{2+}	1*s*	5.6672(+116)	5.6542(−1.4)	5.6554(−0.2)	5.6551(−0.5)	5.6556
Be	2*s*	0.3093(−34)	0.3187(−23.9)	0.3237(−18.9)	0.3224(−20.2)	0.3426
	1*s*	4.733(+200)	4.5892(+56)	4.5439(+11)	4.5405(+8)	4.533
Ne	2*p*	0.852(+57)	0.752(−41)	0.8101(+17)	0.8037(+11)	0.793
	2*s*	1.931(+149)	1.750(−39)	1.8057(+24)	1.7967(+15)	1.782
Mg^{2+}	2*p*	3.0068(+56.9)	2.9217(−28.2)	2.9572(+7.3)	2.9537(+3.8)	2.9499
	2*s*	4.4827	4.3283	4.3632	4.3589	
Mg	3*s*	0.253(−28)	0.267(−14)	0.272(−9)	0.280(−1)	0.281
	2*p*	2.282(+162)	2.117(−3)	2.141(+21)	2.137(+17)	2.12
Ar	3*p*	0.591(+12)	0.563(−16)	0.581(+2)	0.579(≈ 0)	0.579
	3*s*	1.277(+202)	1.111(+36)	1.087(+12)	1.065(−10)	1.075
	3*s*		1.840	1.578	1.544	
σ_{rms} [mH]		81.4	29.3	13.7	10.6	

← ionization energies (atoms)

[M. Degroote, M. Van Neck, C. B. Phys. Rev. A **83**, 042517 (2011); **85**, 012501 (2012)]

NB: energies in Hartree
errors in mHartree

Accuracy of FRPA for simple molecules

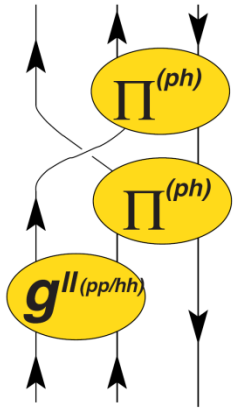
- Diatomic molecules

		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

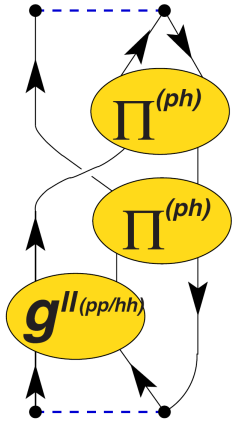
[a] Only up to CCD

[M. Degroote, D. Van Neck, C. B. Phys. Rev. A **83**, 042517 (2011); **85**, 012501 (2012)]

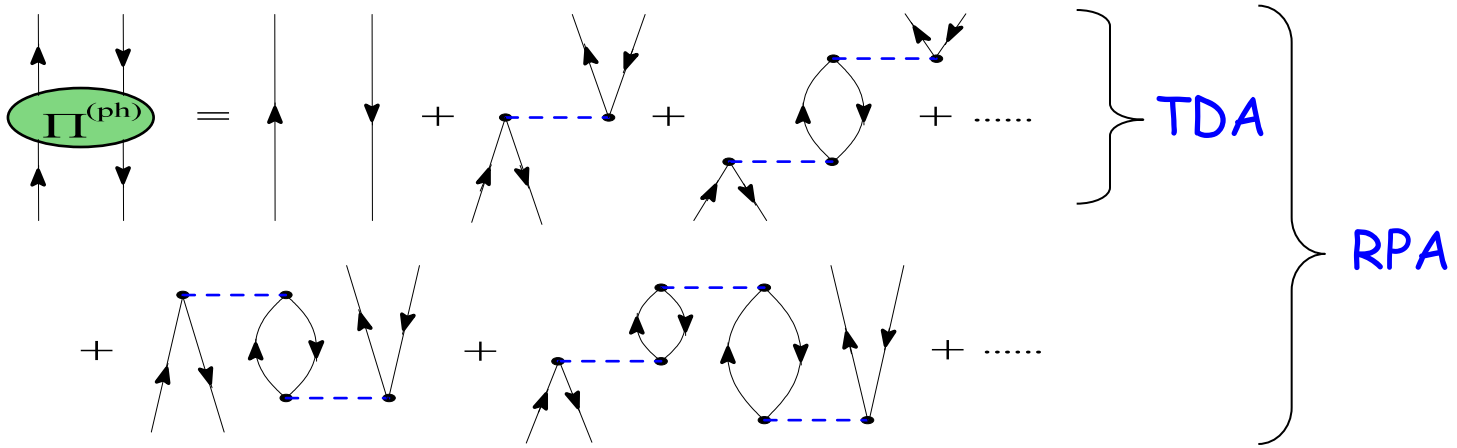
FRPA: Faddeev summation of RPA propagators



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



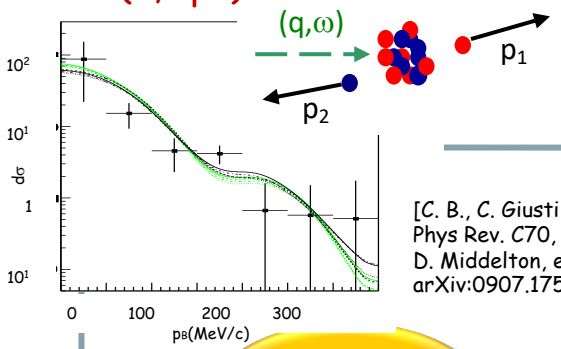
where:



References: CB, et al., Phys. Rev. C**63**, 034313 (2001); Phys. Rev. A**76**, 052503 (2007)
Phys. Rev. C**79**, 064313 (2009)

Self-Consistent Green's Function Approach

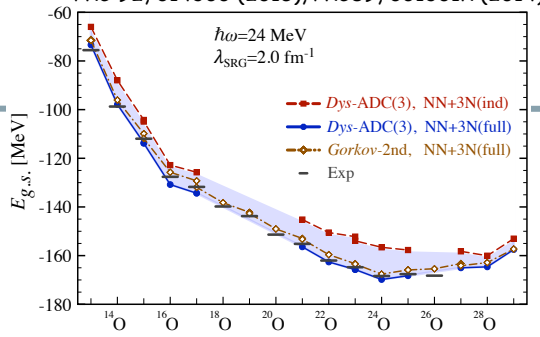
$^{16}O(e,e'pn)^{14}N$ @ MAINZ



[C. B., C. Giusti, et al.
Phys Rev. C70, 014606 (2004)
D. Middelton, et al.
arXiv:0907.1758; EPJA in print]

Binding energies

[PRL. 111, 062501 (2013),
PRC 92, 014306 (2015), PRC89, 061301R (2014)]



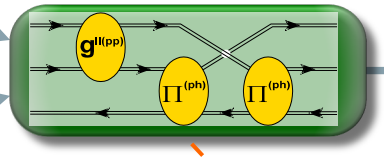
Ionization energies/ affinities, in atoms

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

		Hartree-Fock	FRPAc	Experiment [16, 17]
He:	1s	0.918 (+14)	0.9008 (-2.9)	0.9037
Be^{2+}:	1s	5.6672 (+116)	5.6551 (-0.5)	5.6556
Be:	2s	0.3093 (-34)	0.3224 (-20.2)	0.3426
	1s	4.733 (+200)	4.5405 (+8)	4.533
Ne:	2p	0.852 (+57)	0.8037 (+11)	0.793
	1s	1.931 (+149)	1.7967 (+15)	1.782
Mg^{2+}:	2p	3.0068 (+56.9)	2.9537 (+3.8)	2.9499
	1s	4.4827	4.3589	
Mg:	3s	0.253 (-28)	0.280 (-1)	0.281
	2p	2.282 (+162)	2.137 (+17)	2.12
Ar:	3p	0.591 (+12)	0.579 (≈0)	0.579
	3s	1.277 (+202)	1.065 (-10)	1.075
	3s		1.544	
	2p	9.571 (+411)	9.219 (+59)	9.160

$g^{II}(\omega)$

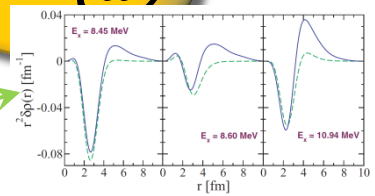
$\Pi^{(ph)}(\omega)$

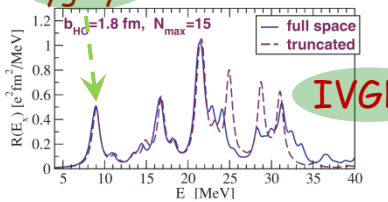


Dyson Eq.

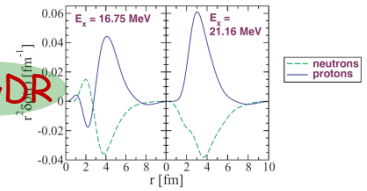
Isovector response for ^{32}Ar, ^{34}Ar

Proton Pygmy



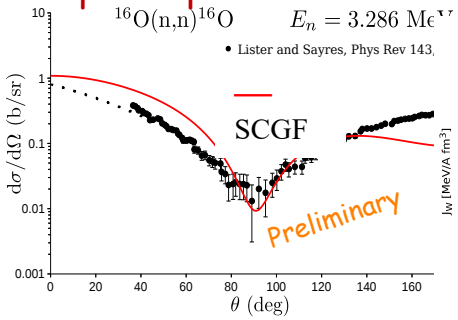


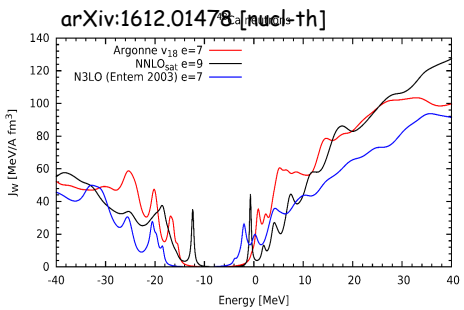
IVGDR



[C. B., K. Langanke, et al., Phys Rev. C77, 024304 (2008)]

Optical potential





Developments needed for Nuclear physics

- Large scale computations of Self-energy ADC(n) - FRPA
- Going to open shell isotopes (Gorkov-SCGF)
- Need for 3-nucleon forces
- Handling strong short-range interactions

Reaching open-Oshell nuclei:

The Gorkov GF approach

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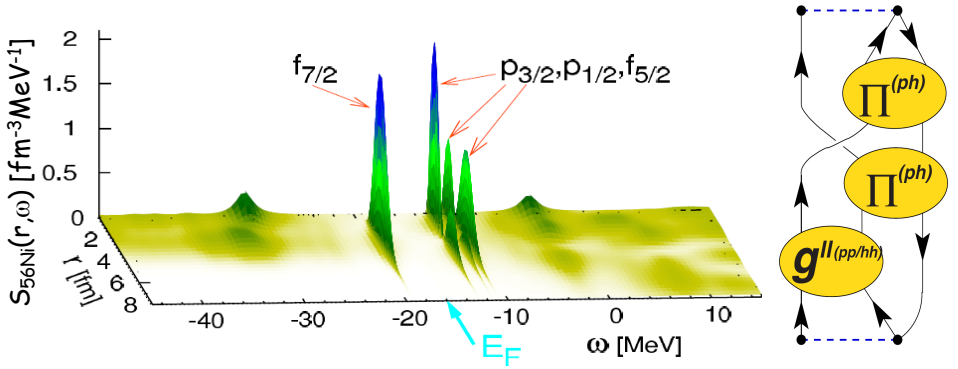
Applications to semi-magic nuclei

✺ Faddeev-RPA approximation for the self-energy [2001-2013]

collective vibrations

particle-vibration coupling



✺ Successful in medium-mass doubly-magic systems

→ Expansion breaks down when pairing instabilities appear

Explicit configuration mixing

Single-reference: Bogoliubov (Gorkov)

Gorkov and symmetry breaking approaches

V. Somà, T. Duguet, CB, Phys. Rev. C **84**, 064317 (2011)
V. Somà, CB, T. Duguet, Phys. Rev. C **87**, 011303R (2013)
V. Somà, CB, T. Duguet, , Phys. Rev. C **89**, 024323 (2014)

- Ansatz $\quad \ldots \approx E_0^{N+2} - E_0^N \approx E_0^N - E_0^{N-2} \approx \ldots \approx 2\mu$

- Auxiliary many-body state $\quad |\Psi_0\rangle \equiv \sum_N^{\text{even}} c_N \, |\psi_0^N\rangle$

  → Mixes various particle numbers

  → Introduce a "grand-canonical" potential $\quad \Omega = H - \mu N$

⇒ $|\Psi_0\rangle$ minimizes $\quad \Omega_0 = \langle\Psi_0|\Omega|\Psi_0\rangle$ under the constraint $\quad N = \langle\Psi_0|N|\Psi_0\rangle$

- This approach leads to the Gorkov equation (that generalizes Dyson)

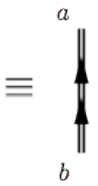
$$\mathbf{G}_{ab}(\omega) = \mathbf{G}^{(0)}_{ab}(\omega) + \sum_{cd} \mathbf{G}^{(0)}_{ac}(\omega)\, \mathbf{\Sigma}^{\star}_{cd}(\omega)\, \mathbf{G}_{db}(\omega)$$

Gorkov Green's functions and equations

[V. Somà, T. Duguet, CB, Pys. Rev. C84, 046317 (2011)]

✺ Set of 4 Green's functions

$$i\,G^{11}_{ab}(t,t') \equiv \langle\Psi_0|T\left\{a_a(t)a^\dagger_b(t')\right\}|\Psi_0\rangle \equiv$$



$$i\,G^{21}_{ab}(t,t') \equiv \langle\Psi_0|T\left\{\bar{a}^\dagger_a(t)a^\dagger_b(t')\right\}|\Psi_0\rangle \equiv$$

$$i\,G^{12}_{ab}(t,t') \equiv \langle\Psi_0|T\left\{a_a(t)\bar{a}_b(t')\right\}|\Psi_0\rangle \equiv$$

$$i\,G^{22}_{ab}(t,t') \equiv \langle\Psi_0|T\left\{\bar{a}^\dagger_a(t)\bar{a}_b(t')\right\}|\Psi_0\rangle \equiv$$

[Gorkov 1958]

$$\mathbf{G}_{ab}(\omega) = \mathbf{G}^{(0)}_{ab}(\omega) + \sum_{cd} \mathbf{G}^{(0)}_{ac}(\omega)\,\mathbf{\Sigma}^\star_{cd}(\omega)\,\mathbf{G}_{db}(\omega)$$

Gorkov equations

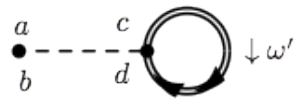
$$\mathbf{\Sigma}^\star_{ab}(\omega) \equiv \begin{pmatrix} \Sigma^{\star\,11}_{ab}(\omega) & \Sigma^{\star\,12}_{ab}(\omega) \\ \Sigma^{\star\,21}_{ab}(\omega) & \Sigma^{\star\,22}_{ab}(\omega) \end{pmatrix}$$

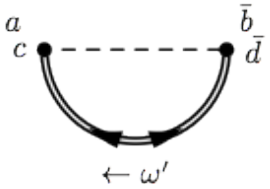
$$\mathbf{\Sigma}^\star_{ab}(\omega) \equiv \mathbf{\Sigma}_{ab}(\omega) - \mathbf{U}_{ab}$$

Open-shells: 1st & 2nd order Gorkov diagrams

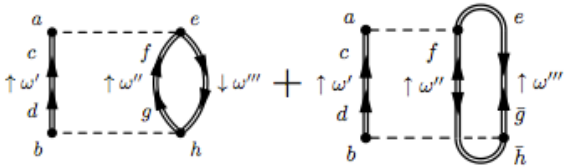
V. Somà, CB, T. Duguet, , Phys. Rev. C **89**, 024323 (2014)
V. Somà, CB, T. Duguet, Phys. Rev. C **87**, 011303R (2013)
V. Somà, T. Duguet, CB, Phys. Rev. C **84**, 064317 (2011)

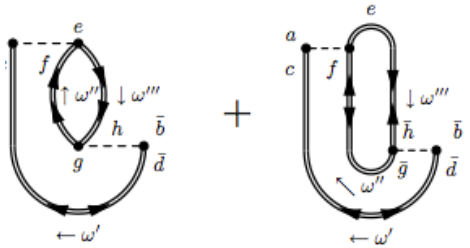
✺ 1st order ➞ energy-independent self-energy

$\Sigma^{11\,(1)}_{ab} =$ 

$\Sigma^{12\,(1)}_{ab} =$ 

✺ 2nd order ➞ energy-dependent self-energy

$\Sigma^{11\,(2)}_{ab}(\omega) =$ 

$\Sigma^{12\,(2)}_{ab}(\omega) =$ 

✺ Gorkov equations ⟶ eigenvalue problem

$$\sum_b \begin{pmatrix} t_{ab} - \mu_{ab} + \Sigma^{11}_{ab}(\omega) & \Sigma^{12}_{ab}(\omega) \\ \Sigma^{21}_{ab}(\omega) & -t_{ab} + \mu_{ab} + \Sigma^{22}_{ab}(\omega) \end{pmatrix}\Bigg|_{\omega_k} \begin{pmatrix} \mathcal{U}^k_b \\ \mathcal{V}^k_b \end{pmatrix} = \omega_k \begin{pmatrix} \mathcal{U}^k_a \\ \mathcal{V}^k_a \end{pmatrix}$$

$$\mathcal{U}^{k*}_a \equiv \langle \Psi_k | \bar{a}^\dagger_a | \Psi_0 \rangle$$
$$\mathcal{V}^{k*}_a \equiv \langle \Psi_k | a_a | \Psi_0 \rangle$$

Espressions for 1st & 2nd order diagrams

[*V. Somà*, T. Duguet, CB, Pys. Rev. C84, 046317 (2011)]

Gorkov equations

[V. Somà, T. Duguet, CB, Pys. Rev. C84, 046317 (2011)]

$$\sum_b \begin{pmatrix} t_{ab} - \mu_{ab} + \Sigma^{11}_{ab}(\omega) & \Sigma^{12}_{ab}(\omega) \\ \Sigma^{21}_{ab}(\omega) & -t_{ab} + \mu_{ab} + \Sigma^{22}_{ab}(\omega) \end{pmatrix} \Bigg|_{\omega_k} \begin{pmatrix} \mathcal{U}^k_b \\ \mathcal{V}^k_b \end{pmatrix} = \omega_k \begin{pmatrix} \mathcal{U}^k_a \\ \mathcal{V}^k_a \end{pmatrix}$$

$$\begin{pmatrix} T - \mu + \Lambda & \tilde{h} & \mathcal{C} & -\mathcal{D}^\dagger \\ \tilde{h}^\dagger & -T + \mu - \Lambda & -\mathcal{D}^\dagger & \mathcal{C} \\ \mathcal{C}^\dagger & -\mathcal{D} & E & 0 \\ -\mathcal{D} & \mathcal{C}^\dagger & 0 & -E \end{pmatrix} \begin{pmatrix} \mathcal{U}^k \\ \mathcal{V}^k \\ \mathcal{W}_k \\ \mathcal{Z}_k \end{pmatrix} = \omega_k \begin{pmatrix} \mathcal{U}^k \\ \mathcal{V}^k \\ \mathcal{W}_k \\ \mathcal{Z}_k \end{pmatrix}$$

Energy *independent* eigenvalue problem

with the normalization condition $\sum_a \left[\left| \mathcal{U}^k_a \right|^2 + \left| \mathcal{V}^k_a \right|^2 \right] + \sum_{k_1 k_2 k_3} \left[\left| \mathcal{W}^{k_1 k_2 k_3}_k \right|^2 + \left| \mathcal{Z}^{k_1 k_2 k_3}_k \right|^2 \right] = 1$

Solving for Dyson

The Dyson / Gorkov eq. is the solved by diagonalizing:

$$\varepsilon^{\pm}\begin{pmatrix}\vec{Z}^{\pm}\\ \vec{W}\\ \\ \vec{U}\end{pmatrix} = \left(\begin{array}{c|c|c} H_0+\mathbf{\Sigma}^{\infty} & \mathbf{M}^{\dagger} & \mathbf{N}^{\dagger} \\ \hline \mathbf{M} & \mathrm{diag}(\mathbf{E}^{fw})+\mathbf{C} & \\ \hline \mathbf{N} & & \mathrm{diag}(\mathbf{E}^{bk})+\mathbf{D} \end{array}\right)\begin{pmatrix}\vec{Z}^{\pm}\\ \vec{W}\\ \\ \vec{U}\end{pmatrix}$$

$$\begin{pmatrix} T-\mu+\Lambda & \tilde{h} & \mathcal{C} & -\mathcal{D}^{\dagger} \\ \tilde{h}^{\dagger} & -T+\mu-\Lambda & -\mathcal{D}^{\dagger} & \mathcal{C} \\ \mathcal{C}^{\dagger} & -\mathcal{D} & E & 0 \\ -\mathcal{D} & \mathcal{C}^{\dagger} & 0 & -E \end{pmatrix}\begin{pmatrix}\mathcal{U}^k\\ \mathcal{V}^k\\ \mathcal{W}_k\\ \mathcal{Z}_k\end{pmatrix} = \omega_k\begin{pmatrix}\mathcal{U}^k\\ \mathcal{V}^k\\ \mathcal{W}_k\\ \mathcal{Z}_k\end{pmatrix}$$

Use a Lanczos reduction for the big part of the matrix:

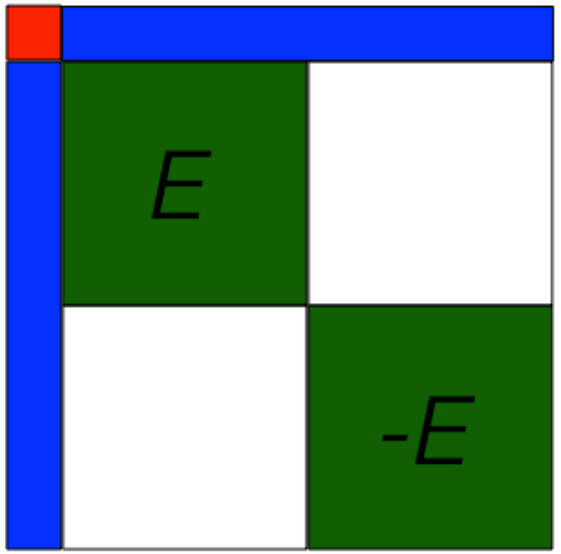
Lanczos reduction of self-energy

V. Somà, CB, T. Duguet, , Phys. Rev. C **89**, 024323 (2014)

$$\begin{pmatrix} T-\mu+\Lambda & \tilde{h} & \mathcal{C} & -\mathcal{D}^\dagger \\ \tilde{h}^\dagger & -T+\mu-\Lambda & -\mathcal{D}^\dagger & \mathcal{C} \\ \mathcal{C}^\dagger & -\mathcal{D} & E & 0 \\ -\mathcal{D} & \mathcal{C}^\dagger & 0 & -E \end{pmatrix} \begin{pmatrix} \mathcal{U}^k \\ \mathcal{V}^k \\ \mathcal{W}_k \\ \mathcal{Z}_k \end{pmatrix} = \omega_k \begin{pmatrix} \mathcal{U}^k \\ \mathcal{V}^k \\ \mathcal{W}_k \\ \mathcal{Z}_k \end{pmatrix}$$

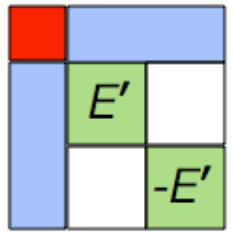
- Conserves moments of spectral functions
- Equivalent to exact diagonalization for $N_L \rightarrow$ dim(E)

HFB



Lanczos

HFB



Numerical challenge:

Matrix E (is huge and) is diagonal in Gorkov ADC(2)
but becomes extremely dense in Gorkov-ADC(3)

Lanczos reduction of self-energy

V. Somà, CB, T. Duguet, , Phys. Rev. C **89**, 024323 (2014)

$$\begin{pmatrix} T-\mu+\Lambda & \tilde{h} & \mathcal{C} & -\mathcal{D}^\dagger \\ \tilde{h}^\dagger & -T+\mu-\Lambda & -\mathcal{D}^\dagger & \mathcal{C} \\ \mathcal{C}^\dagger & -\mathcal{D} & E & 0 \\ -\mathcal{D} & \mathcal{C}^\dagger & 0 & -E \end{pmatrix} \begin{pmatrix} \mathcal{U}^k \\ \mathcal{V}^k \\ \mathcal{W}_k \\ \mathcal{Z}_k \end{pmatrix} = \omega_k \begin{pmatrix} \mathcal{U}^k \\ \mathcal{V}^k \\ \mathcal{W}_k \\ \mathcal{Z}_k \end{pmatrix}$$

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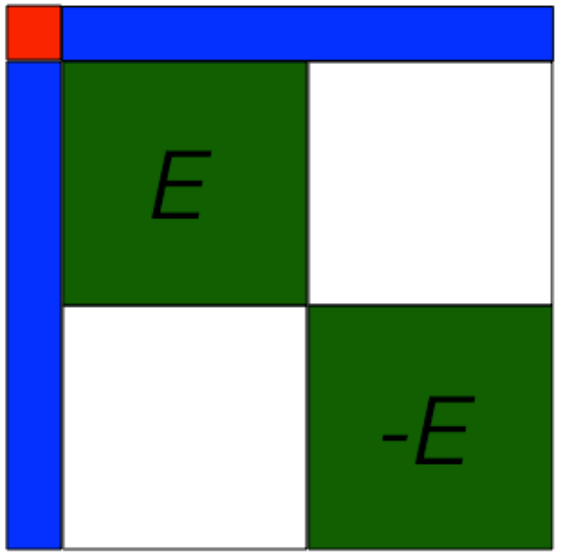
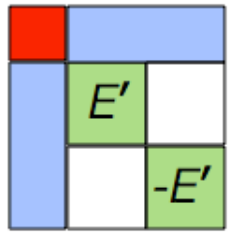
HFB

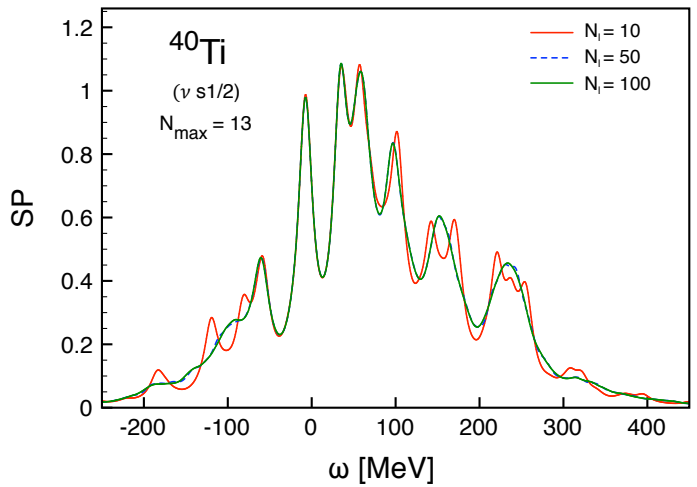


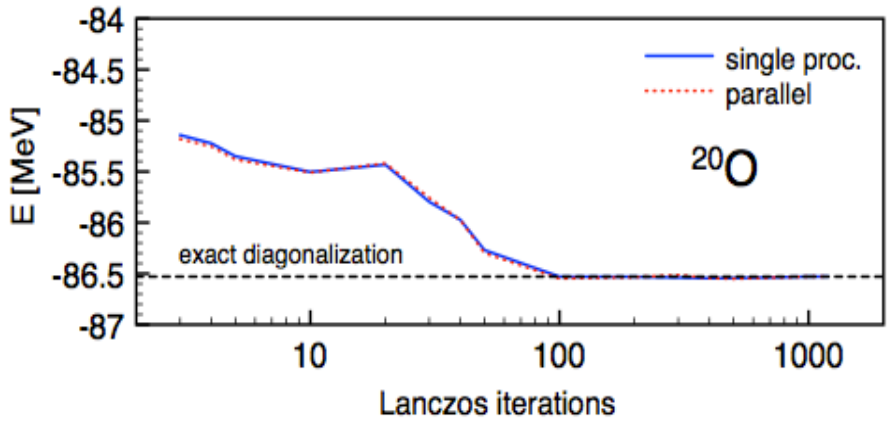
Lanczos

HFB



Spectral strength



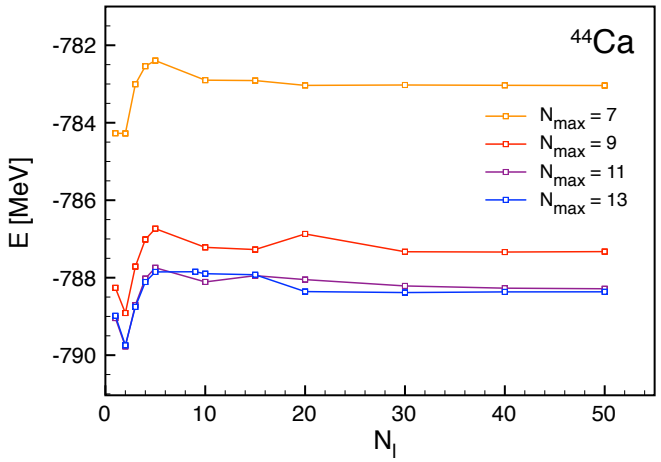


Testing Krylov projection

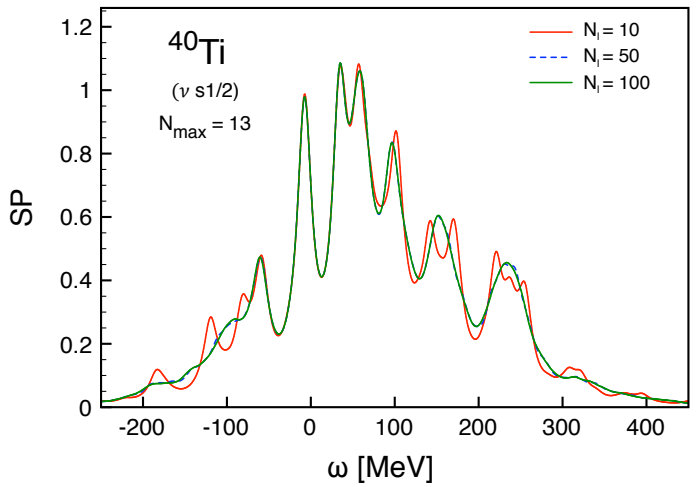
V. Somà, CB, T. Duguet, , Phys. Rev. C **89**, 024323 (2014)

- Energy and spectra independent of the projection
- Same behavior for all model spaces

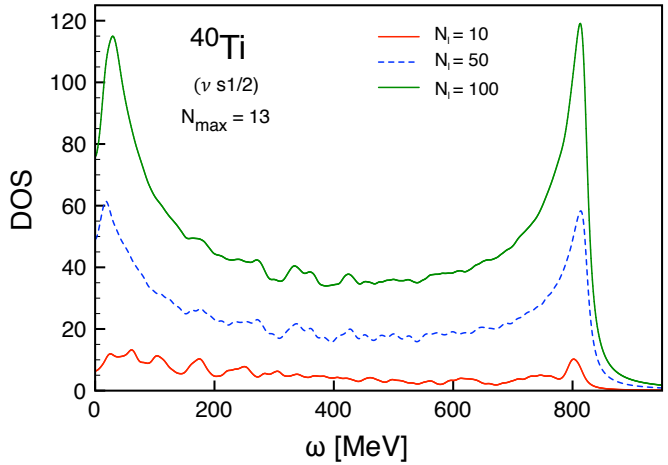
Favourable scaling



Spectral strength



Deinsity of states



Adding three-nucleon interactions

→ application to nuclei
→ need new formalism for many-body forces

A. Carbone, A. Cipollone, CB, A. Rios, A. Polls, Phys. Rev. C**88**, 054326 (2013)
A. Cipollone, CB, P. Navrátil, Phys. Rev. Lett. **111**, 062501 (2013)
F. Raimondi, CB, Phys. Rev. C**97**, 054308 (2018)

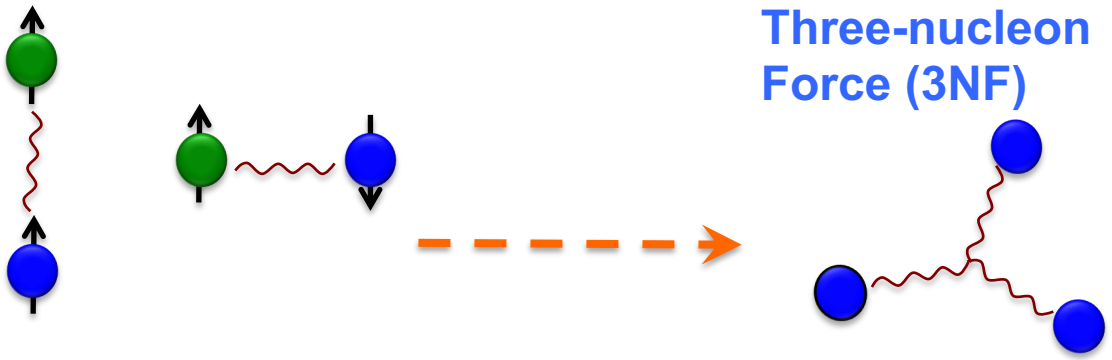
Some key features of the nuclear force

Fundamental features of the nuclear Hamiltonian (and, hence, nuclei):

$$\hat{H}_{nuclear} \approx \hat{T} + V^{NN}_{central}(r) + \ldots + V^{NN}_{tensor}(r)\hat{S}_{12} + \ldots + W^{3N}_{\substack{repulsive \\ FujMiyaz}}(r_{12}, r_{23})$$

Symmetric matter:
N ≈ Z

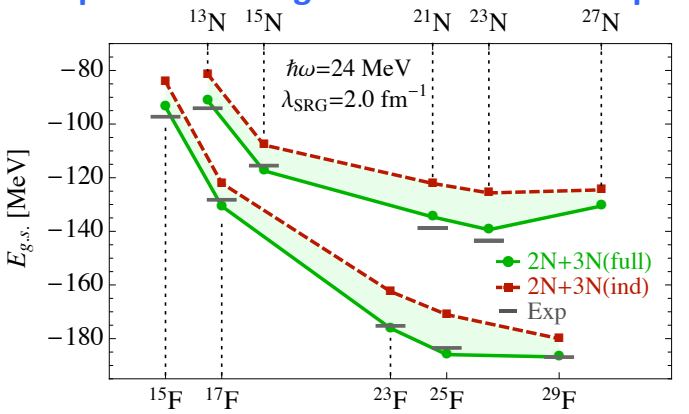
Tensor force (p-n)



Three-nucleon Force (3NF)

Neutron-rich matter (N ≫ Z):
- **Neutron star matter EoS**
- **Symmetry energy**
- **new shell closures**

Driplines of nitrogen and fluorine isotopes



[A. Cipollone, CB, P. Navrátil, Phys. Rev. Lett. **111**, 062501 (2013)]

Change of regime from stable to dripline isotopes !

Feynman rules with 3NF

$\underbrace{a^I_\delta(t) a^{I\dagger}_\gamma(t')} \equiv \left\langle \Phi^N_0 \left| \mathcal{T}\left[a^I_\delta(t) a^{I\dagger}_\gamma(t')\right] \right| \Phi^N_0 \right\rangle = i\hbar\, G^{(0)}_{\delta\gamma}(t-t').$

Applying the Wick theorem to any such arbitrary diagram, results in the following Feynman rules.

Rule 1: Draw all, topologically distinct and connected diagrams with k vertices, and p incoming and p outgoing external lines, using directed arrows. For interaction vertices the external lines are not present.

Rule 2: Each oriented fermion line represents a Wick contraction, leading to the unperturbed propagator $i\hbar G^{(0)}_{\alpha\beta}(t-t')$ [or $i\hbar G^{(0)}_{\alpha\beta}(\omega_i)$]. In time formulation, the t and t' label the times of the vertices at the end and at the beginning of the line. In energy formulation, ω_i denotes the energy carried by the propagator.

Rule 3: Each fermion line starting from and ending at the *same* vertex is an equal-time propagator, $-i\hbar G^{(0)}_{\alpha\beta}(0^-) = \rho^{(0)}_{\alpha\beta}$.

Rule 4: For each 1B, 2B or 3B vertex, write down a factor $\frac{i}{\hbar}U_{\alpha\beta}$, $-\frac{i}{\hbar}V_{\alpha\gamma,\beta\delta}$ or $-\frac{i}{\hbar}W_{\alpha\gamma\xi,\beta\delta\theta}$, respectively. For effective interactions, the factors are $-\frac{\mathrm{i}}{\hbar}\widetilde{U}_{\alpha\beta}$, $-\frac{\mathrm{i}}{\hbar}\widetilde{V}_{\alpha\gamma,\beta\delta}$.

Rule 5: Include a factor $(-1)^L$ where L is the number of closed fermion loops. This sign comes from the odd permutation of operators needed to create a loop and does not include loops of a single propagator, already accounted for by Rule 3.

Rule 6: For a diagram representing a $2p$-point GF, add a factor $(-i/\hbar)$, whereas for a $2p$-point interaction vertex without external lines (such as $\Sigma^\star$ and Γ^{2p-pt}) add a factor $i\hbar$.

The next two rules require a distinction between the time and the energy representation. In the time representation,

Rule 7: Assign a time to each interaction vertex. All the fermion lines connected to the same vertex i share the same time t_i.

Rule 8: Sum over all the internal quantum numbers and integrate over all internal times from $-\infty$ to $+\infty$.

Alternatively, in energy representation,

Rule 7′: Label each fermion line with an energy ω_i, under the *constraint* that the total incoming energy equals the total outgoing energy at each interaction vertex, $\sum_i \omega_i^{\mathrm{in}} = \sum_i \omega_i^{\mathrm{out}}$.

Rule 8′: Sum over all the internal quantum numbers and integrate over each independent internal energy, with an extra factor $\frac{1}{2\pi}$, i.e., $\int_{-\infty}^{+\infty}\frac{d\omega_i}{2\pi}$.

Each diagram is then multiplied by a combinatorial factor S that originates from the number of equivalent Wick contractions that lead to it. This symmetry factor represents the order of the symmetry group for one specific diagram or, in other words, the order of the permutation group of both open and closed lines, once the vertices are fixed. Its structure, assuming only 2BFs and 3BFs, is the following:

$$S = \frac{1}{k!}\frac{1}{[(2!)^2]^q[(3!)^2]^{k-q}}\binom{k}{q} C = \prod_i S_i. \qquad \text{(A1)}$$

Rule 9: For each group of n symmetric lines, or symmetric groups of lines as defined below, multiply by a symmetry factor $S_i = \frac{1}{n!}$. The overall symmetry factor of the diagram will be $S = \prod_i S_i$. Possible cases include the following:

(i) *Equivalent lines*. n equally oriented fermion lines are said to be equivalent if they start from the same initial vertex and end on the same final vertex.

(ii) *Symmetric and interacting lines*. n equally oriented fermion lines that start from the same initial vertex and end on the same final vertex, but are linked via an interaction vertex to one or more close fermion line blocks. The factor arises as long as the diagram is *invariant* under the permutation of the two blocks.

(iii) *Equivalent groups of lines*. These are blocks of interacting lines (e.g., series of bubbles) that are equal to each other: They all start from the same initial vertex and end on the same final vertex.

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A. Carbone, CB, et al., Phys. Rev. C88, 054326 (2013)

Feynman rules with 3NF

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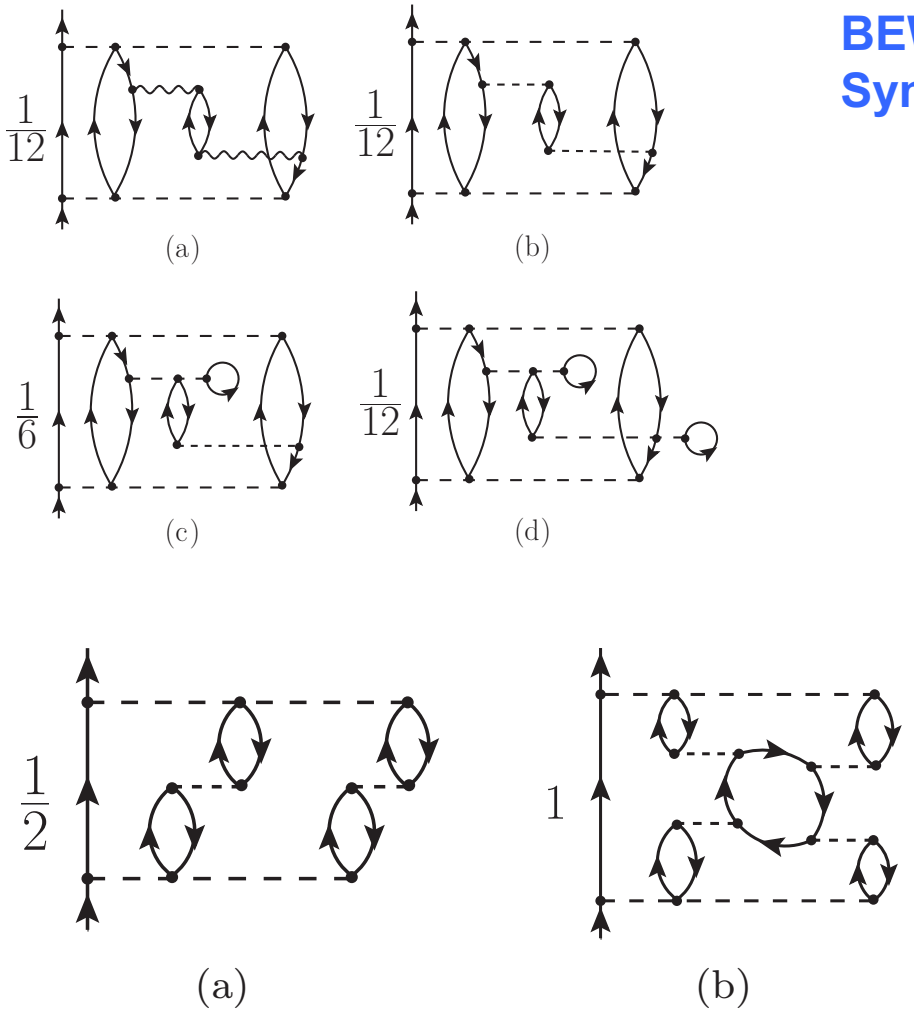


BEWARE of Symmetry factors!

A. Carbone, CB, et al., Phys. Rev. C88, 054326 (2013)

Feynman rules with 3NF

Each diagram is then multiplied by a combinatorial factor S that originates from the number of equivalent Wick contractions that lead to it. This symmetry factor represents the order of the symmetry group for one specific diagram or, in other words, the order of the permutation group of both open and closed lines, once the vertices are fixed. Its structure, assuming only 2BFs and 3BFs, is the following:

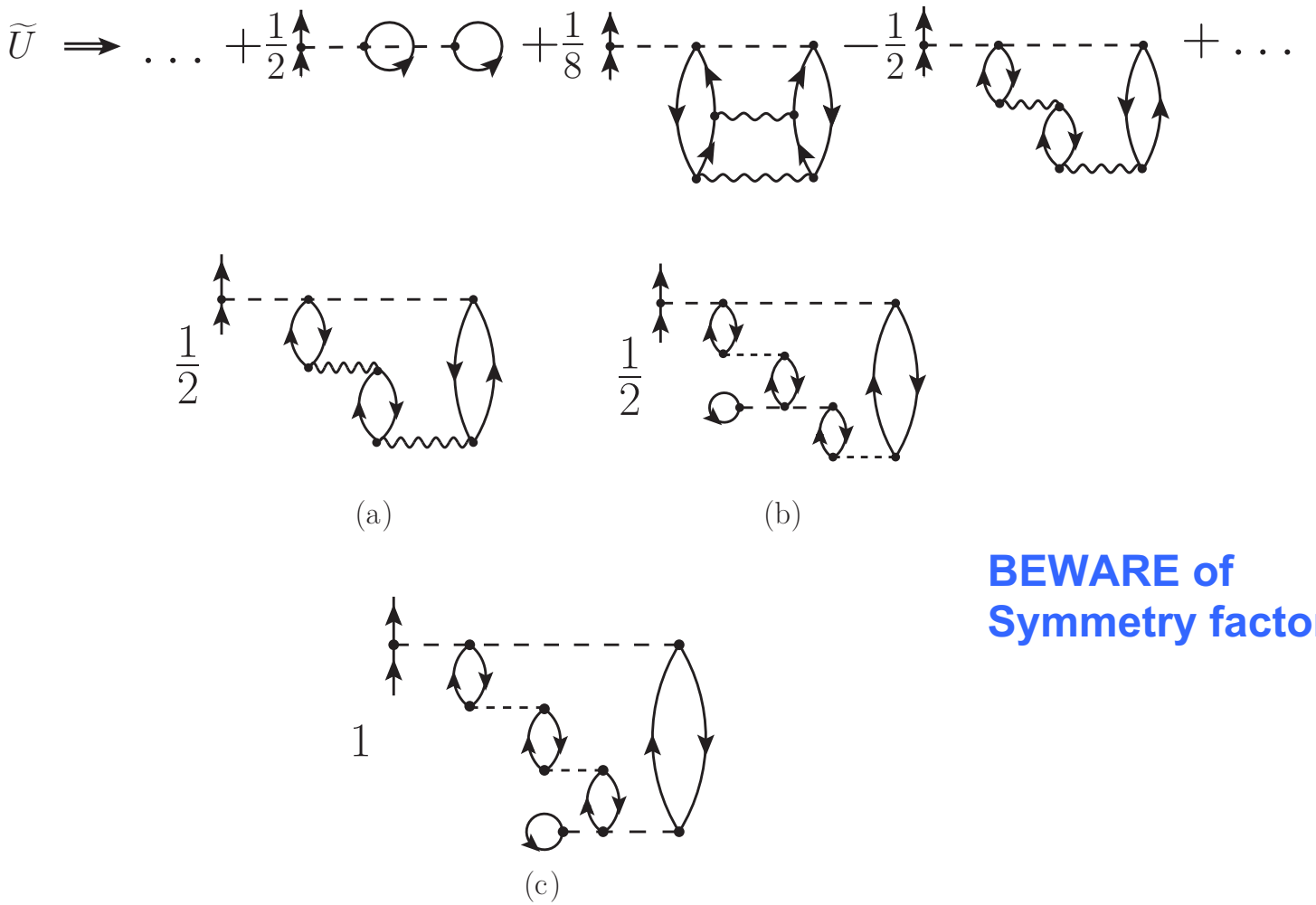
$$S = \frac{1}{k!}\frac{1}{[(2!)^2]^q[(3!)^2]^{k-q}}\binom{k}{q} C = \prod_i S_i . \qquad \text{(A1)}$$

Rule 9: For each group of n symmetric lines, or symmetric groups of lines as defined below, multiply by a symmetry factor $S_i = \frac{1}{n!}$. The overall symmetry factor of the diagram will be $S = \prod_i S_i$. Possible cases include the following:

(i) *Equivalent lines*. n equally oriented fermion lines are said to be equivalent if they start from the same initial vertex and end on the same final vertex.

(ii) *Symmetric and interacting lines*. n equally oriented fermion lines that start from the same initial vertex and end on the same final vertex, but are linked via an interaction vertex to one or more close fermion line blocks. The factor arises as long as the diagram is *invariant* under the permutation of the two blocks.

(iii) *Equivalent groups of lines*. These are blocks of interacting lines (e.g., series of bubbles) that are equal to each other: They all start from the same initial vertex and end on the same final vertex.



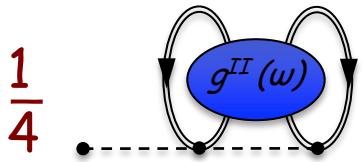
BEWARE of Symmetry factors!

A. Carbone, CB, et al., Phys. Rev. C88, 054326 (2013)

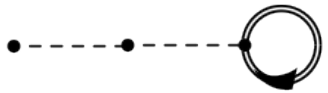
Inclusion of NNN forces

A. Carbone, CB, et al., Phys. Rev. C88, 054326 (2013)

✺ NNN forces can enter diagrams in three different ways:



Correction to external 1-Body interaction



Correction to *non-contracted* 2-Body interaction

pure 3-Body contribution

- Contractions are with *fully correlated density matrices* (BEYOND a normal ordering…)

Inclusion of NNN forces

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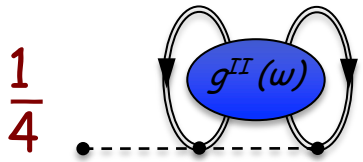

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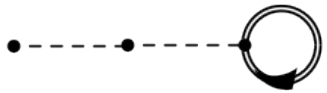

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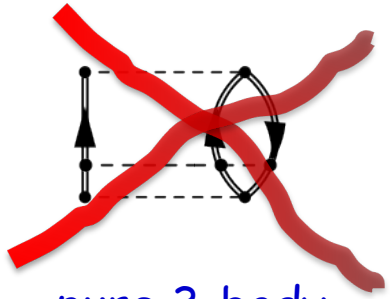

pure 3-body contribution (small)

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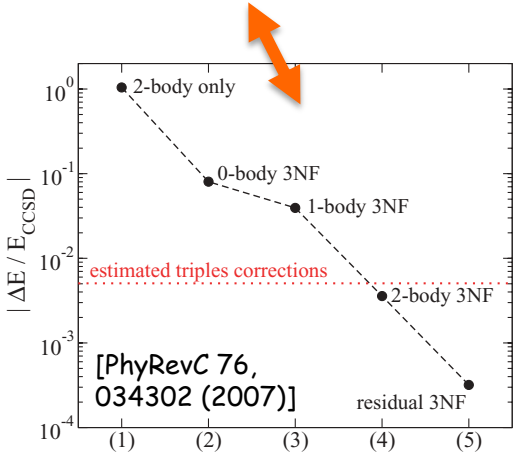

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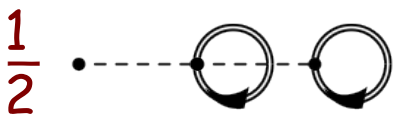

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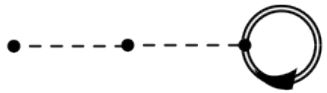

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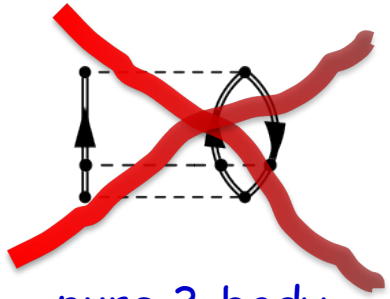

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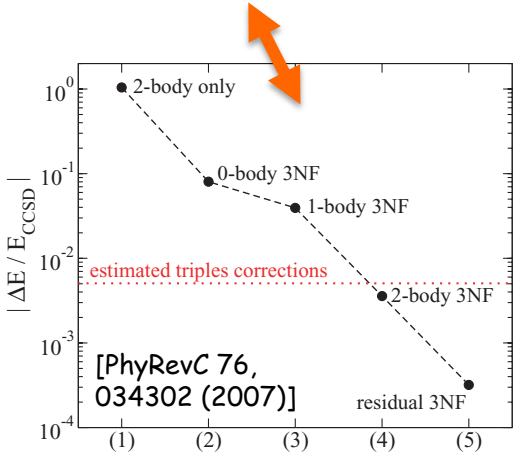

Inclusion of NNN forces

A. Carbone, CB, et al., Phys. Rev. C88, 054326 (2013)

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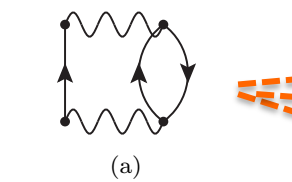
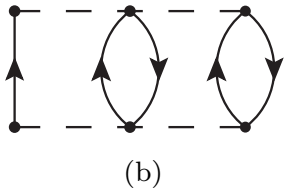




effectively:

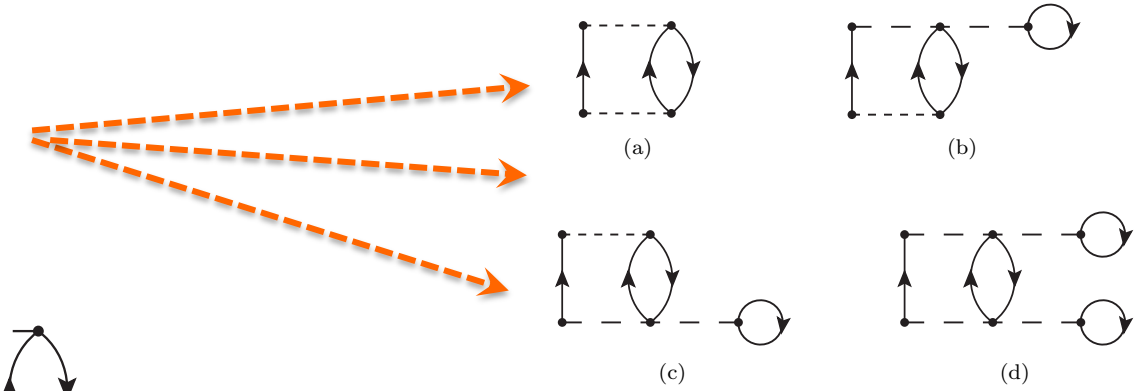
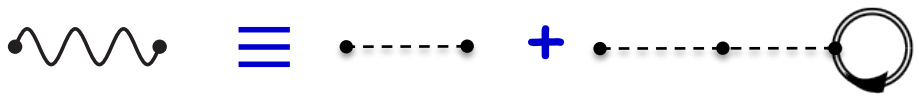


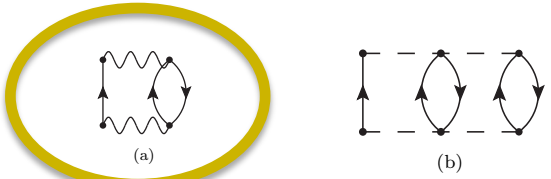
FIG. 4. The one *interaction irreducible* diagrams (a) and the three *interaction reducible* ones (b, c and d) that are contained in Fig. 3a.

NNN forces in the SCGF formalism

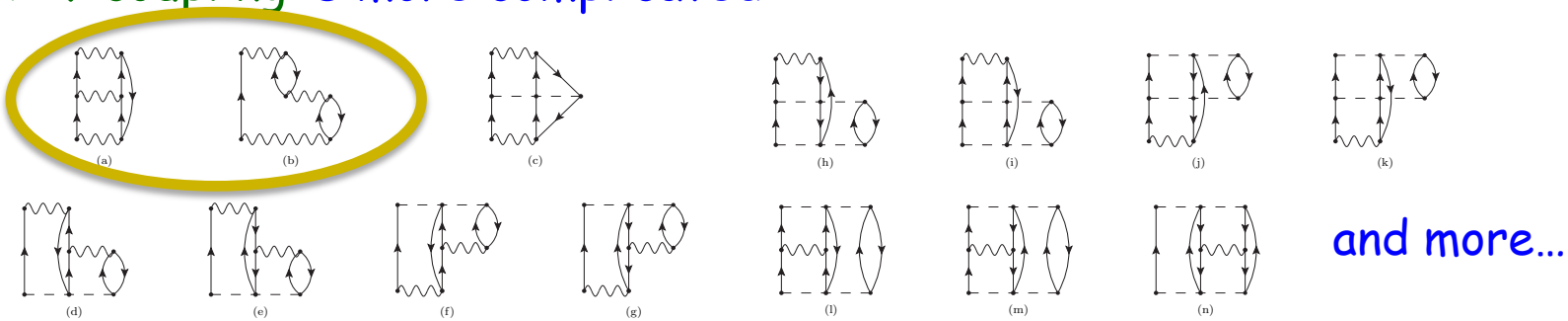
- Introduce effective (system dependent 2-body) interactions. E.g.:



- Complex 3p2h/3h/2p configurations with 3BFs appear earlier:



- P-V coupling is more complicated:



and more…

A. Carbone, CB, et al., Phys. Rev. C**88**, 054326 (2013)

F. Raimondi, CB, Phys Rev C**97**, 054308 (2018)

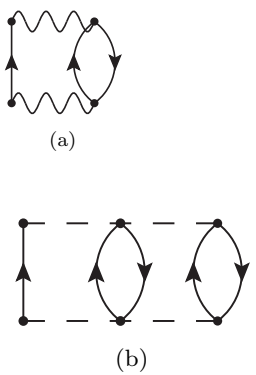
A. Carbone, A. Polls, Phy Rev. C**90**, 044302 (2013)

A. Carbone, A. Rios, A. Polls, Phy Rev. C**90**, 054322 (2014)

} infinite nuclear matter

Inclusion of NNN forces

- Second order PT diagrams with 3BFs:



➔ Use of irreducible 2-body interactions

➔ Need to correct the Koltun sum rule (for energy)

➔ 3p2h/3h2p terms relevant to next-generation high-precision methods.

A. Carbone, CB, et al., Phys. Rev. C88, 054326 (2013)
and F. Raimondi, CB, Phys. Rev. C97, 054308 (2018)

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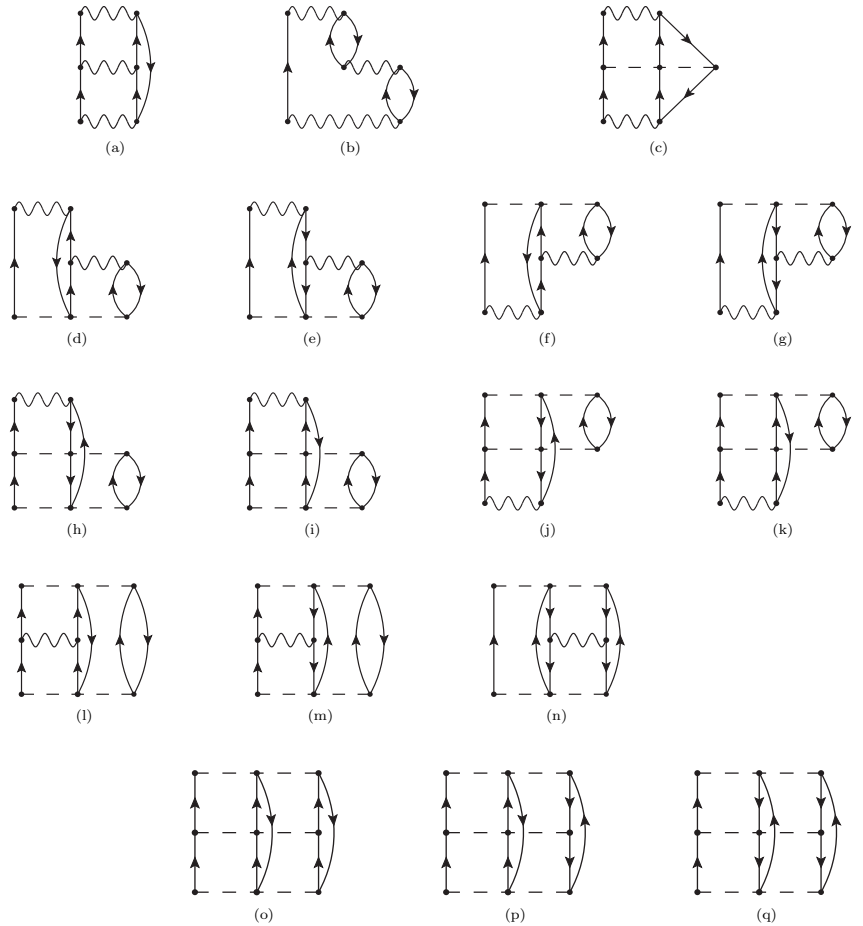

FIG. 5. 1PI, *skeleton* and *interaction irreducible* self-energy diagrams appearing at 3^{rd}-order in perturbative expansion (7), making use of the effective hamiltonian of Eq. (9).

Inclusion of NNN forces

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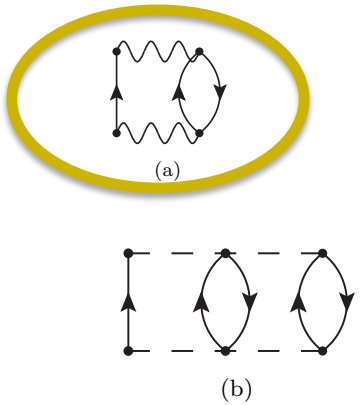

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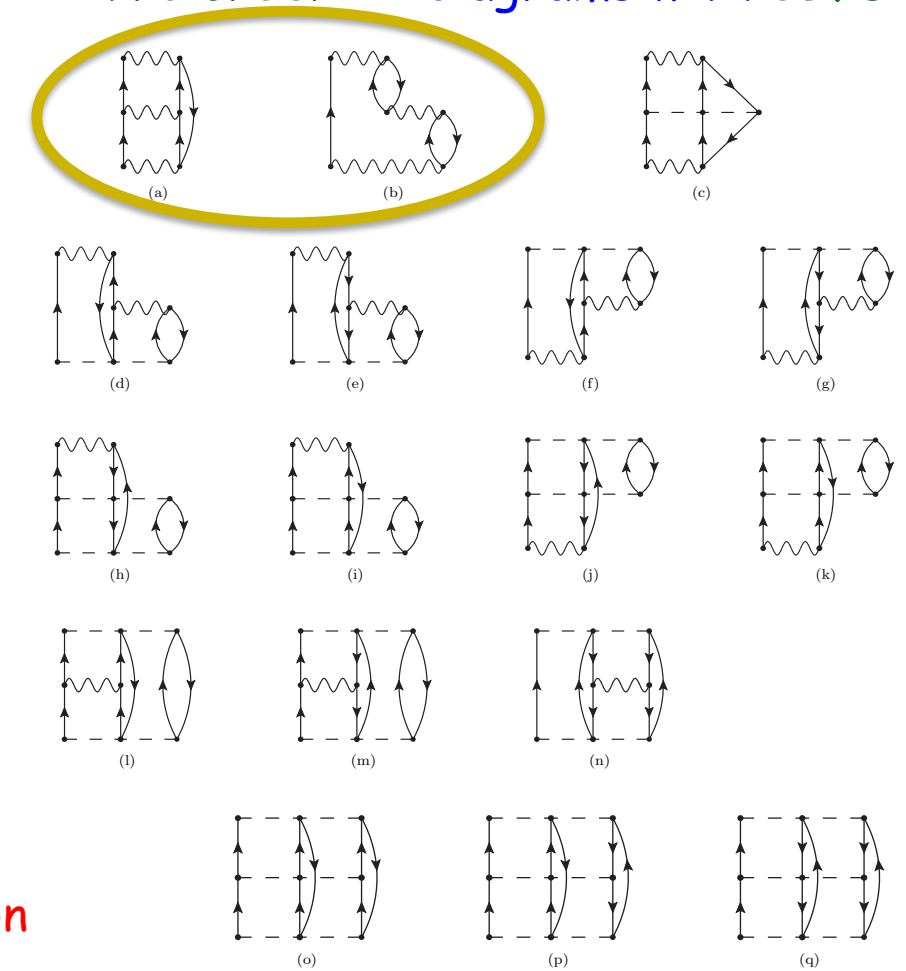

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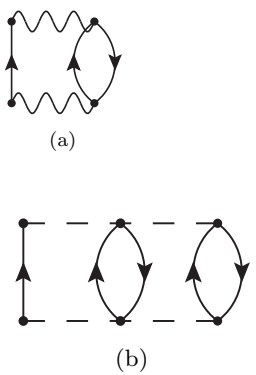

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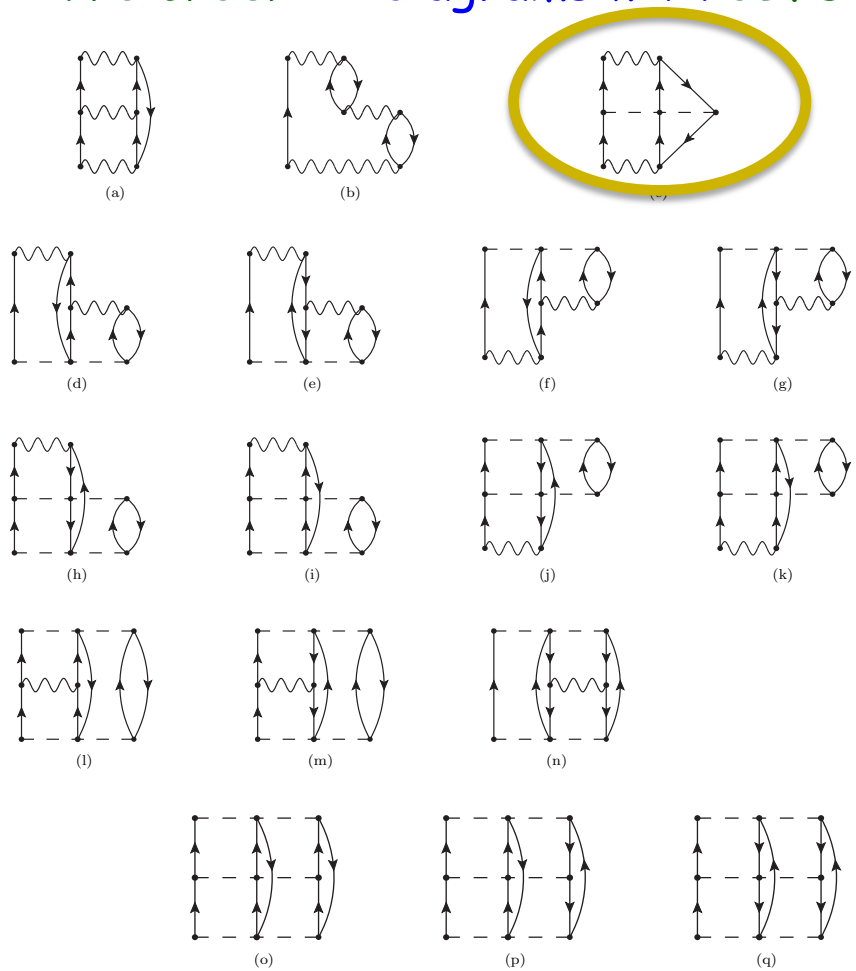

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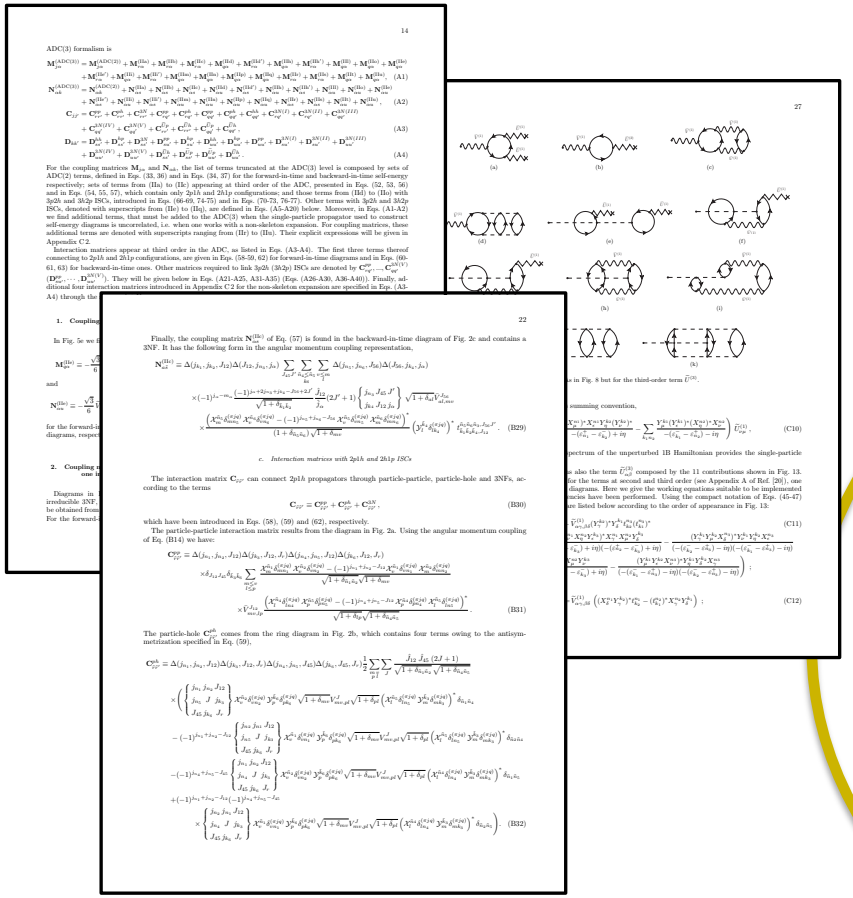

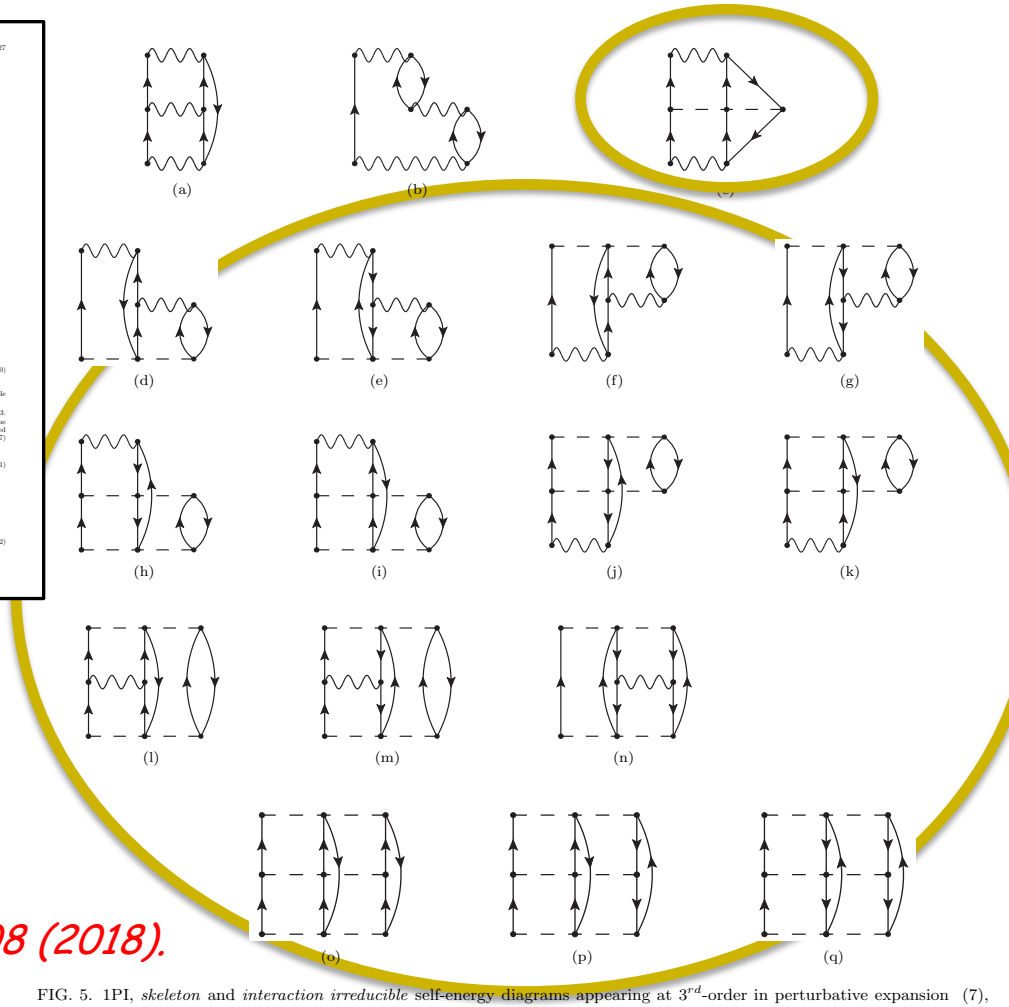

Formalism already laid out:
F. Raimondi, CB, Phys. Rev. C97, 054308 (2018).

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(Galitskii-Migdal-Boffi-) Koltun sumrule

✺ Koltun sum rule (with NNN interactions):

$$\sum_\alpha \frac{1}{\pi}\int_{-\infty}^{\bar{\epsilon_F}} d\omega\, \omega\, \mathrm{Im}\, G_{\alpha\alpha}(\omega) = \langle\Psi_0^N|\hat{T}|\Psi_0^N\rangle + 2\langle\Psi_0^N|\hat{V}|\Psi_0^N\rangle + 3\langle\Psi_0^N|\hat{W}|\Psi_0^N\rangle$$

two-body three-body

✺ Thus, need an extra correction:

$$E_0^N = \frac{1}{3\pi}\int_{-\infty}^{\bar{\epsilon_F}} \mathrm{d}\omega \sum_{\alpha\beta}(2T_{\alpha\beta} + \omega\delta_{\alpha\beta})\mathrm{Im}\, G_{\beta\alpha}(\omega) + \frac{1}{3}\langle\Psi_0^N|\widehat{V}|\Psi_0^N\rangle$$

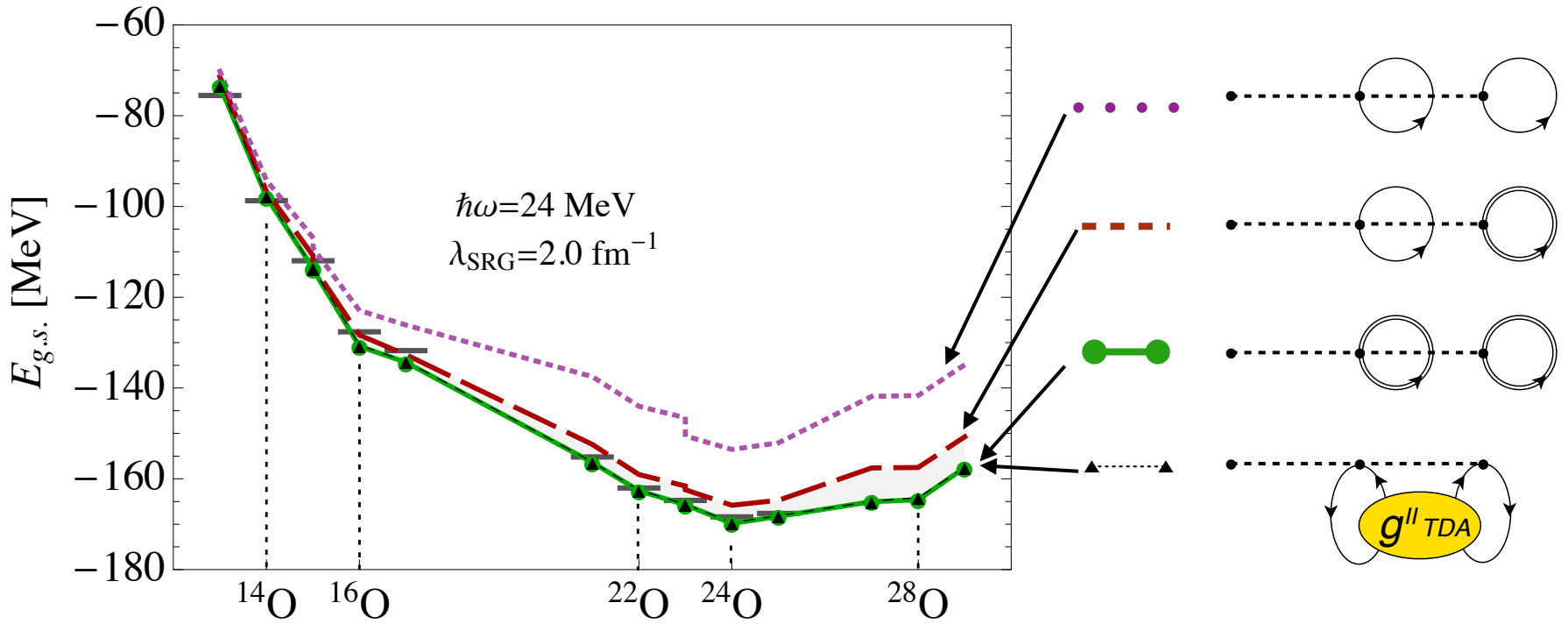
or

$$E_0^N = \frac{1}{2\pi}\int_{-\infty}^{\bar{\epsilon_F}} \mathrm{d}\omega \sum_{\alpha\beta}(T_{\alpha\beta} + \omega\delta_{\alpha\beta})\mathrm{Im}\, G_{\beta\alpha}(\omega) - \frac{1}{2}\langle\Psi_0^N|\widehat{W}|\Psi_0^N\rangle$$

$\langle\Psi_0^N|\widehat{W}|\Psi_0^N\rangle \approx \frac{1}{6}$ 

3N forces in FRPA/FTDA formalism

→ Ladder contributions to static self-energy are negligible (in oxygen)



CB, *arXiv:1405.3002v2 [nucl-th]* (2014)

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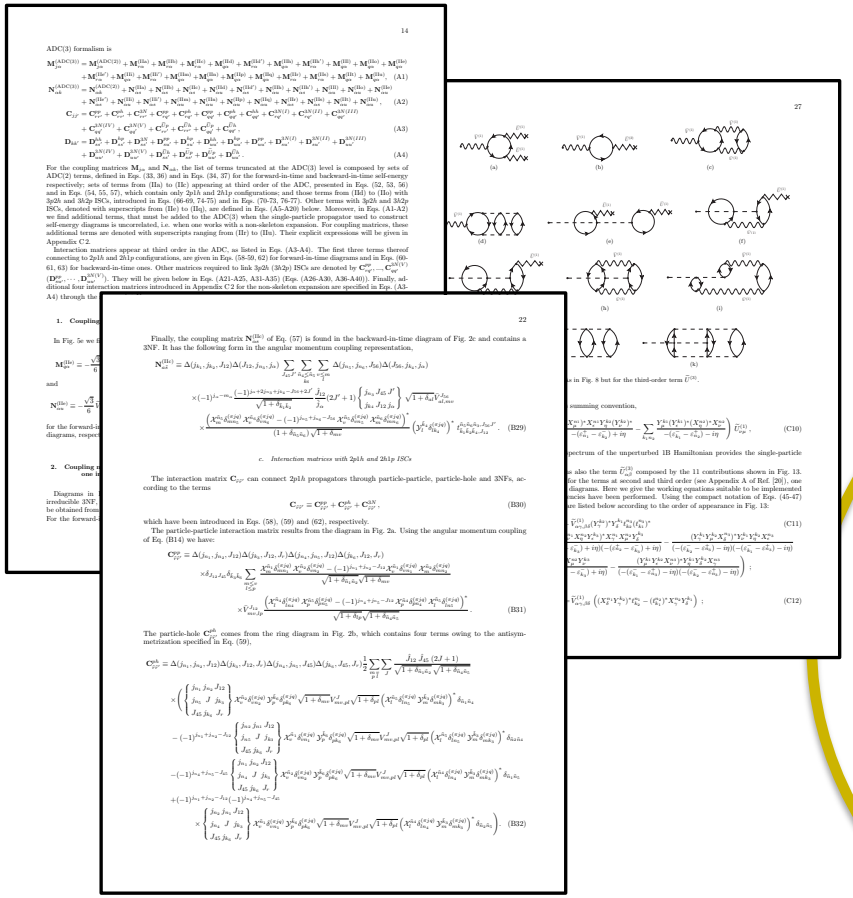

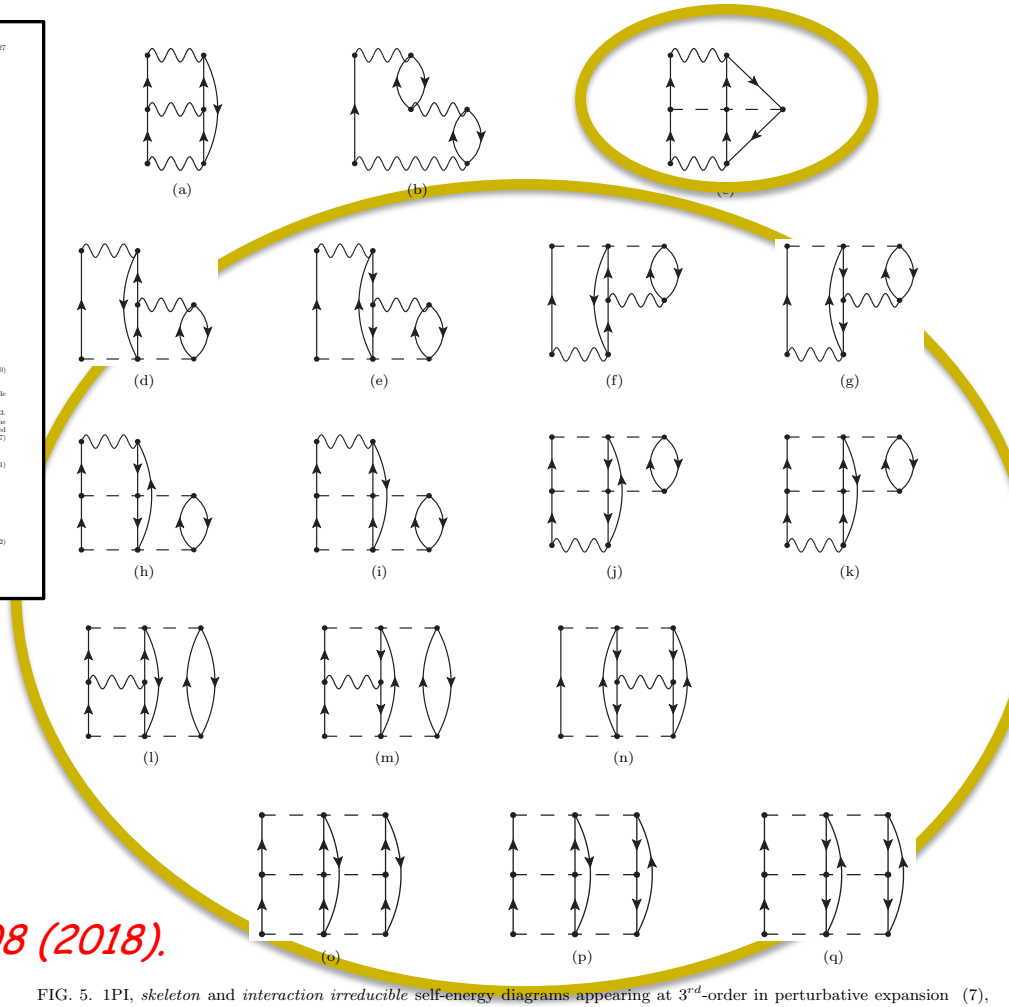

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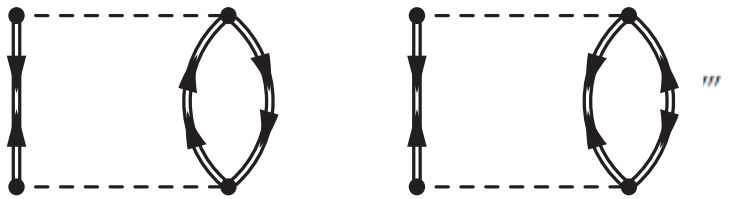
FIG. 5. 1PI, *skeleton* and *interaction irreducible* self-energy diagrams appearing at 3^{rd}-order in perturbative expansion (7), making use of the effective hamiltonian of Eq. (9).

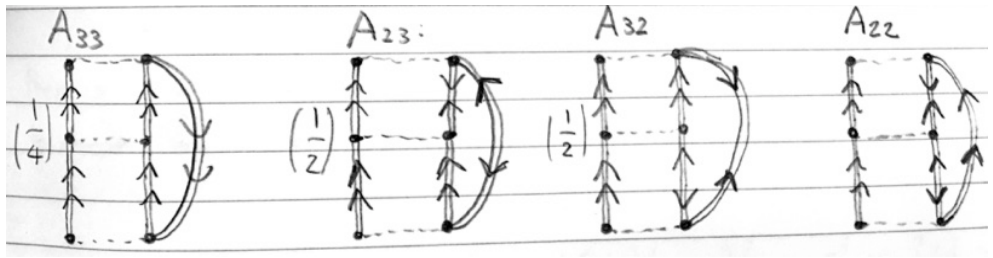
Reaching (Gorkov – 3NF – higher ordes…) is a mess

Gorkov at 2nd order and ONLY NN forces:

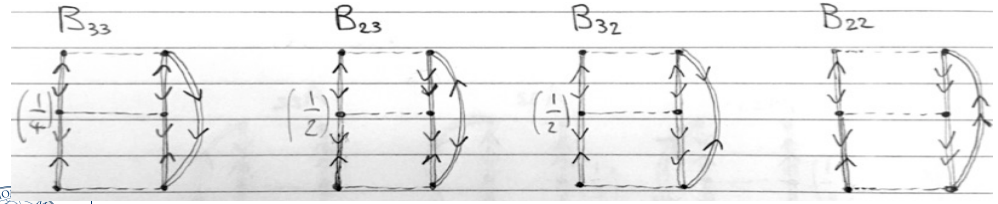
$$\Sigma_{ab}^{11\,(2)}(\omega) =$$  ,,,

Gorkov at 3rd order and ONLY NN forces:

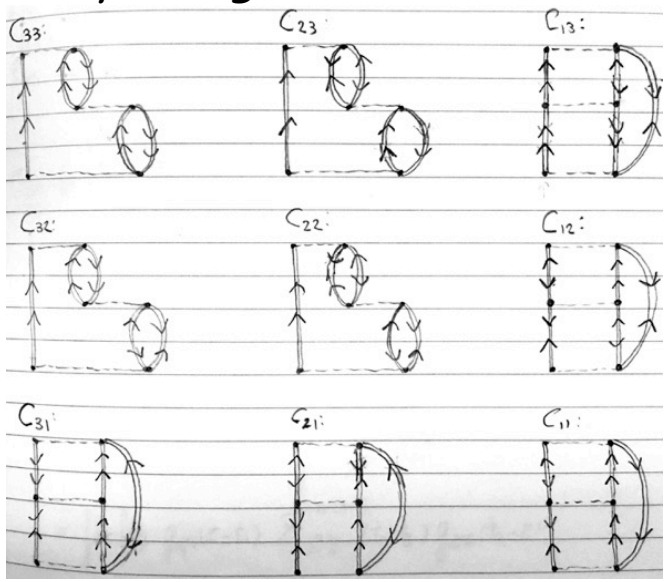
pp/hh-ladders:



hh-interactions (hh int. among pp ladders!!!)



ph-rings:



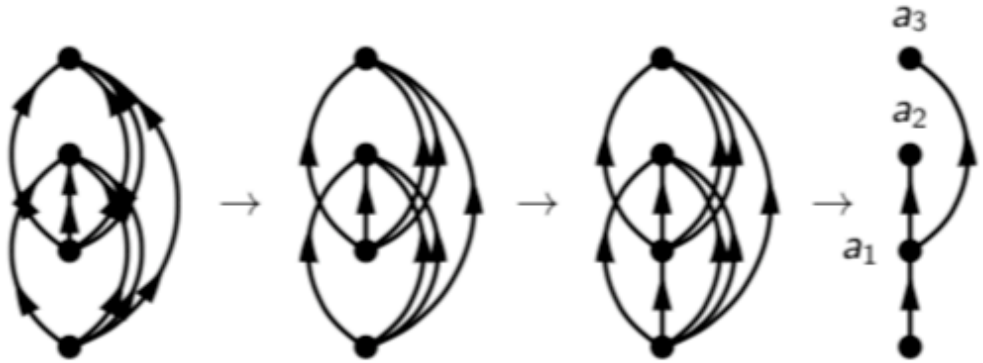
Automatic generation of diagram needed for 3NF and beyond…
➔ F. Raimondi and P. Arthuis, in progress…

Automated generation of BMBPT diagrams

Symmetry-broken many-body perturbation theory expanded in imaginary time:

$$E_0^A - \lambda A = \langle \Psi_0^A | \Omega | \Phi \rangle_c = \lim_{\tau \to \infty} \langle \Phi | T e^{-\int_0^\tau d\tau \Omega_1(\tau)} \Omega | \Phi \rangle_c$$

Tree structure of B-MBPT diagrams:



Github-hosted open-source code ADG

https://github.com/adgproject/adg

Order		0	1	2	3	4	5
0/2/4-leg vertex	General	1	2	8	59	568	6 805
	HFB vacuum	1	1	1	10	82	938
0/2/4/6-leg vertex	General	1	3	23	396	10716	+ 100 000
	HFB vacuum	1	2	8	77	5 055	+ 100 000

P. Arthuis, T. Duguet, A. Tichai, R.-D. Lasseri, J.-P. Ebran, *CPC* **40** (2019)

Automatic Diagrammatic Generation (ADG) of the self-energy

Goal: Drawing of self-energy Feynman diagrams and derivation of corresponding algebraic expressions are performed automatically

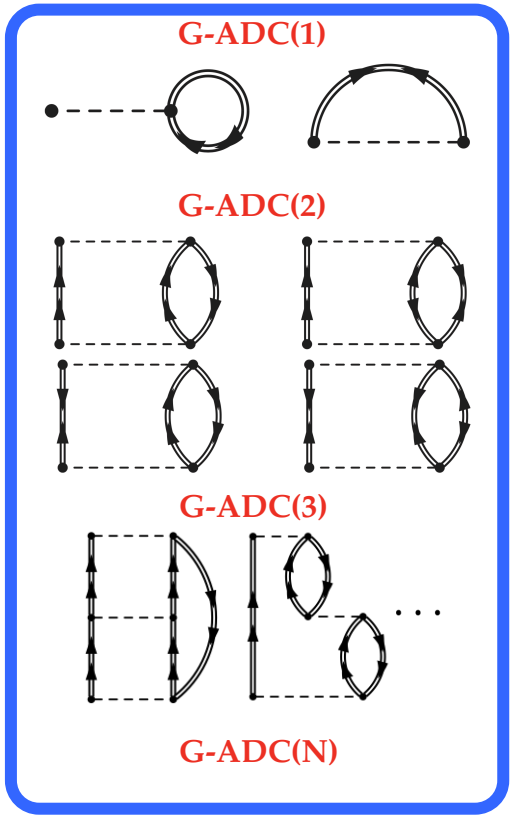
Background: ADG of the BMBPT expansion (P. Arthuis *et al* Comp. Phys. Comm. **240**, 202 (2019))

Feynman rules for Gorkov's self-energy
(V. Somà *et al* . Phys. Rev. C **84**, 064317 (2011))

→

- **Symbolic computation** (`Python`)
- **Graph theory** (`NetworkX` package)
- **Formatting and drawing tools** (`LaTeX`, `TikZ` package)

→



Features:

- Reach arbitrary order in the self-energy expansion
- Different treatments of the self-energy enabled:
  perturbative/nonperturbative(ADC); Dyson/Gorkov; interaction reducible/irreducible, etc
- Faster and less error-prone than "human" derivation

Status:

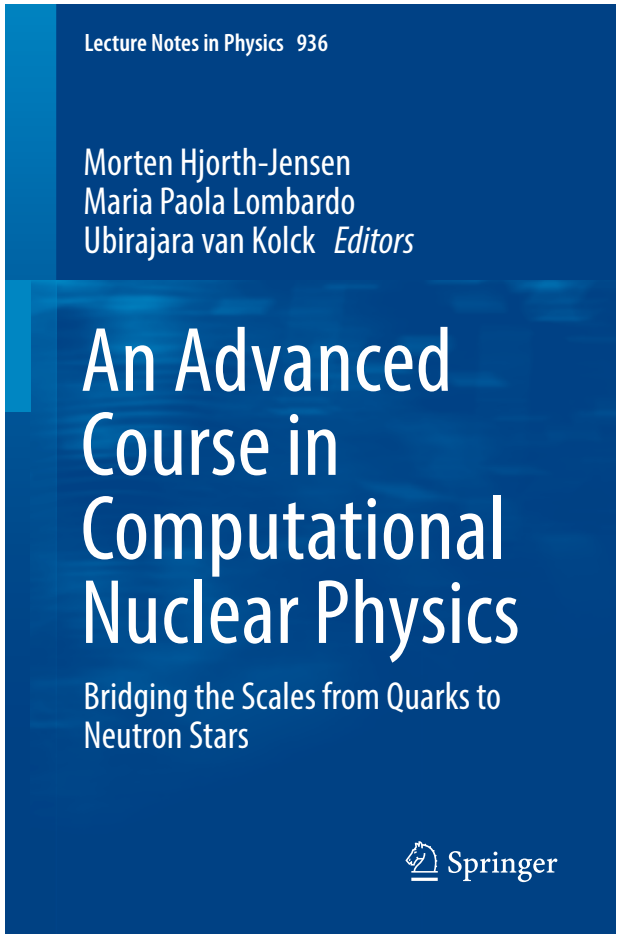
- Drawing of the valid self-energy Feynman diagrams at arbitrary order completed
- Implementation of the rules to obtain algebraic expressions for the diagrams in progress

UNIVERSITÀ DEGLI STUDI DI MILANO
DIPARTIMENTO DI FISICA

*Work in progress by **F. Raimondi**, CEA, Saclay*

Ab-initio Nuclear Computation & BcDor code

Self-consistent Green's function formalism and methods for Nuclear Physics

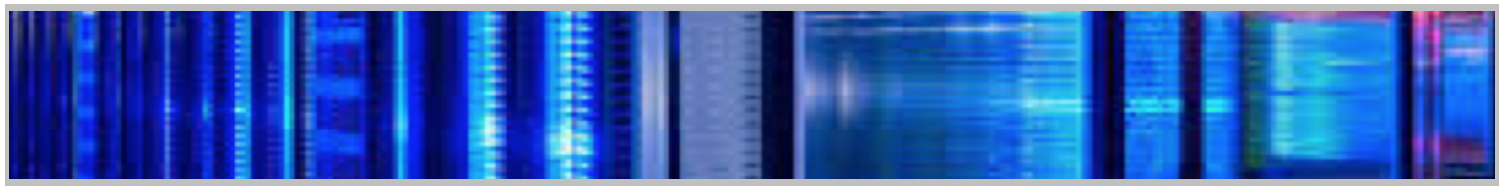


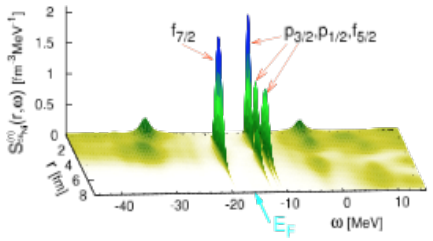
CB and A. Carbone,
chapter 11 of
Lecture Notes in Physics 936 (2017)

http://personal.ph.surrey.ac.uk/~cb0023/bcdor/

https://github.com/craolus/BoccaDorata-public

Computational Many-Body Physics





Download

Documentation

Welcome

From here you can download a public version of my self-consistent Green's function (SCGF) code for nuclear physics. This is a code in J-coupled scheme that allows the calculation of the single particle propagators (a.k.a. one-body Green's functions) and other many-body properties of spherical nuclei.

This version allows to:

- Perform Hartree-Fock calculations.
- Calculate the the correlation energy at second order in perturbation theory (MBPT2).
- Solve the Dyson equation for propagators (self consistently) up to second order in the self-energy.
- Solve coupled cluster CCD (doubles only!) equations.

When using this code you are kindly invited to follow the creative commons license agreement, as detailed at the weblinks below. In particular, we kindly ask you to refer to the publications that led the development of this software.

Relevant references (which can also help in using this code) are:

Prog. Part. Nucl. Phys. 52, p. 377 (2004),
Phys. Rev. A76, 052503 (2007),
Phys. Rev. C79, 064313 (2009),
Phys. Rev. C89, 024323 (2014)

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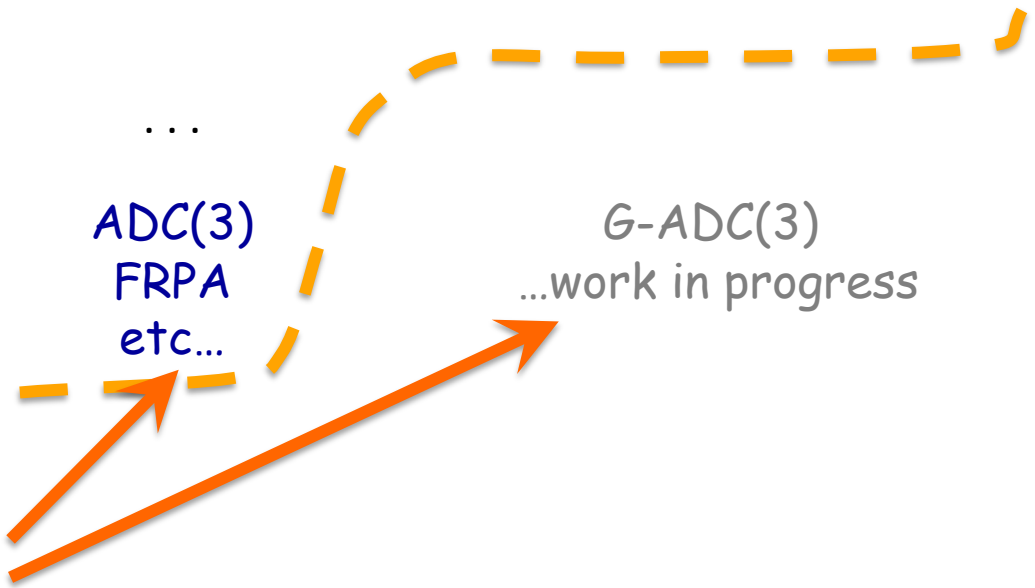
Approaches in GF theory

Truncation scheme:	Dyson formulation (closed shells)	Gorkov formulation (semi-/doubly-magic)
1st order:	Hartree-Fock	HF-Bogolioubov
2nd order:	2nd order	2nd order (w/ pairing)
. . .	. . .	
3rd and all-orders sums, P-V coupling:	ADC(3) FRPA etc…	G-ADC(3) …work in progress



This is a ***non-perturbative all-orders resummation*** — NOT a PT truncation!

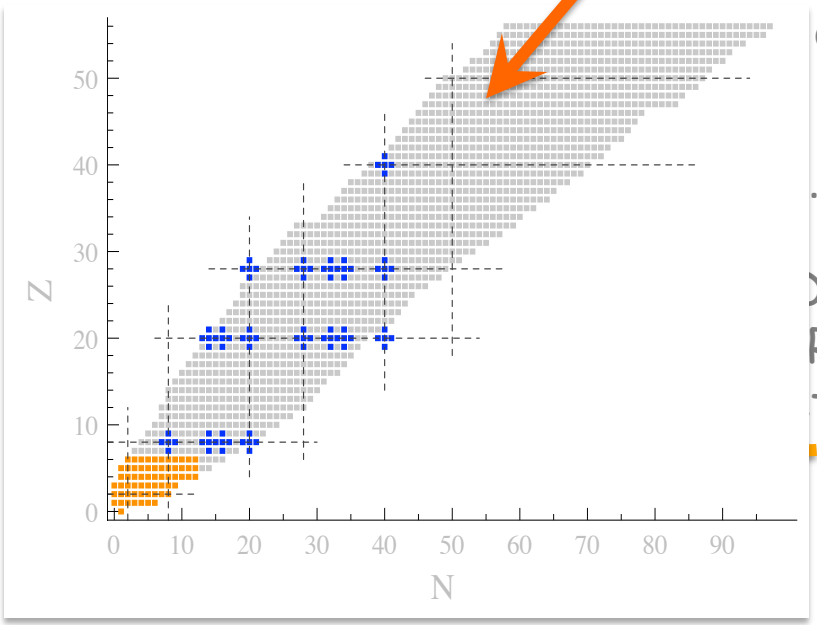
Approaches in GF theory

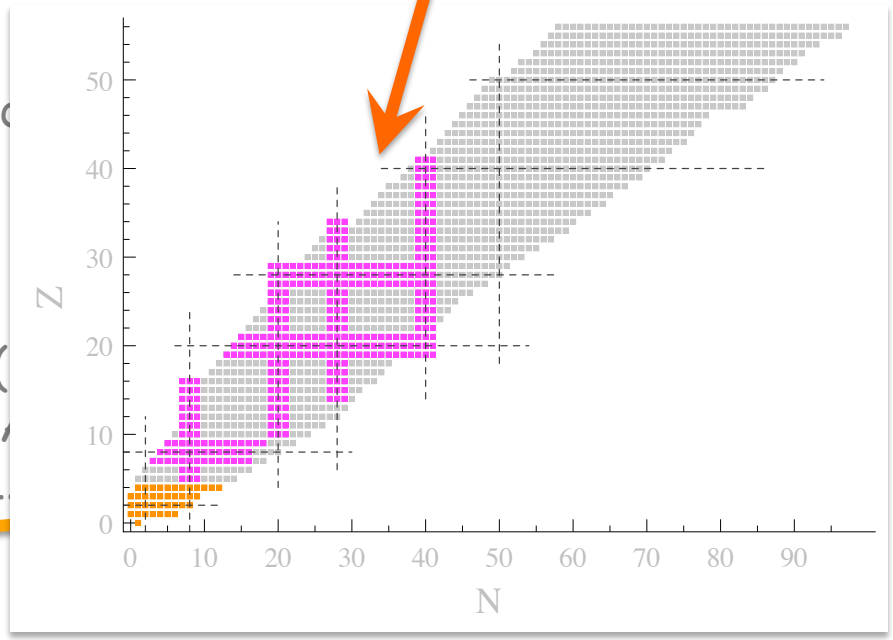
Truncation scheme:

Dyson formulation (closed shells)

Gorkov formulation (semi-/doubly-magic)

1st order: Hartree-Fock HF-Bogolioubov



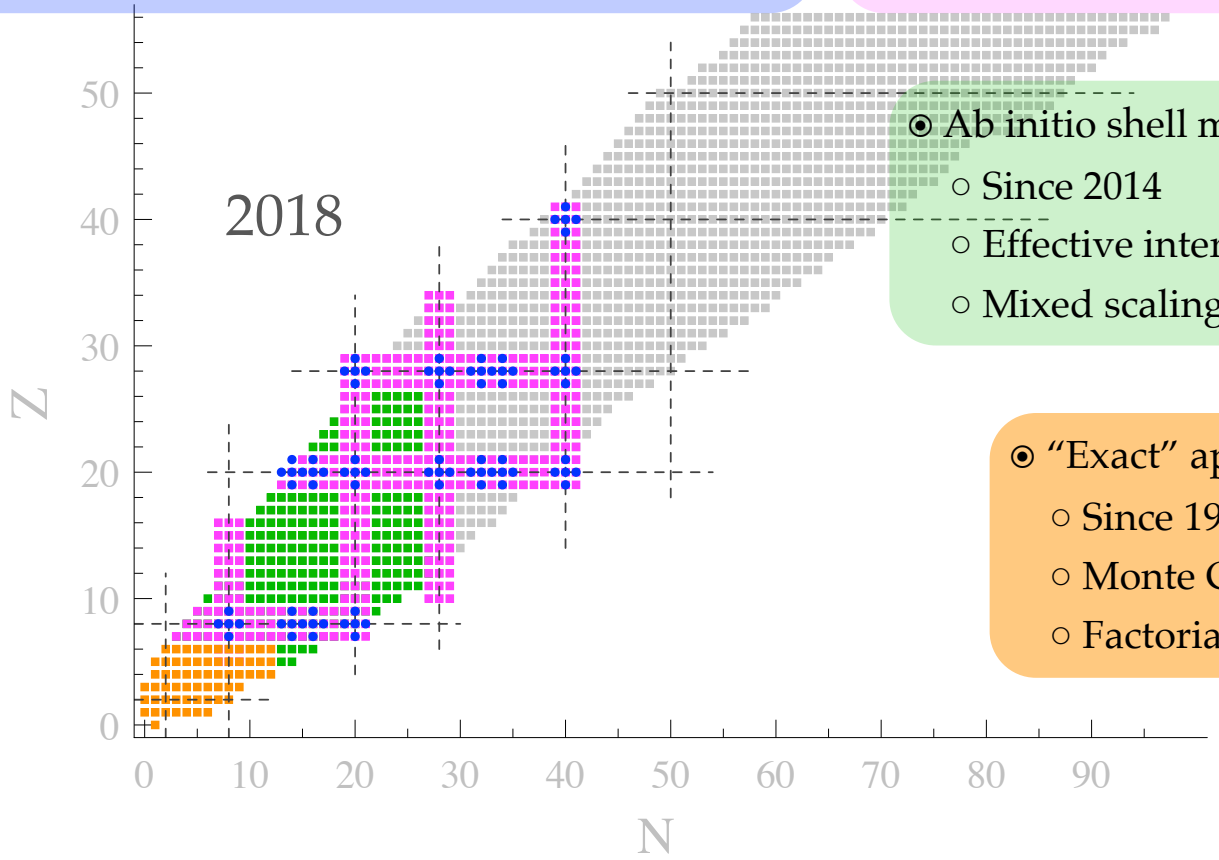


pics. credits: V. Somà

Reach of ab initio methods across the nuclear chart

- Approximate approaches for closed-shell nuclei
  - Since 2000's
  - SCGF, CC, IMSRG
  - Polynomial scaling

- Approximate approaches for open-shells
  - Since 2010's
  - GGF, BCC, MR-IMSRG
  - Polynomial scaling



- Ab initio shell model
  - Since 2014
  - Effective interaction via CC/IMSRG
  - Mixed scaling

- "Exact" approaches
  - Since 1980's
  - Monte Carlo, CI, …
  - Factorial scaling

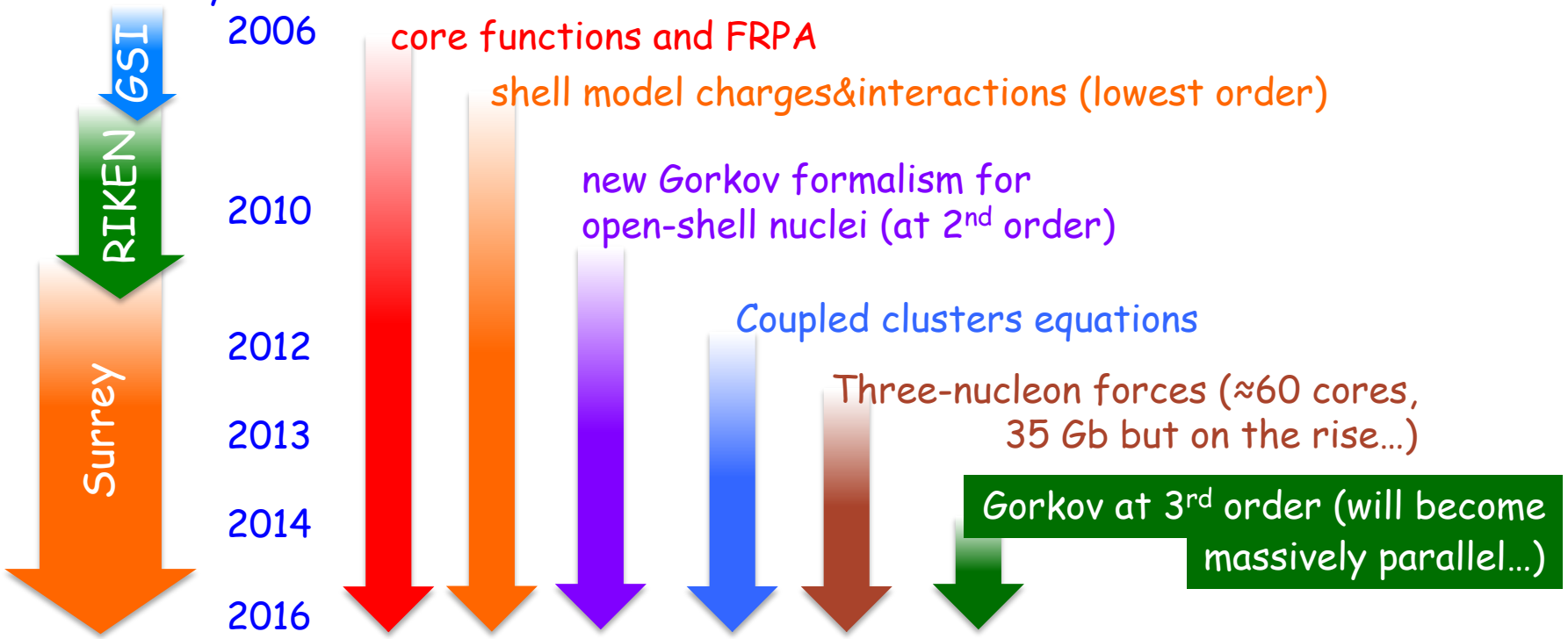
Slide, courtesy of V. Somà

Ab-initio Nuclear Computation & BcDor code

BoccaDorata code:
(C. Barbieri 2006-16
V. Somà 2010-15
A. Cipollone 2011-14)

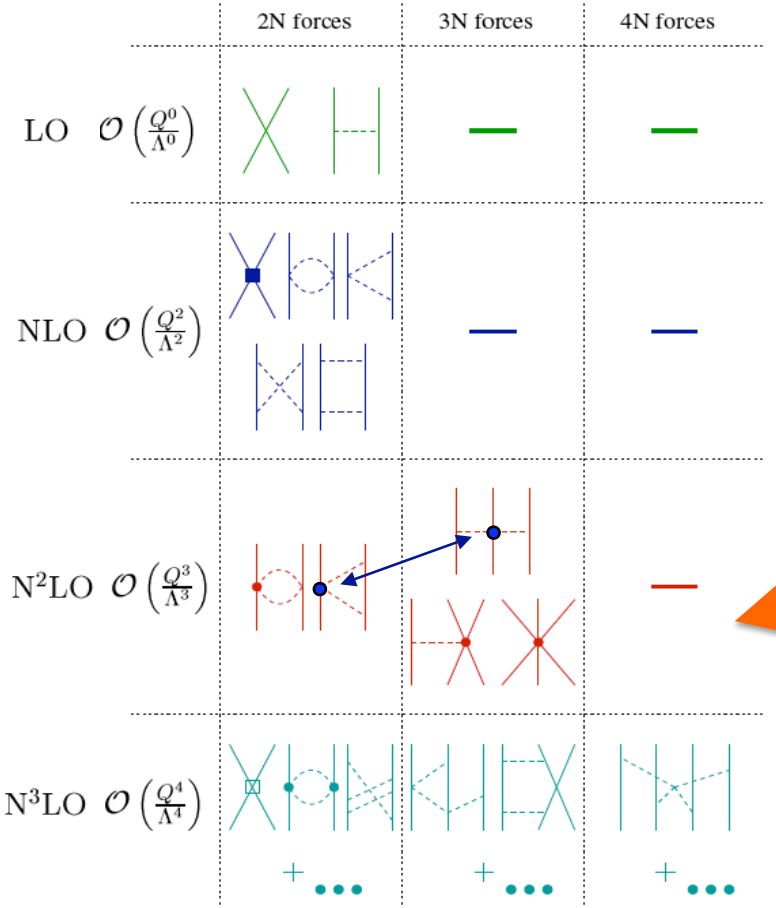
- Provides a *C++ class library* for handling many-body propagators (≈40,000 lines, MPI&OpenMP based).
- Allows to solve for nuclear spectral functions, many-body propagators, RPA responses, coupled cluster equations and effective interaction/charges for the shell model.

Code history:



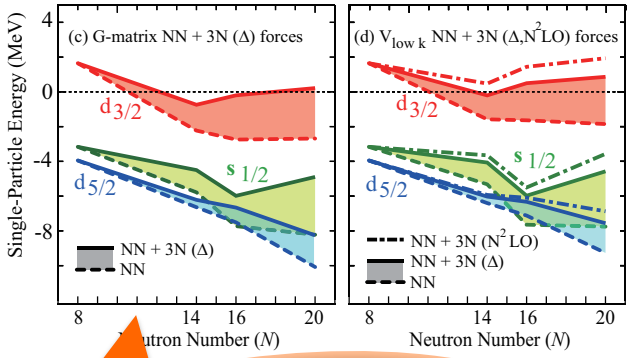
Realistic nuclear forces form Chiral EFT

Chiral EFT for nuclear forces:



(3NFs arise naturally at N2LO)

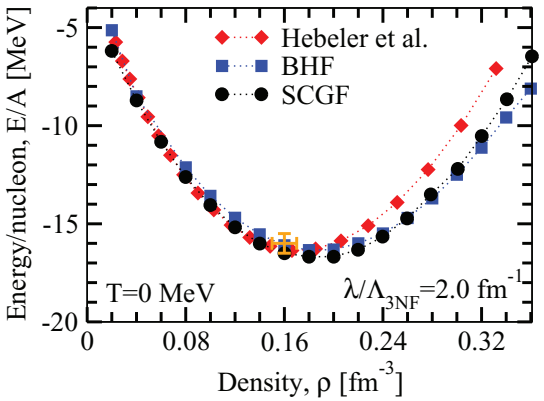
Single particle spectrum at E_{fermi}:



[T. Otsuka et al., Phys Rev. Lett **105**, 032501 (2010)]

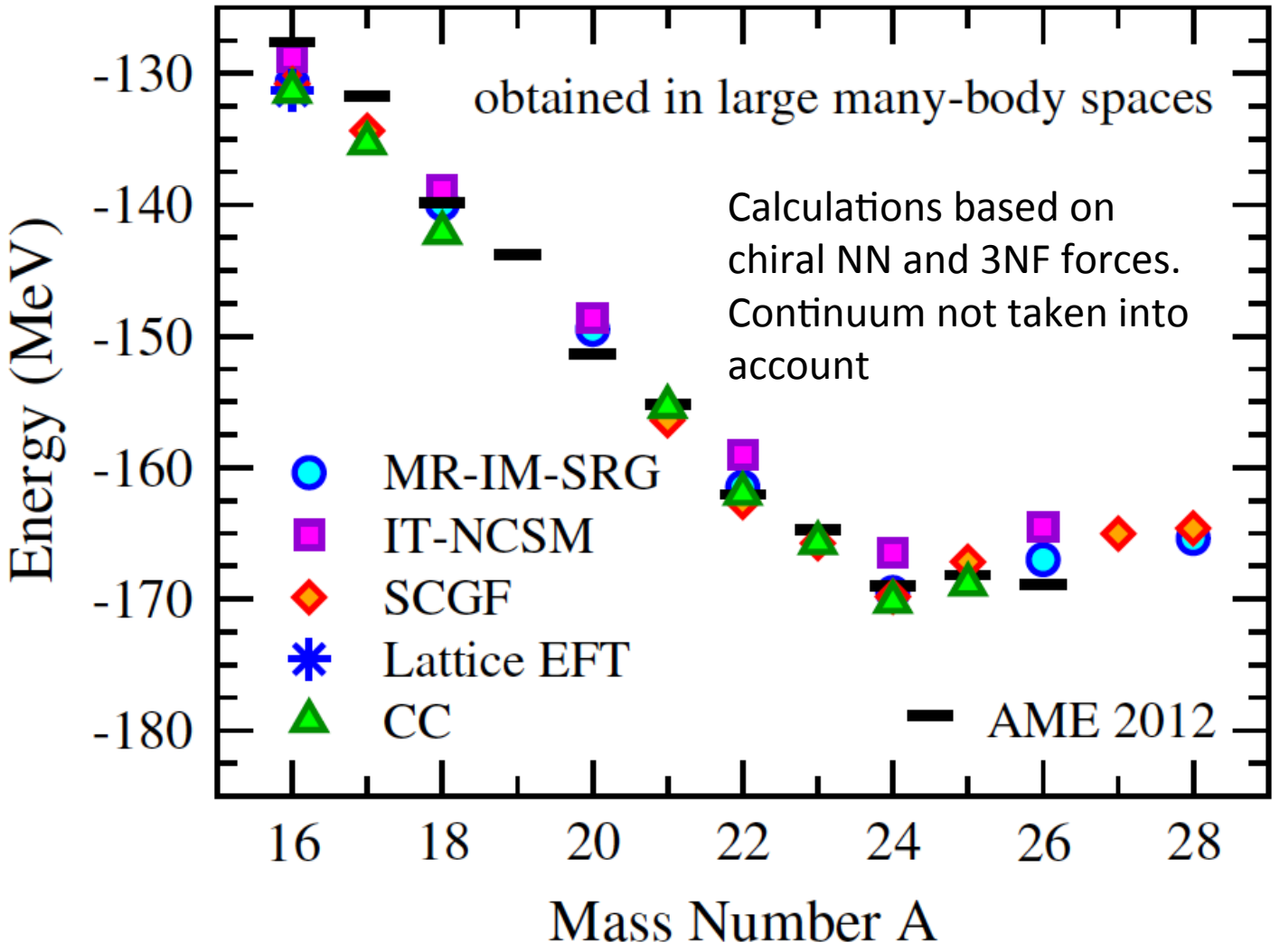
Need at LEAST 3NF!!!
("cannot" do RNB physics without…)

Saturation of nuclear matter:



[A. Carbone et al., Phy.s Rev. C **88**, 044302 (2013)]

Benchmark of ab-initio methods for oxygen isotopic chain

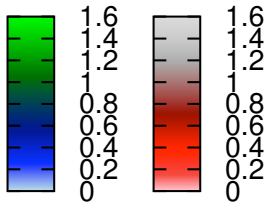


Hebeler, Holt, Menendez, Schwenk, Ann. Rev. Nucl. Part. Sci. in press (2015)

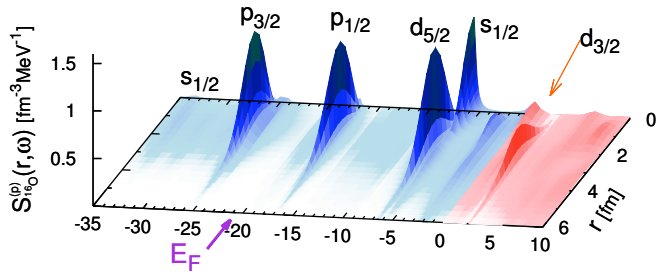
N3LO (Λ = 500Mev/c) chiral NN interaction evolved to 2N + 3N forces (2.0fm^{-1})
N2LO (Λ = 400Mev/c) chiral 3N interaction evolved (2.0fm^{-1})

Neutron spectral function of Oxygens

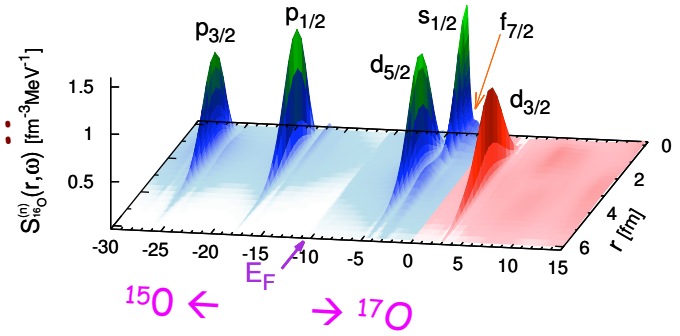
A. Cipollone, CB, P. Navrátil, *Phys. Rev. C* ***92***, *014306 (2015)*



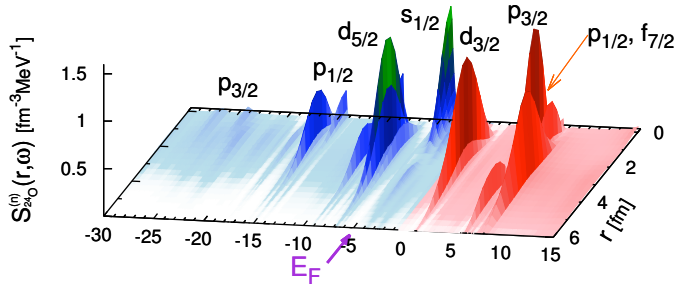
^{14}O:



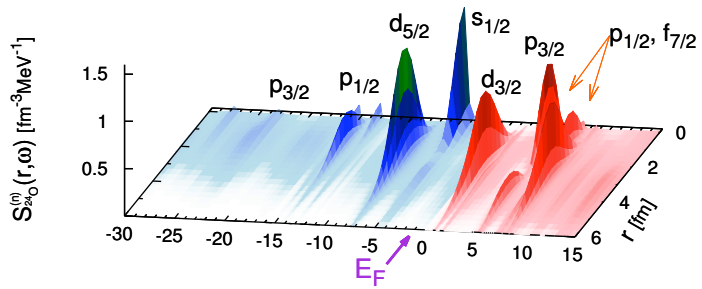
^{16}O:



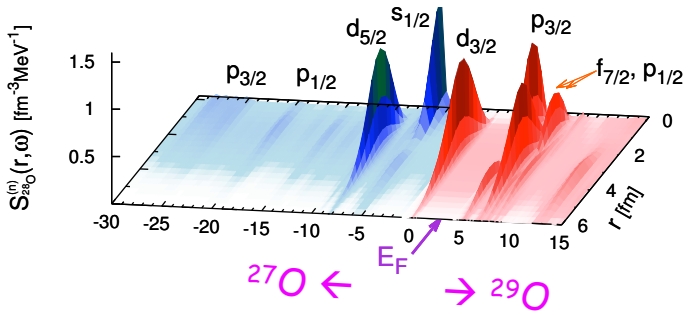
^{22}O:



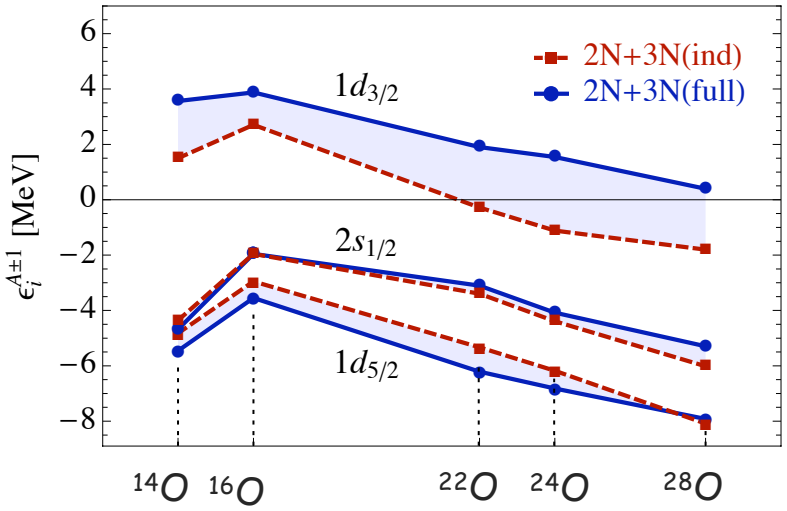
^{24}O:



^{28}O:



Neutron quasiparticle energies



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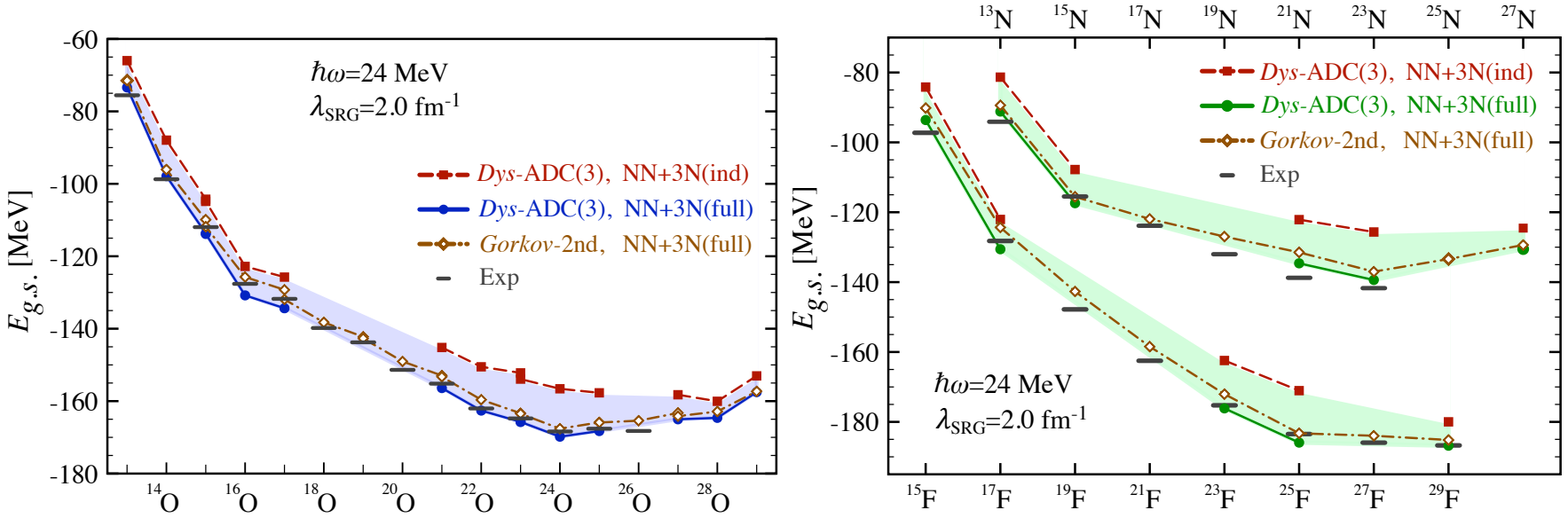
Results for the N-O-F chains

A. Cipollone, CB, P. Navrátil, Phys. Rev. Lett. **111**, 062501 (2013)
and Phys. Rev. C **92**, 014306 (2015)



→ 3NF crucial for reproducing binding energies and driplines around oxygen

→ cf. microscopic shell model [Otsuka et al, PRL**105**, 032501 (2010).]

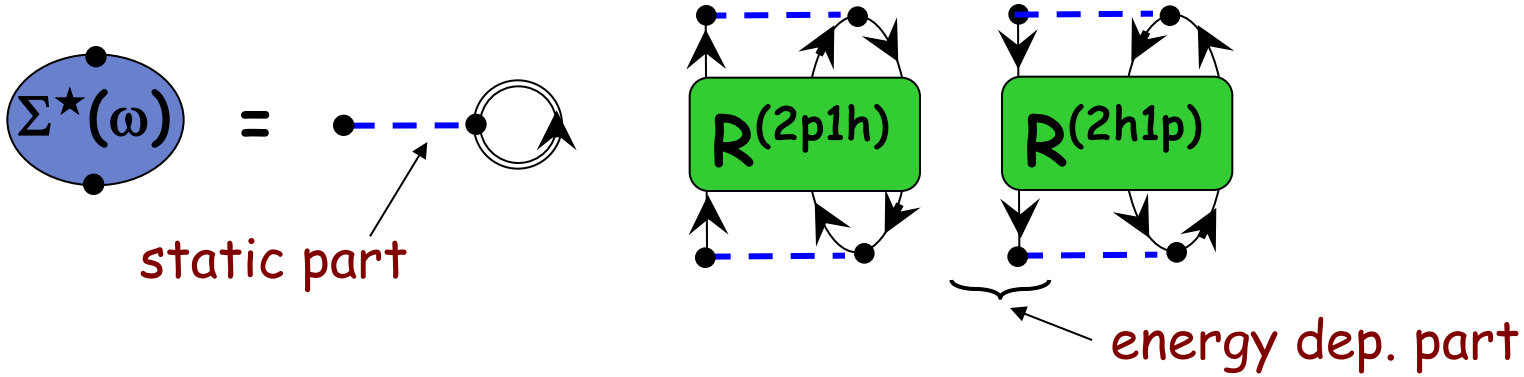
N3LO (Λ = 500Mev/c) chiral NN interaction evolved to 2N + 3N forces (2.0fm^{-1})
N2LO (Λ = 400Mev/c) chiral 3N interaction evolved (2.0fm^{-1})

Using the G-matrix for renormalizing SRC
(i.e., using potentials with hard cores)

- Strong short-range cores require "renormalizing" the interaction:
  - G-matrix, SRG, Lee Suzuki, Bloch-Horowitz, …
- Long-range correlations → *FRPA/ADC(3) !!*

Treating short-range correlations directly…

- Non perturbative expansion of the self-energy:



Treating short-range correlations directly…

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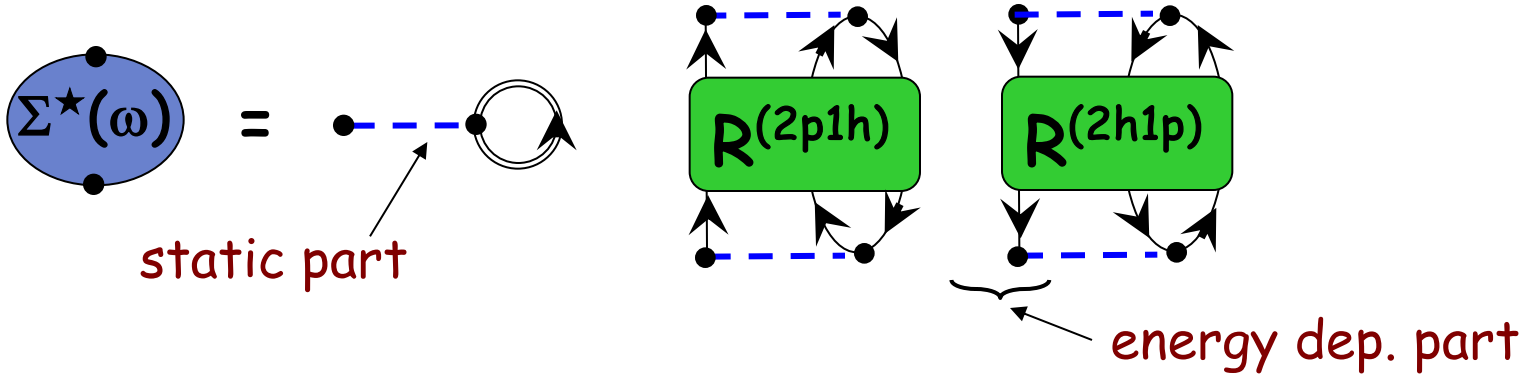
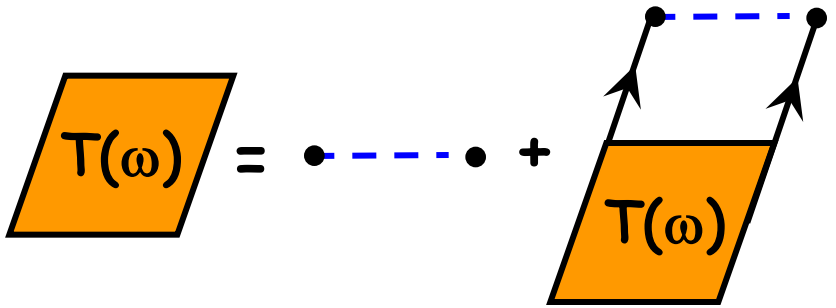


- 2 nucleons in free space: → solve for the scatt. matrix…

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



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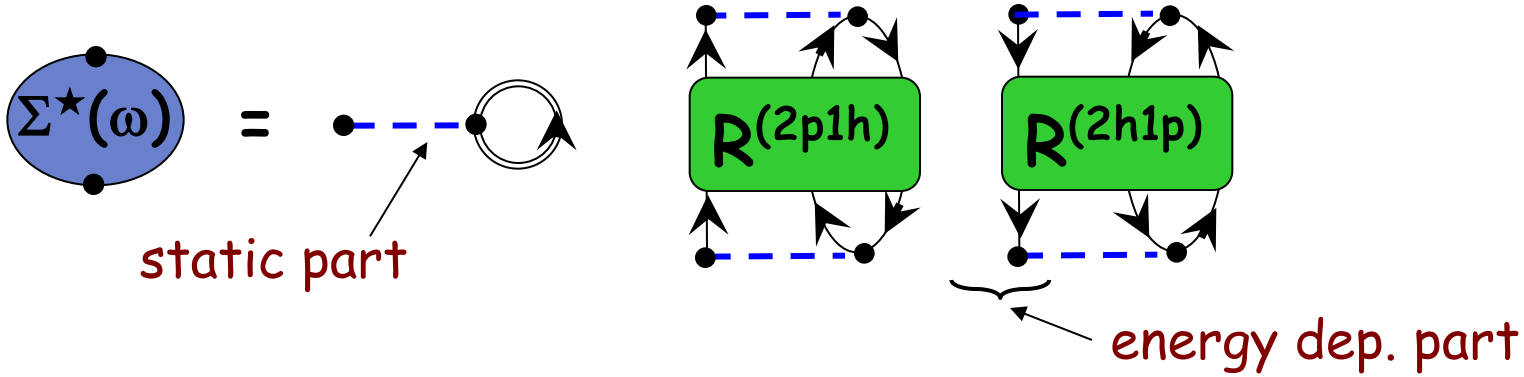
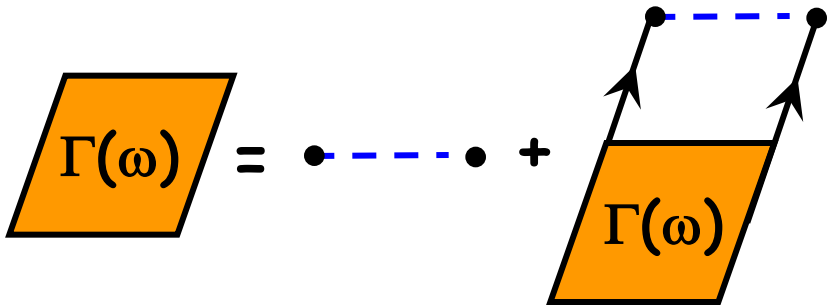


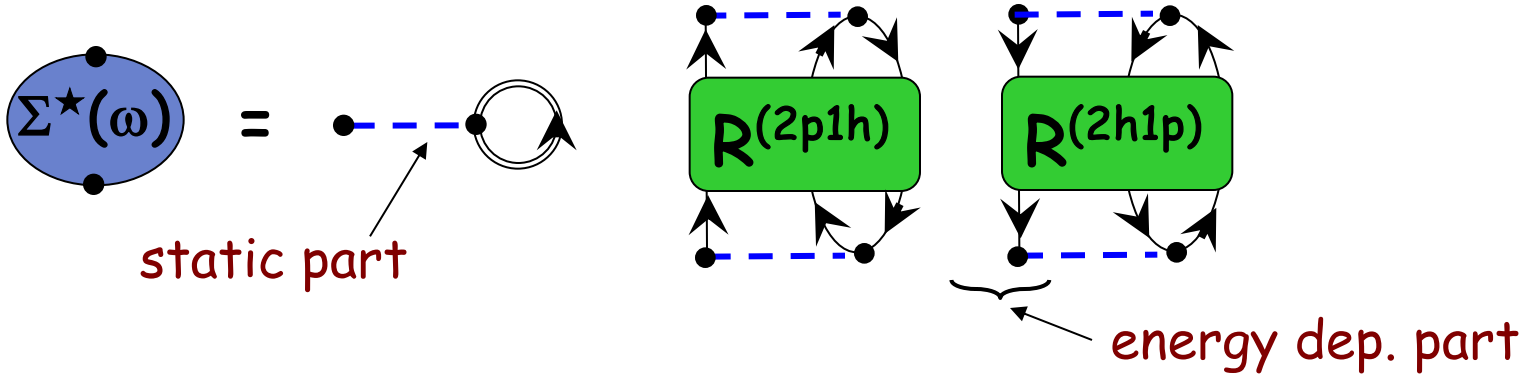
- 2 nucleons in medium: → resum pp ladders…

$$\Gamma(\omega) \approx V + V \frac{[1-n(k_a)][1-n(k_b)]}{\omega - (k_a^2 + k_b^2)/2m + i\eta} \Gamma(\omega)$$

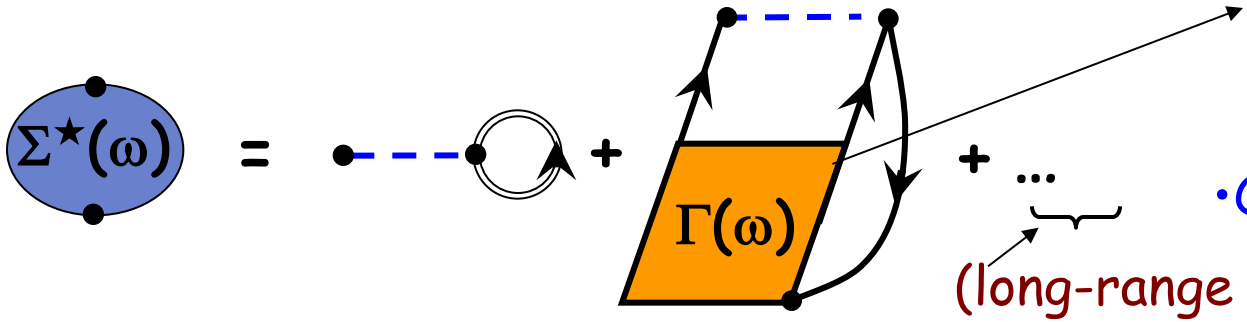


Treating short-range correlations directly…

- Non perturbative expansion of the self-energy:



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

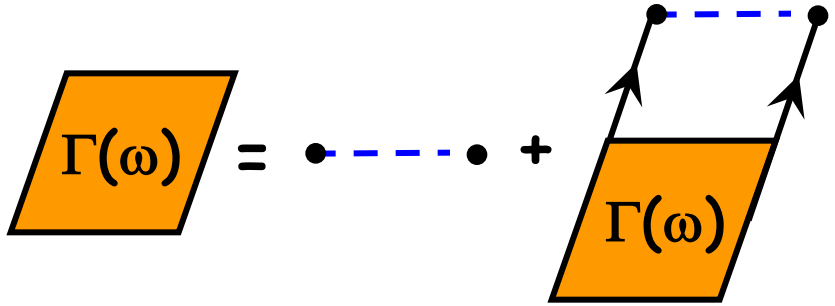


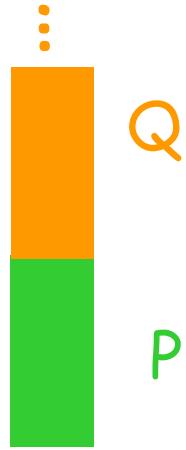
- Inside the MS:
  → ladders already accouted by FRPA
- Outside the MS:
  → one still NEEDS to resum ladders

Treating short-range corr. with a G-matrix

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

$$\Gamma(\omega) \approx V + V \frac{[1-n(k_a)][1-n(k_b)]}{\omega - (k_a^2 + k_b^2)/2m + i\eta} \Gamma(\omega)$$

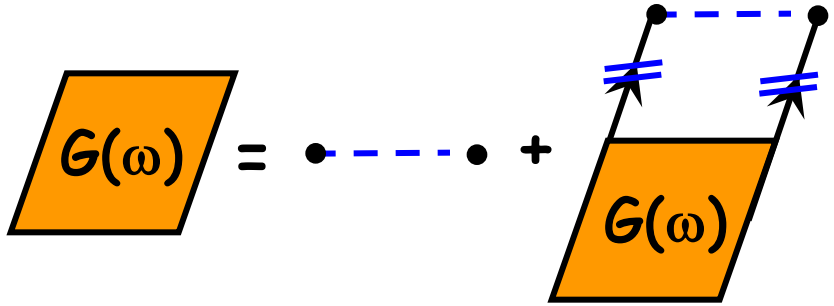


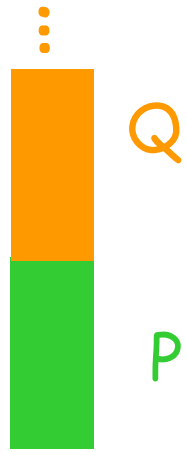


Treating short-range corr. with a G-matrix

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

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

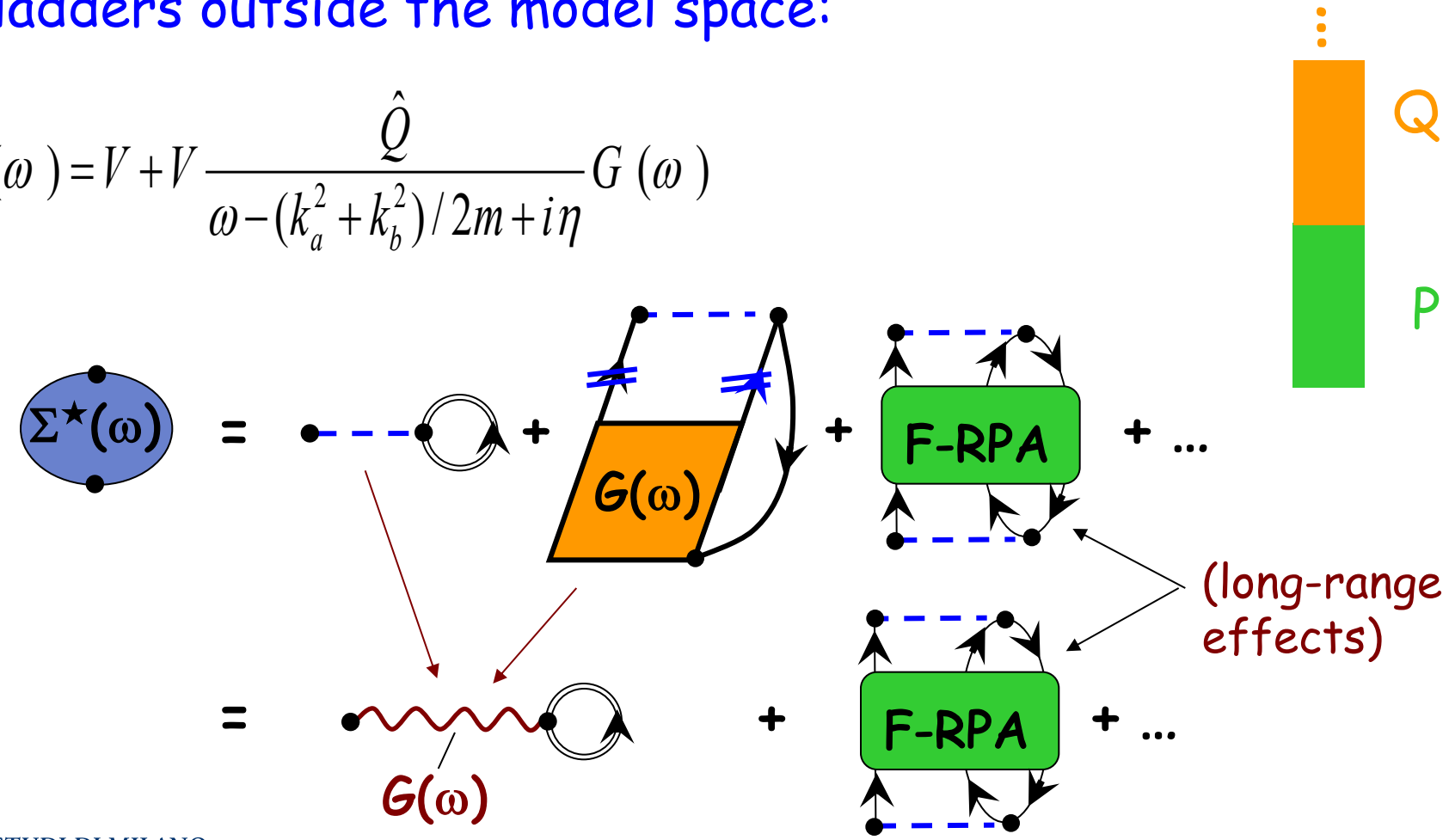




Treating short-range corr. with a G-matrix

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

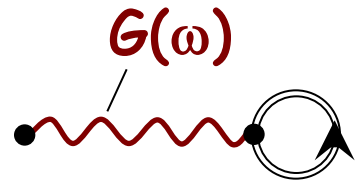
$$G(\omega) = V + V \frac{\hat{Q}}{\omega - (k_a^2 + k_b^2)/2m + i\eta} G(\omega)$$

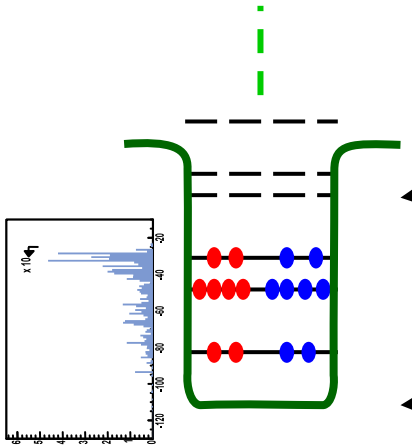


Treating short-range corr. with a G-matrix

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

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





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

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

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

(Galitskii-Migdal) Koltun sumrule

Koltun sum rule (with NNN interactions):

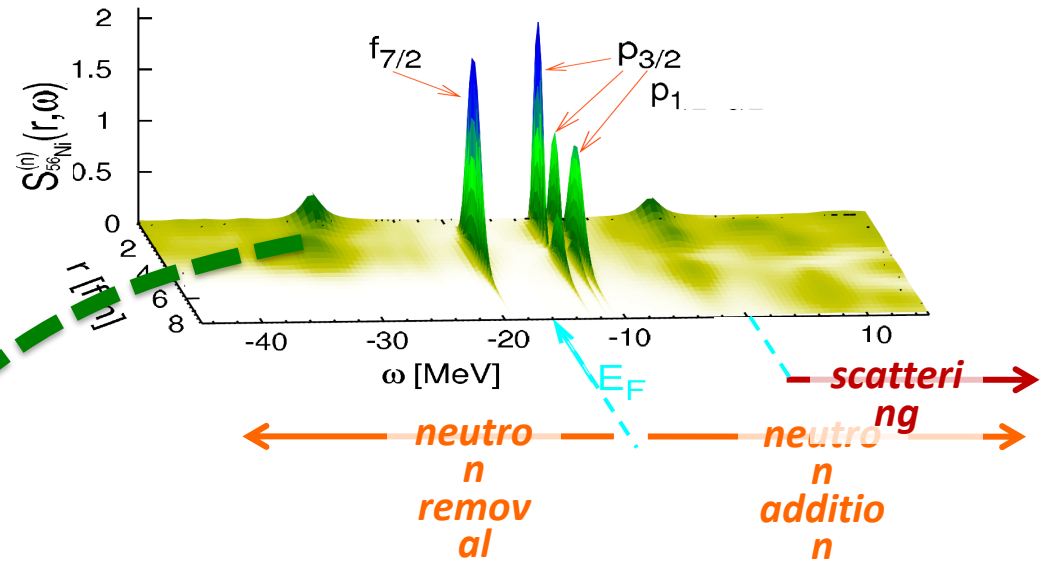
$$\sum_\alpha \frac{1}{\pi}\int_{-\infty}^{\epsilon_F} d\omega\, \omega\, \mathrm{Im}\, G_{\alpha\alpha}(\omega) = \langle \Psi_0^N|\hat{T}|\Psi_0^N\rangle + 2\langle \Psi_0^N|\hat{V}|\Psi_0^N\rangle + 3\langle \Psi_0^N|\hat{W}|\Psi_0^N\rangle$$

two-body

three-body

$$E_0^N = \frac{1}{2\pi}\int_{-\infty}^{\epsilon_F} \mathrm{d}\omega \sum_{\alpha\beta}(T_{\alpha\beta}+\omega\delta_{\alpha\beta})\mathrm{Im}\, G_{\beta\alpha}(\omega) - \frac{1}{2}\langle \Psi_0^N|\widehat{W}|\Psi_0^N\rangle$$

High-k and missing energy tail from SRC… (currently neglected in calculating Koltun SR)



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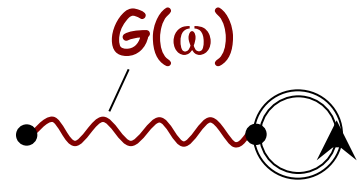
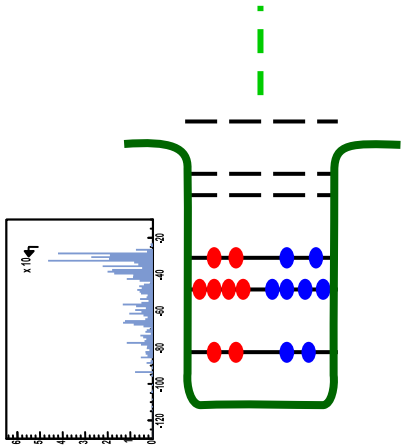




$$\Sigma^{\star}(\mathbf{r},\mathbf{r}';\omega) = \Sigma^{MF}(\mathbf{r},\mathbf{r}';\omega) + \tilde{\Sigma}(\mathbf{r},\mathbf{r}';\omega)\ .$$

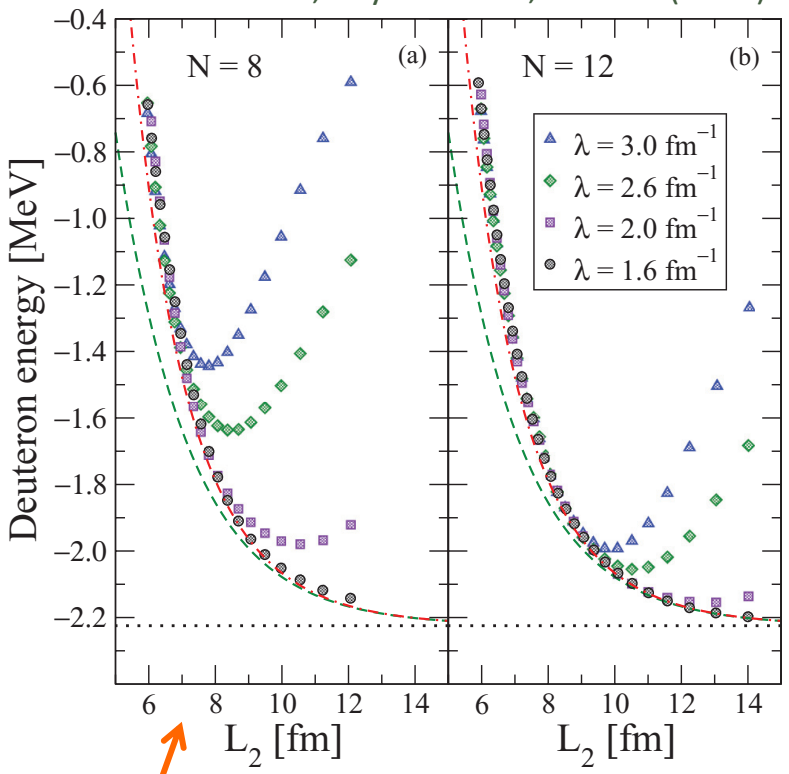
$$Z_\alpha = \int d\mathbf{r}\,|\psi^{A\pm1}_\alpha(\mathbf{r})|^2 = \left.\frac{1}{1-\dfrac{\partial\Sigma^{\star}_{\hat{\alpha}\hat{\alpha}}(\omega)}{\partial\omega}}\right|_{\omega=\pm(E^{A\pm1}_\alpha - E^A_0)}$$

Two contributions to the derivative:

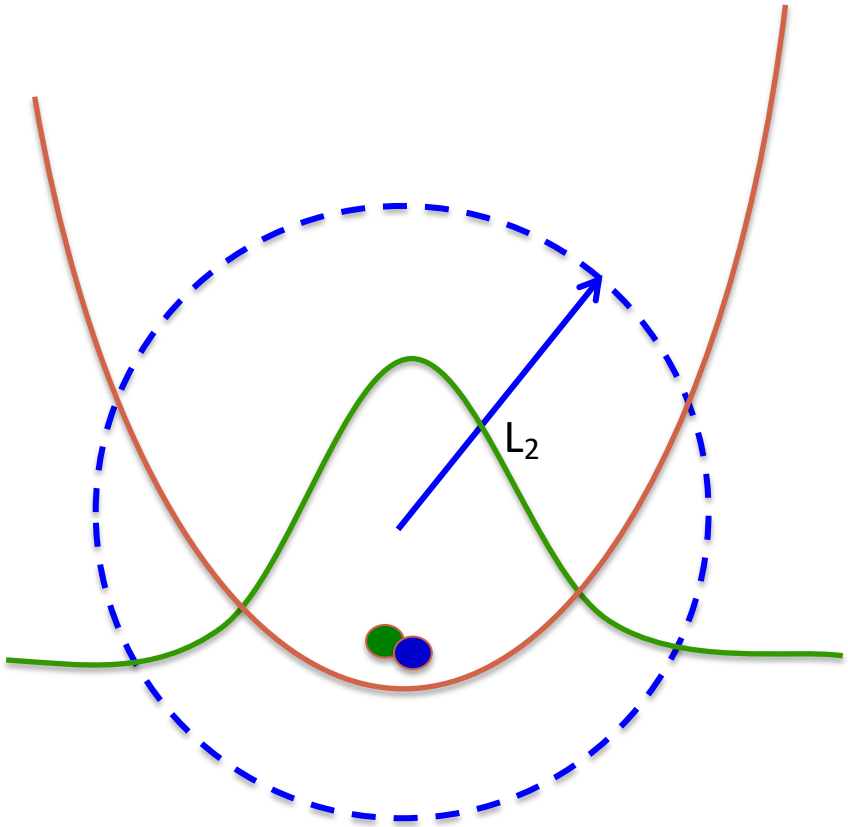
- $\Sigma^{\mathrm{MF}}_{\alpha\beta}(\omega)$ is due to scattering to (high-k) states in the Q space
- $\Sigma(\mathbf{r},\mathbf{r}';\omega)$ accounts for low-energy (long range) correlations

Infrared convergence

S. N. More et al., Phy. Rev. C**87**, 044326 (2013)



Deuteron g.s. Energy
EM(500) – N3LO two-nucleon force

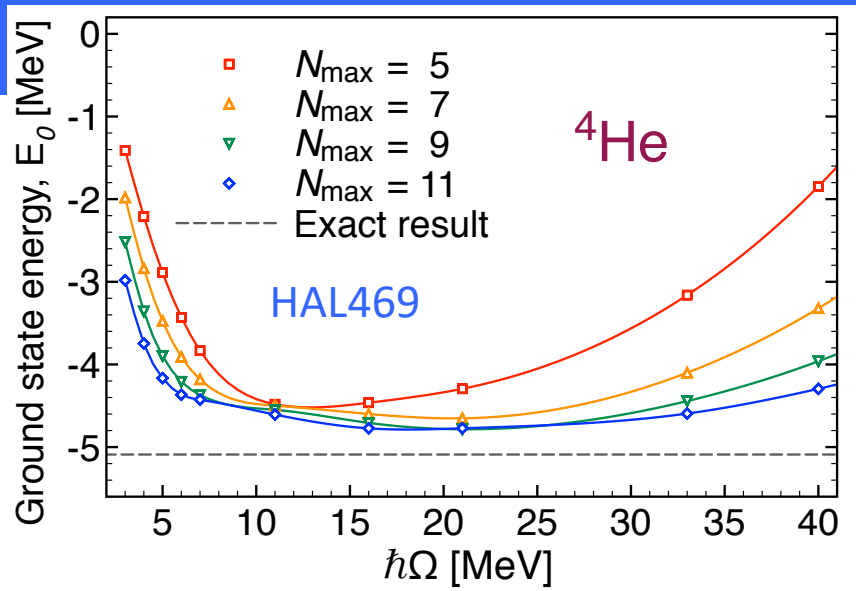


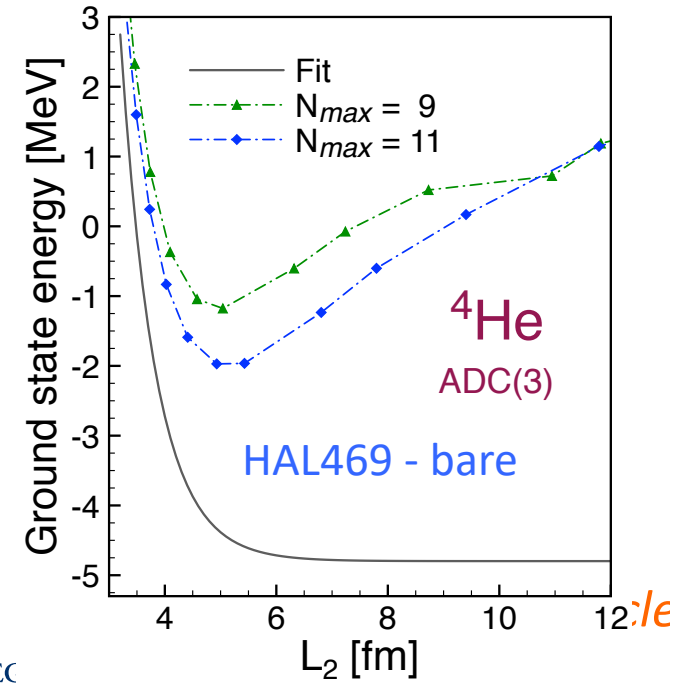
$$L_2 = \sqrt{2(N + 3/2 + 2)}b$$

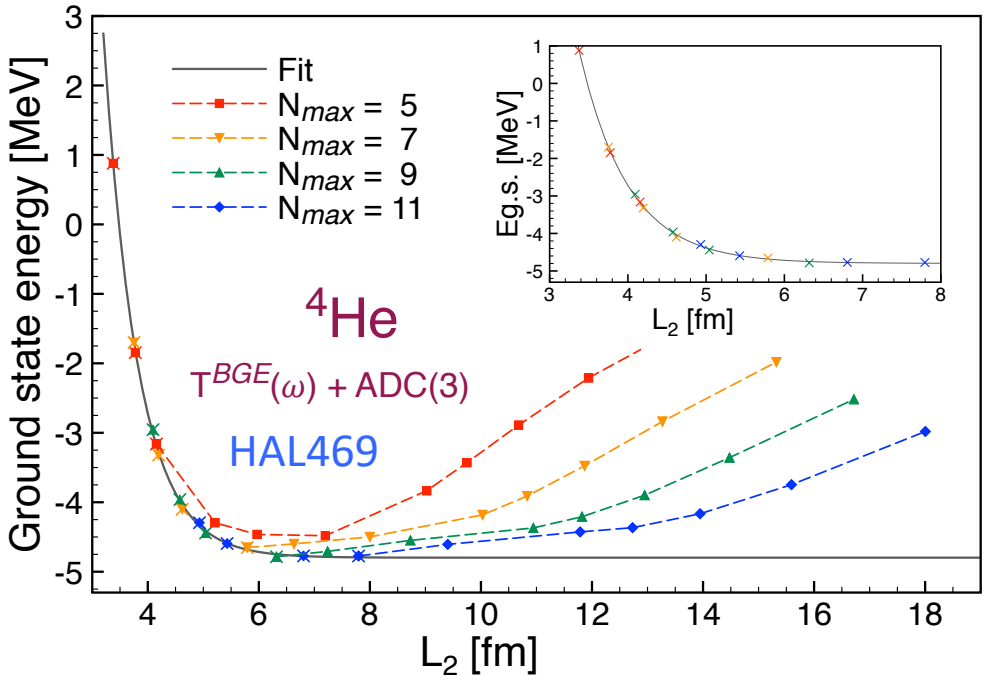
Infrared convergence

Short-range repulsion in the HALQCD-type potentials can be tamed correctly even for large nuclei.

C. McIlroy, CB, et al., Phys. Rev. C**97**, 021303(R) (2018)



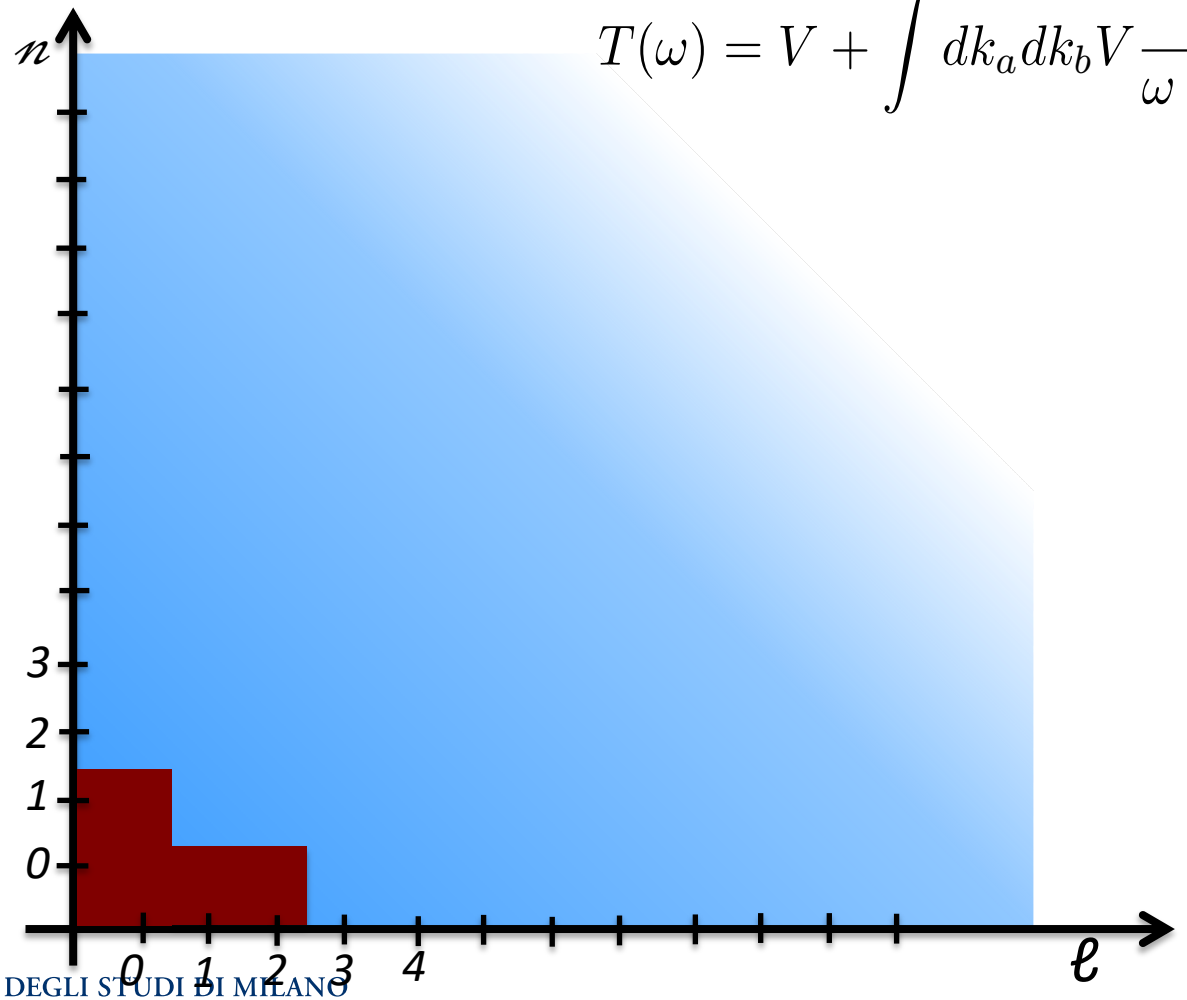


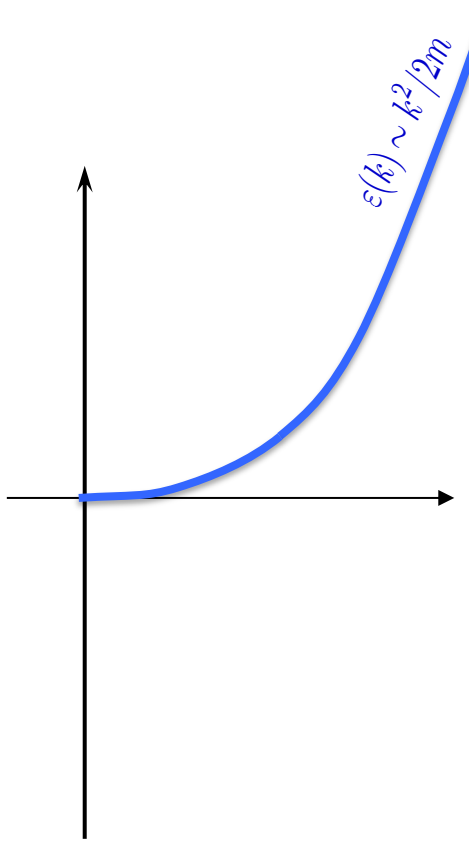


Analysis of Brueckner HF

Scattering of two nucleon in free space:

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

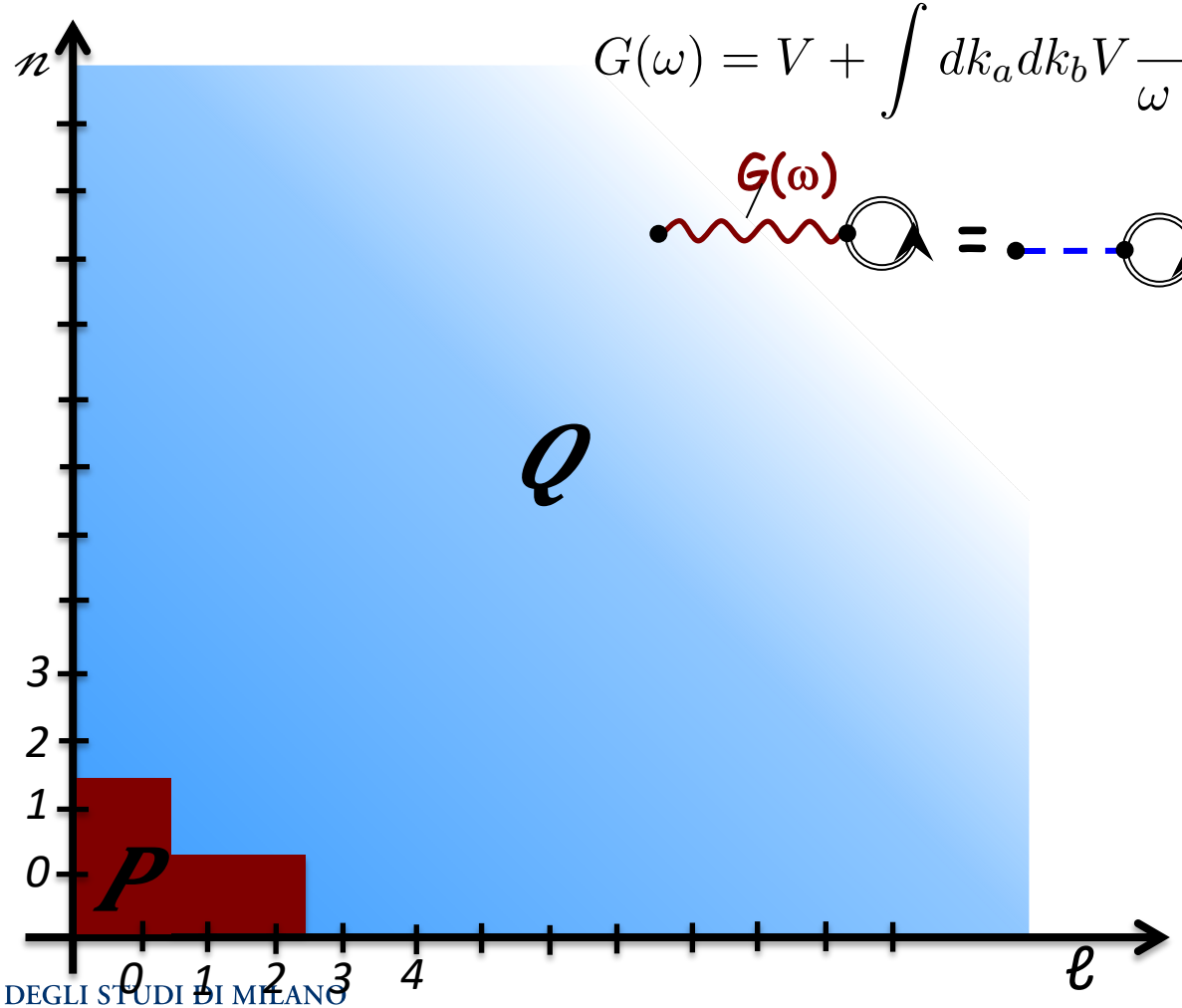


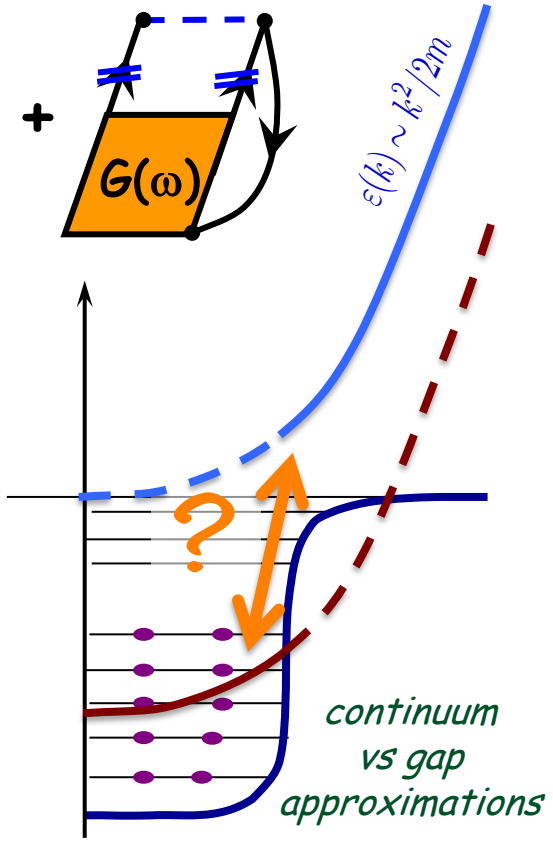


Analysis of Brueckner HF

Scattering of two nucleons outside the Fermi sea (➔BHF):

$$G(\omega) = V + \int dk_a dk_b V \frac{\hat{Q}}{\omega - \varepsilon(k_a) - \varepsilon(k_b) + i\eta} G(\omega)$$

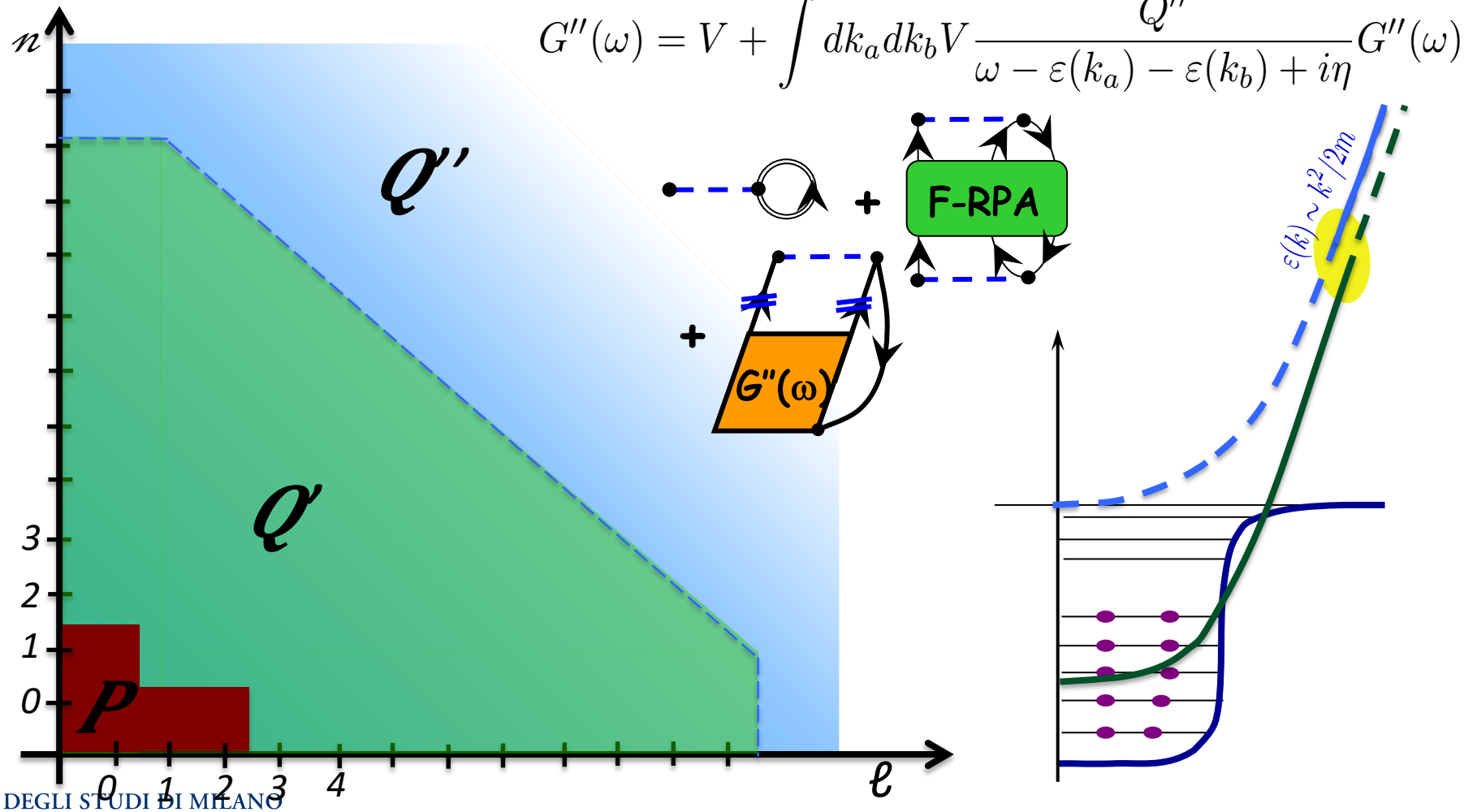




Mixed SCGF-Brueckner approach

Solve full many-body dynamics in model space (P+Q') and the Goldstone's ladders outside it (i.e. in Q'' only):

$$G''(\omega) = V + \int dk_a dk_b V \frac{\hat{Q}''}{\omega - \varepsilon(k_a) - \varepsilon(k_b) + i\eta} G''(\omega)$$



The Faddeev random phase approximation method (FRPA)

CB et al.,
*Phys. Rev. C**63**, 034313 (2001)*
*Phys. Rev. A**76**, 052503 (2007)*
*Phys. Rev. C**79**, 064313 (2009)*

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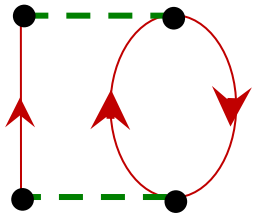
DIPARTIMENTO DI FISICA

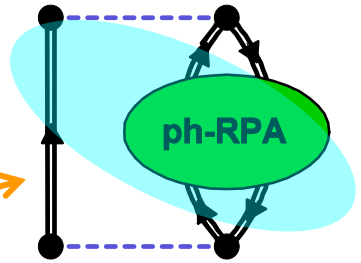
Approximations for the Self-energy

Diagrams of some common approximations for the self- energy:

- 2nd

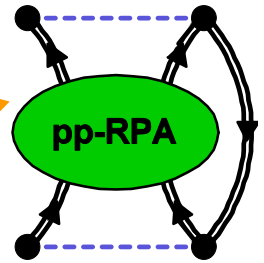


- ph "rings"



GW approach; particle-vibration coupling

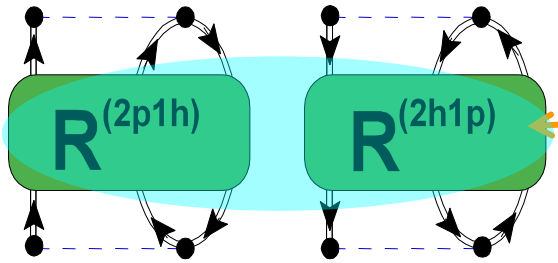
- pp "ladders"



Pairing-like effects; Used for nuclear matter

Keep in mind that in certain cases these two interfere and should not be used separately from each other…

- R^{2p1h}



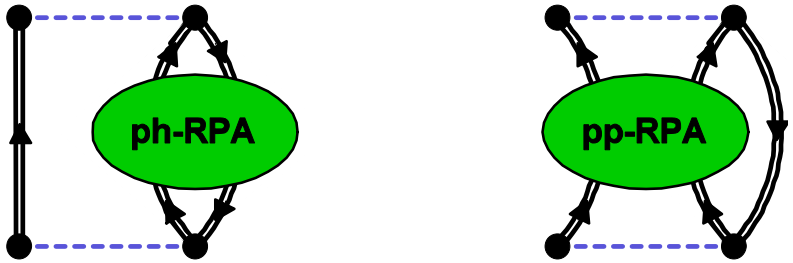
This is the most complete, including both pp and ph correlations and their interference

Faddeev RPA method

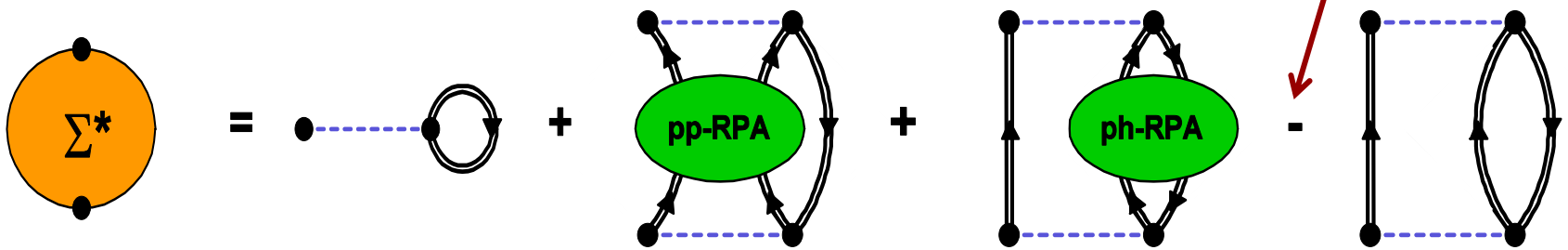
The following two diagram can be equally important. However summing them would not work well:

-They both contain $\Sigma^{2nd}_{\alpha\beta}(\omega)$, which would be over counted

-They would not interfere…

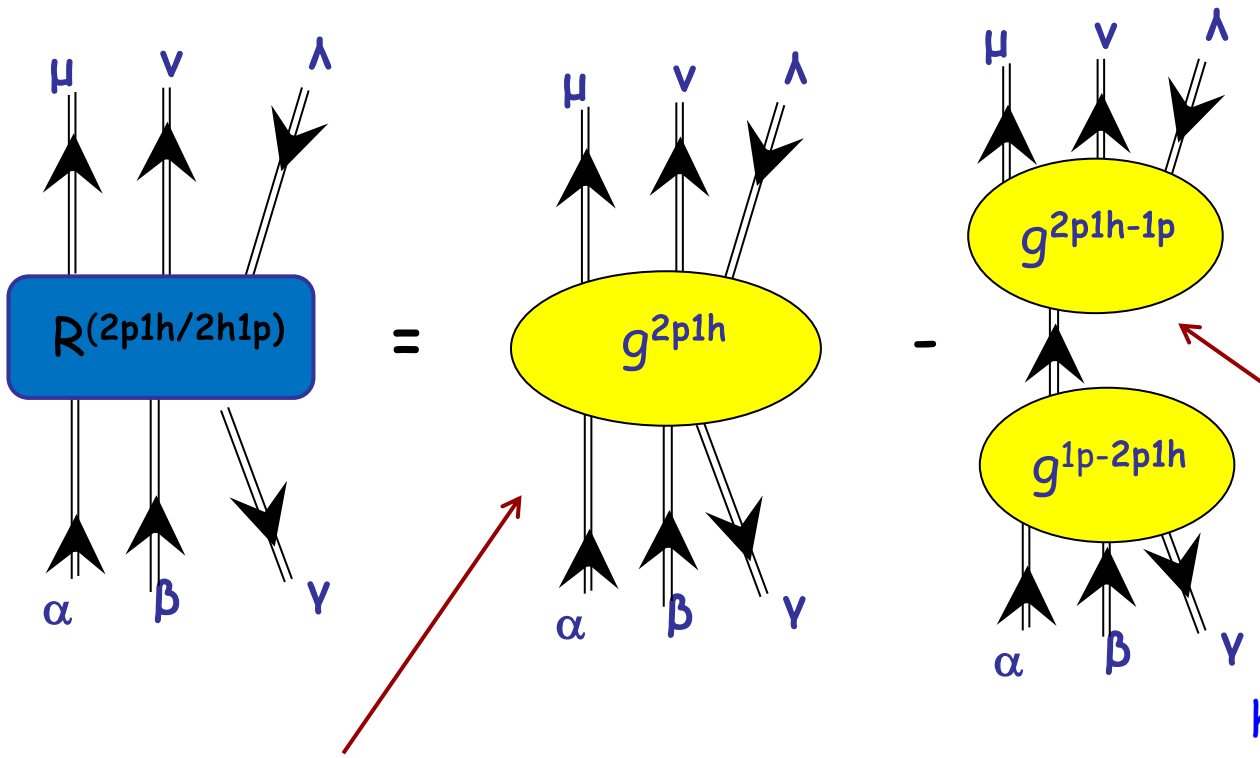


So, the following is NOT good:



Self-energy and 2p1h/2h1p propagator

Graphic representation of the 2p1h/2h1p irreducible propagator R(ω):



Propagation of 3 excitations

Subtract the contribution in which a particle-hole anihilate each other → The Dyson equation will account for it!

Self-energy and 2p1h/2h1p propagator

Using the EOM of both *t* and *t'*, one finds again the Dyson equation with self-energy given (in a symmetric form) by

$$\Sigma^{\star}_{\alpha\beta}(t-t') \;=\; \Sigma^{HF}_{\alpha\beta} \;+\; v_{\alpha\lambda,\mu\nu}\; R_{\mu\nu\lambda,\gamma\delta\zeta}(t,t')\; v_{\gamma\delta,\beta\zeta}\;,$$

where:

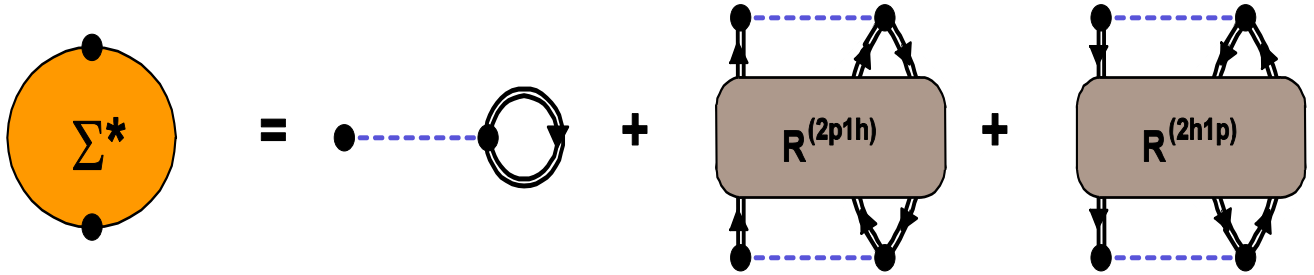
Irreducible 2p1h/2h1p propagator

$$R_{\mu\nu\lambda,\alpha\beta\gamma}(t;t') \;\equiv g^{2p1h}_{\mu\nu\lambda,\alpha\beta\gamma}(t;t') - g^{2p1h-1p}_{\mu\nu\lambda,\eta}(t,t_1)\; g^{-1}_{\eta\sigma}(t_1-t_2)\; g^{1p-2p1h}_{\sigma,\alpha\beta\gamma}(t_2,t')$$

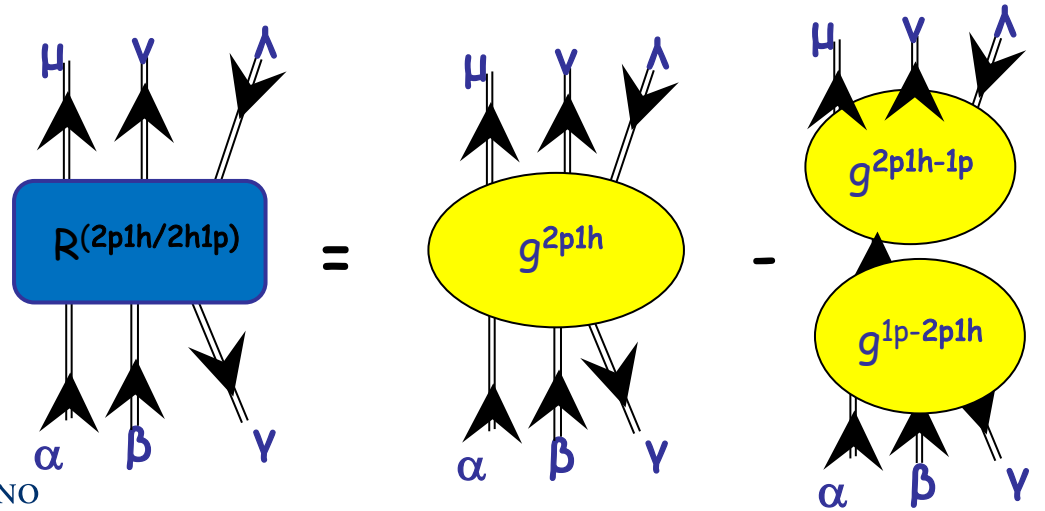
$$g^{1p-2p1h}_{\alpha,\mu\nu\lambda}(t-t') \equiv -\frac{i}{\hbar}\langle\Psi^N_0|\; T[c_\alpha(t)c^\dagger_\mu(t')c^\dagger_\nu(t')c_\lambda(t')]|\Psi^N_0\rangle$$

Faddeev RPA method

Thus, to include both "ladder" and "ring" correlations one must calculate the full 2p1h/2h1p propagator

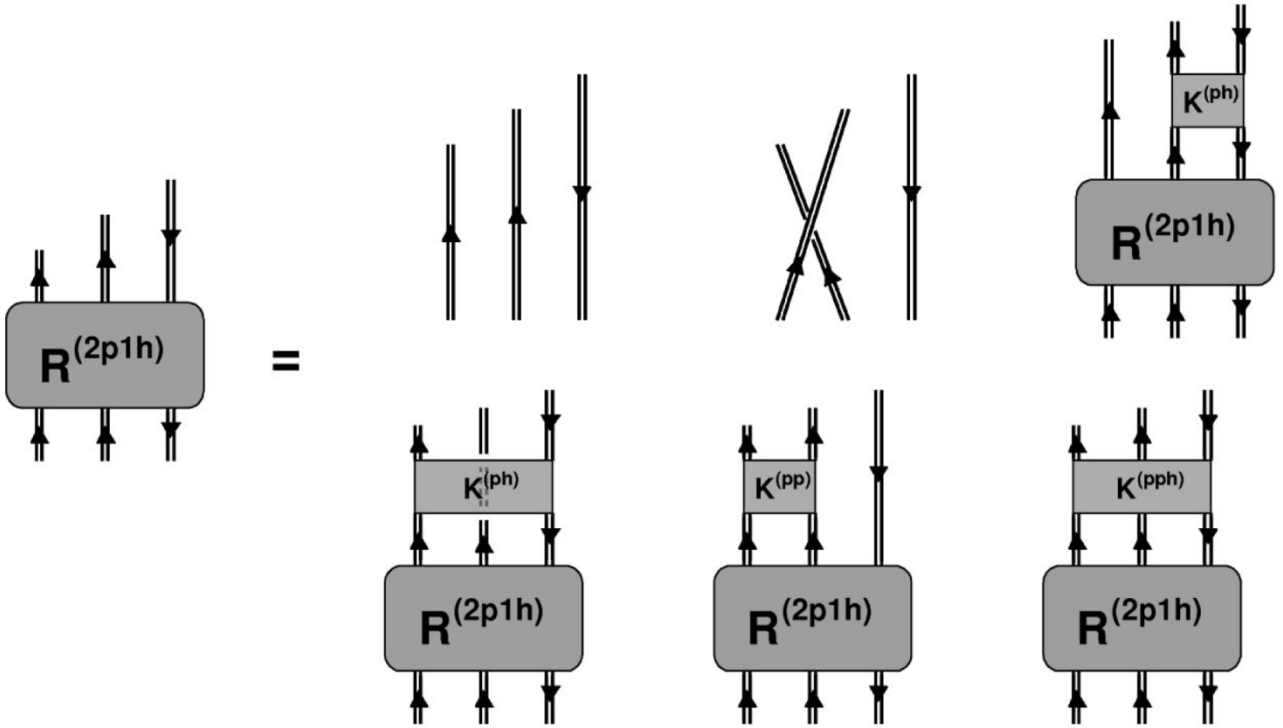


In general this is exact if one can calculate the full 6-points Green's function (see lecture of Apr. 13th):



Faddeev RPA method

The full 2p1h/2h1p polarization propagator also satisfies a Bethe-Salpeter-like equation:



However, this depends on 4-tmes (3 frequancies) and it is much more complicatde than the p-h Bethe-Salpeter.

Faddeev RPA method

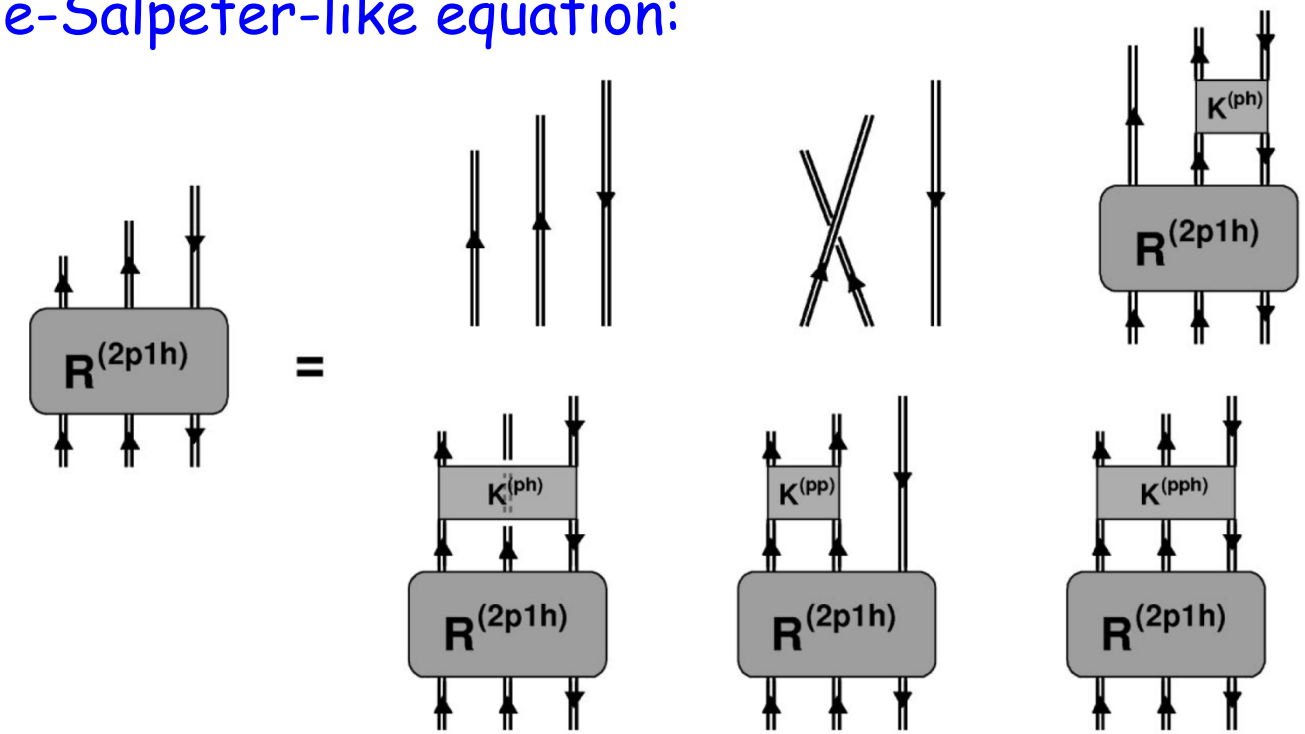
The full 2p1h/2h1p polarization propagator also satisfies a Bethe-Salpeter-like equation:

$$
\begin{aligned}
R_{\alpha\beta\gamma,\mu\nu\lambda}(\omega_1,\omega_2,\omega_3) = {} & [g_{\alpha\mu}(\omega_1)g_{\beta\nu}(\omega_2) - g_{\beta\mu}(\omega_2)g_{\alpha\nu}(\omega_1)]g_{\lambda\gamma}(-\omega_3) \\
& + \Bigg(g_{\beta\beta_1}(\omega_2)g_{\gamma_1\gamma}(-\omega_3)V_{\beta_1\sigma,\gamma_1\rho}\int \frac{ds}{2\pi i} R_{\alpha\rho\sigma,\mu\nu\lambda}(\omega_1,s,\omega_2+\omega_3-s) \\
& + g_{\alpha\alpha_1}(\omega_1)g_{\gamma_1\gamma}(-\omega_3)V_{\alpha_1\sigma,\gamma_1\rho}\int \frac{ds}{2\pi i} R_{\rho\beta\sigma,\mu\nu\lambda}(s,\omega_2,\omega_1+\omega_3-s) \\
& + \frac{1}{2} g_{\alpha\alpha_1}(\omega_1)g_{\beta\beta_1}(\omega_2)V_{\alpha_1\beta_1,\rho\sigma}\int \frac{ds}{-2\pi i} R_{\rho\sigma\gamma,\mu\nu\lambda}(s,\omega_1+\omega_2-s,\omega_3) \Bigg)
\end{aligned}
$$

However, this depends on 4-tmes (3 frequancies) and it is much more complicatde than the p-h Bethe-Salpeter.

Faddeev RPA method

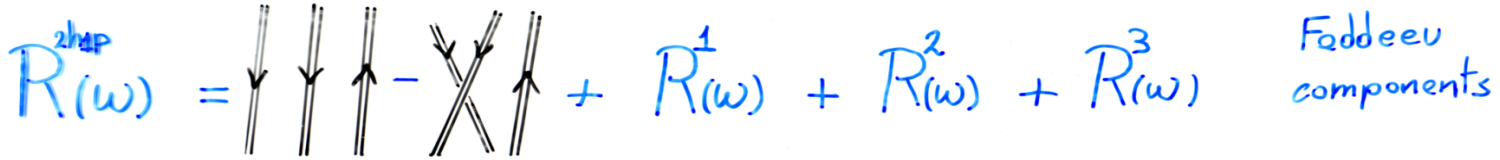
The full 2p1h/2h1p polarization propagator also satisfies a Bethe-Salpeter-like equation:

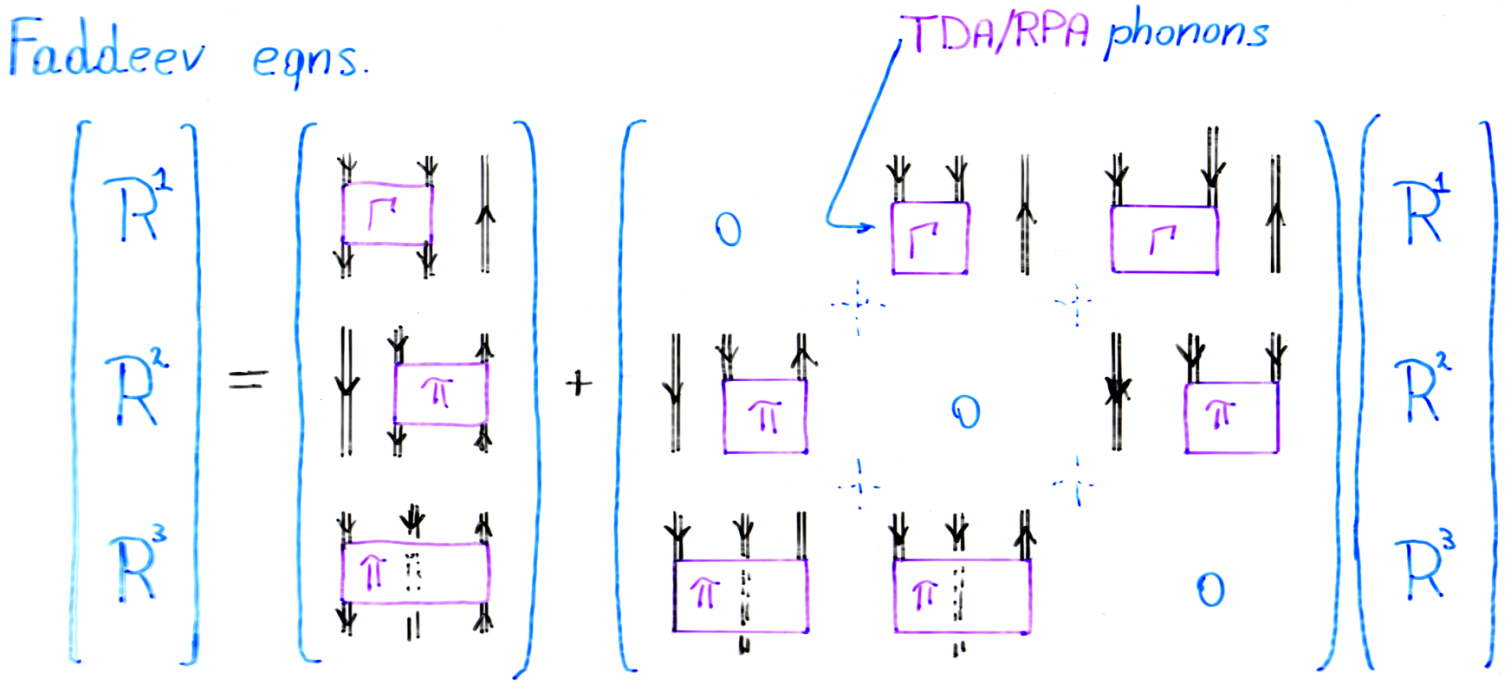


Strategy: solve each "pp" and "ph" channel separately, by solving the (simpler) DRPA equations. Then couple to a third line and mix the corresponding amplitudes ➔ Faddeev eqs.!!

Faddeev equations for the 2h1p motion

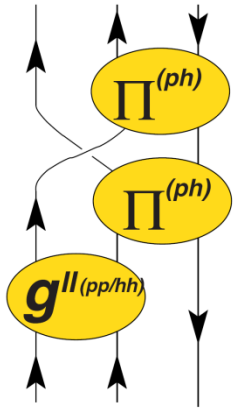
Strategy: solve each "pp" and "ph" channel separately, by solving the (simpler) DRPA equations. Then couple to a third line and mix the corresponding amplitudes ➔ Faddeev eqs.!!



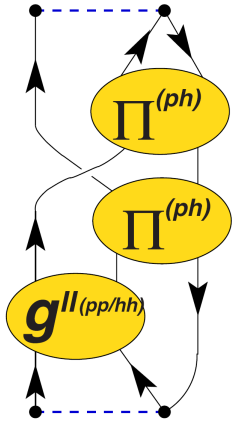


References: CB, et al., Phys. Rev. C**63**, 034313 (2001); Phys. Rev. A**76**, 052503 (2007)
Phys. Rev. C**79**, 064313 (2009)

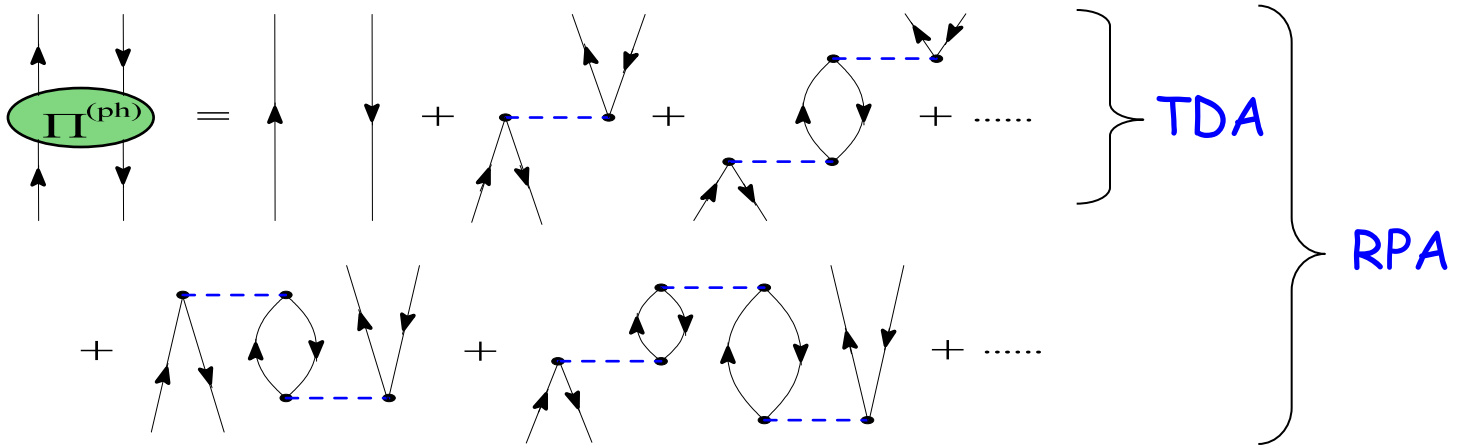
FRPA: Faddeev summation of RPA propagators



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



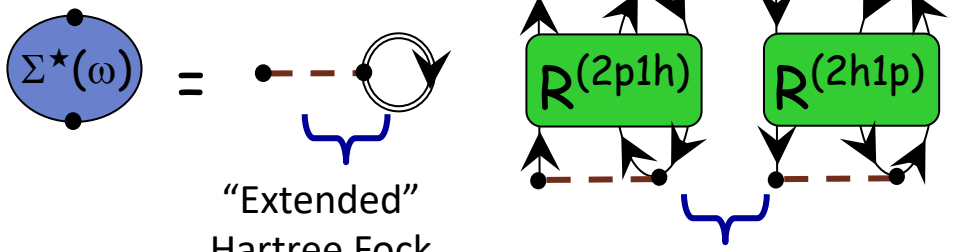
where:



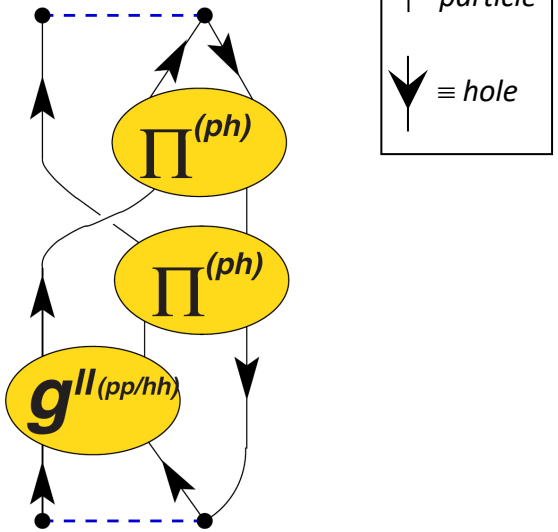
References: CB, et al., Phys. Rev. C**63**, 034313 (2001); Phys. Rev. A**76**, 052503 (2007)
Phys. Rev. C**79**, 064313 (2009)

Faddeev-RPA in two words…

Self-energy (optical potential):



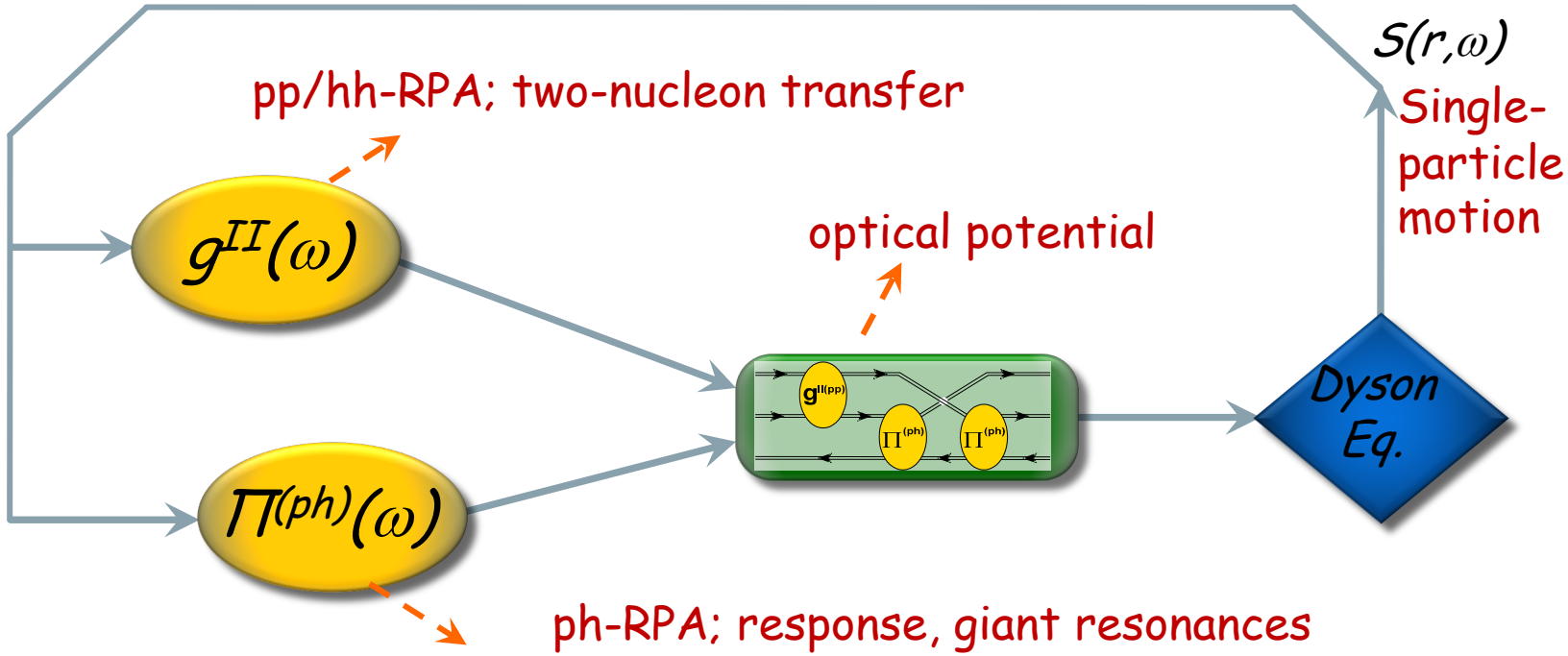
Faddeev-RPA:



- A complete expansion requires *all types* of particle-vibration coupling:
  - ✓ $g^{II}(\omega)$ → pairing effects, two-nucleon transfer
  - ✓ $\Pi^{(ph)}(\omega)$ → collective motion, using RPA or beyond
  - ✓ Pauli exchange effects
- The Self-energy $\Sigma^{\star}(\omega)$ yields *both* single-particle states and scattering
- Finite nuclei:→ require high-performance computing

Phys. Rev. C63, 034313 (2001); Phys. Rev. C65, 064313 (2002)
Phys. Rev. A76, 052503 (2007); Phys. Rev. C79, 064313 (2009)

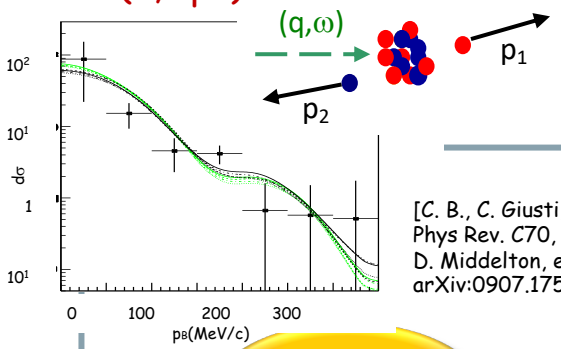
Self-Consistent Green's Function Approach



- Global picture of nuclear dynamics
- Reciprocal correlations among effective modes
- Guaranties *macroscopic conservation laws*

Self-Consistent Green's Function Approach

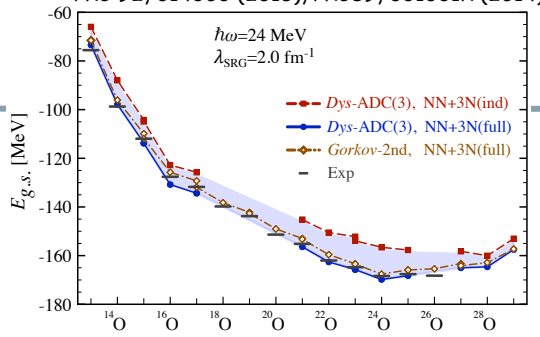
$^{16}O(e,e'pn)^{14}N$ @ MAINZ



[C. B., C. Giusti, et al.
Phys Rev. C70, 014606 (2004)
D. Middelton, et al.
arXiv:0907.1758; EPJA in print]

Binding energies

[PRL. 111, 062501 (2013),
PRC 92, 014306 (2015), PRC89, 061301R (2014)]



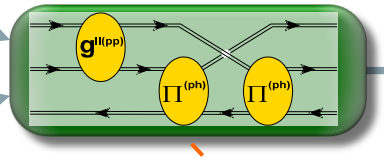
Ionization energies/ affinities, in atoms

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

		Hartree-Fock	FRPAc	Experiment [16, 17]
He:	1s	0.918 (+14)	0.9008 (-2.9)	0.9037
Be^{2+}:	1s	5.6672 (+116)	5.6551 (-0.5)	5.6556
Be:	2s	0.3093 (-34)	0.3224 (-20.2)	0.3426
	1s	4.733 (+200)	4.5405 (+8)	4.533
Ne:	2p	0.852 (+57)	0.8037 (+11)	0.793
	1s	1.931 (+149)	1.7967 (+15)	1.782
Mg^{2+}:	2p	3.0068 (+56.9)	2.9537 (+3.8)	2.9499
	1s	4.4827	4.3589	
Mg:	3s	0.253 (-28)	0.280 (-1)	0.281
	2p	2.282 (+162)	2.137 (+17)	2.12
Ar:	3p	0.591 (+12)	0.579 (≈0)	0.579
	3s	1.277 (+202)	1.065 (-10)	1.075
	3s		1.544	
	2p	9.571 (+411)	9.219 (+59)	9.160

$g^{II}(\omega)$

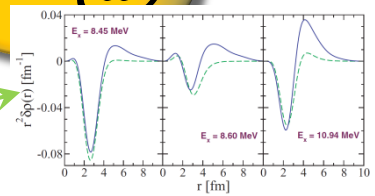
$\Pi^{(ph)}(\omega)$

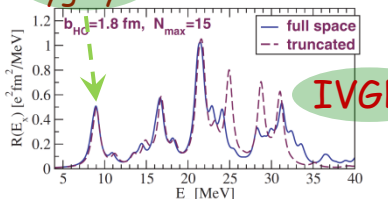


Dyson Eq.

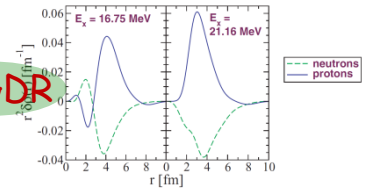
Isovector response for ^{32}Ar, ^{34}Ar

Proton Pygmy





IVGDR



[C. B., K. Langanke, et al., Phys Rev. C77, 024304 (2008)]

Optical potential