TALENT Course no. 2: Many-Body Methods for Nuclear Physics

Self-consistent Green's function in Finite Nuclei and related things…
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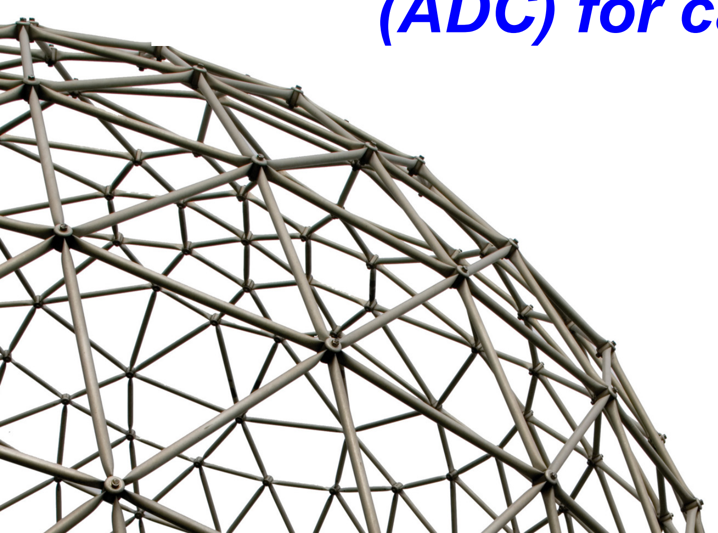
Lecture III

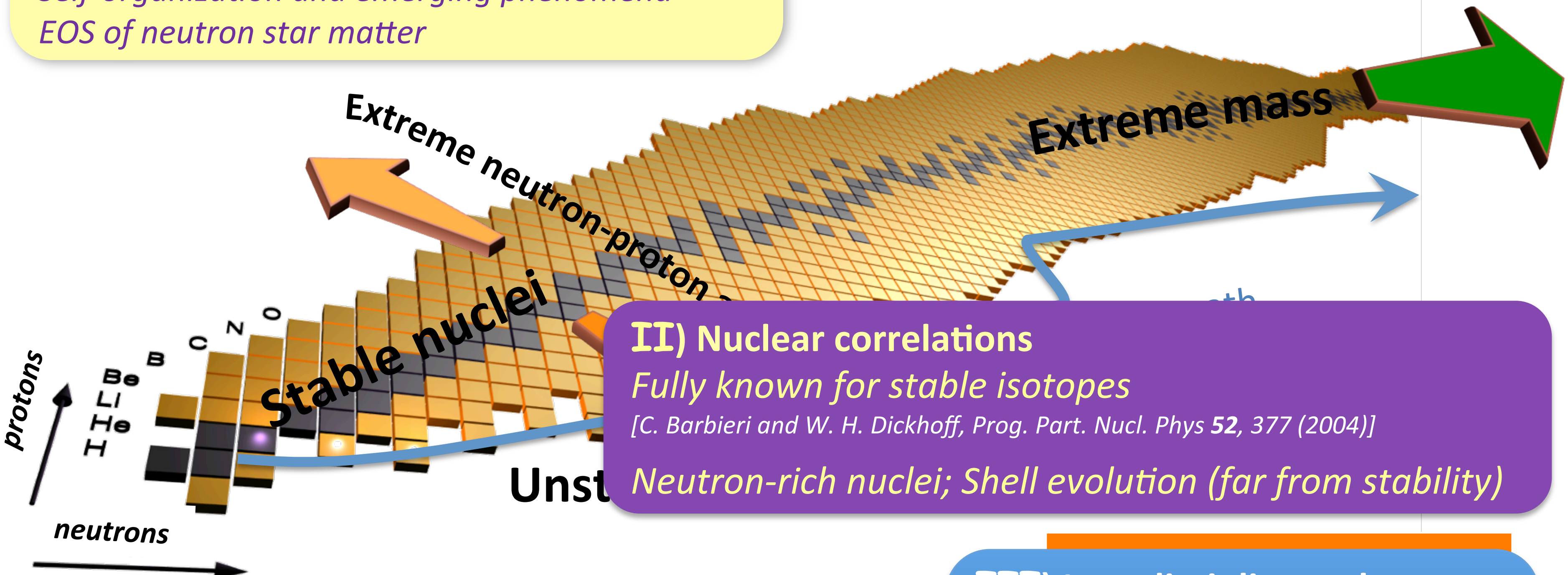
Algebraic Diagramatic Construction method (ADC) for calculating the self- energy



Current Status of low-energy nuclear physics

Composite system of interacting fermions
Binding and limits of stability
Coexistence of individual and collective behaviors
Self-organization and emerging phenomena
EOS of neutron star matter

Experimental programs
RIKEN, FAIR, FRIB



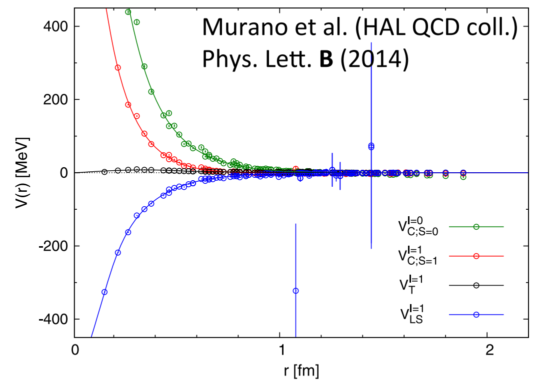
II) Nuclear correlations
Fully known for stable isotopes
*[C. Barbieri and W. H. Dickhoff, Prog. Part. Nucl. Phys **52**, 377 (2004)]*
Neutron-rich nuclei; Shell evolution (far from stability)

I) Understanding the nuclear force
QCD-derived; 3-nucleon forces (3NFs)
First principle (ab-initio) predictions

III) Interdisciplinary character
Astrophysics
Tests of the standard model
Other fermionic systems:
ultracold gasses; molecules;

Nuclear forces in exotic nuclei

Nucleon interactions are very complex and difficult to handle

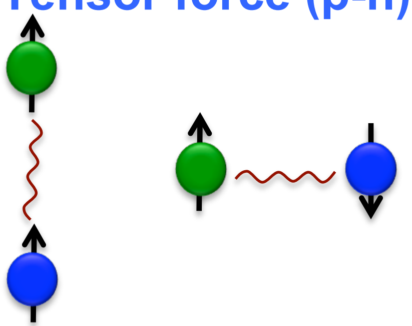


Change of regime from stable to dripline isotopes !

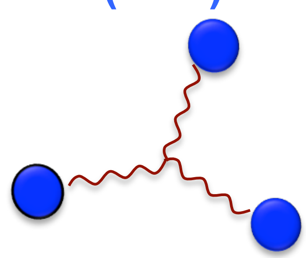
Symmetric matter:
N ≈ Z

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

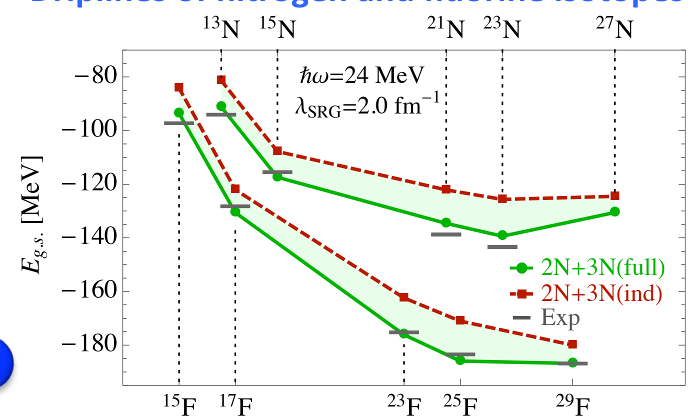
Tensor force (p-n)



Three-nucleon Force (3NF)



Driplines of nitrogen and fluorine isotopes



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

Why want to look at spectral function?

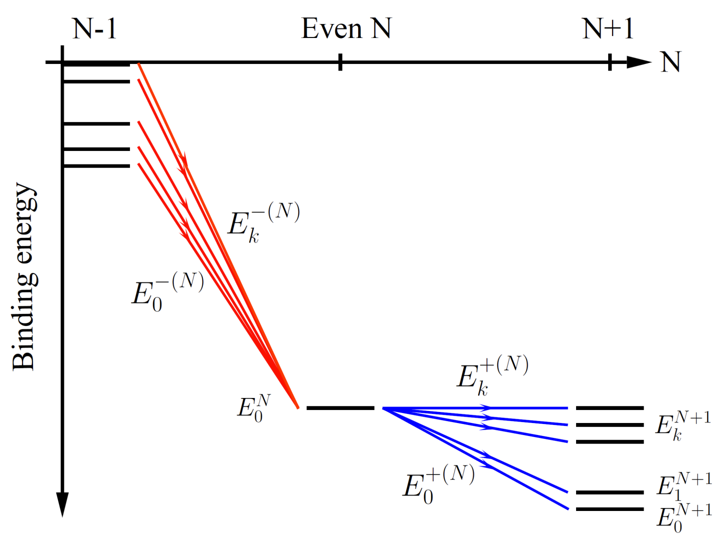
- Strong insight in to the structure (can be done the "ab-initio" way but it also gives qualitative understanding)
- Koltun SR links E_0^A and S^h in a "deep" manner
- Describes hole states (structure) and particle region (scattering) naturally
- Response to excitations, and particle addition/removal
- Useful to investigate changes shell structure

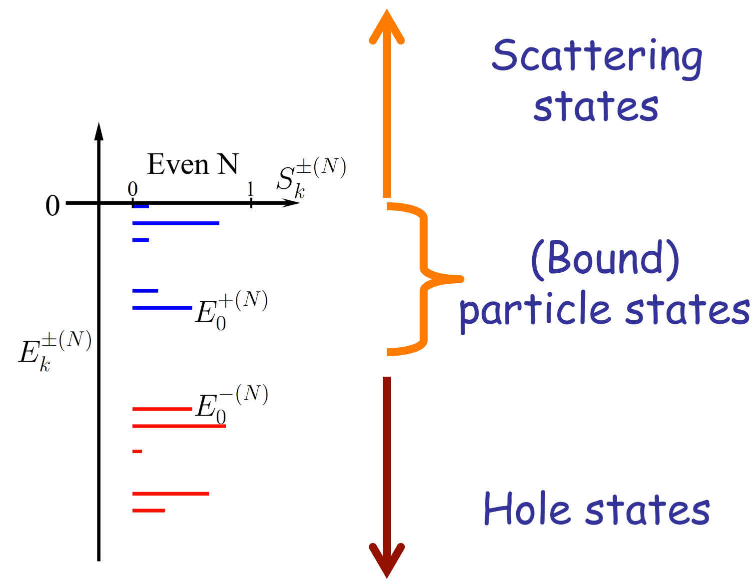
Green's functions in many-body theory

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 <u>all the structure information</u> probed by nucleon transfer (spectral function):





Separation energies and transfer strengths

[pic. J. Sadoudi]

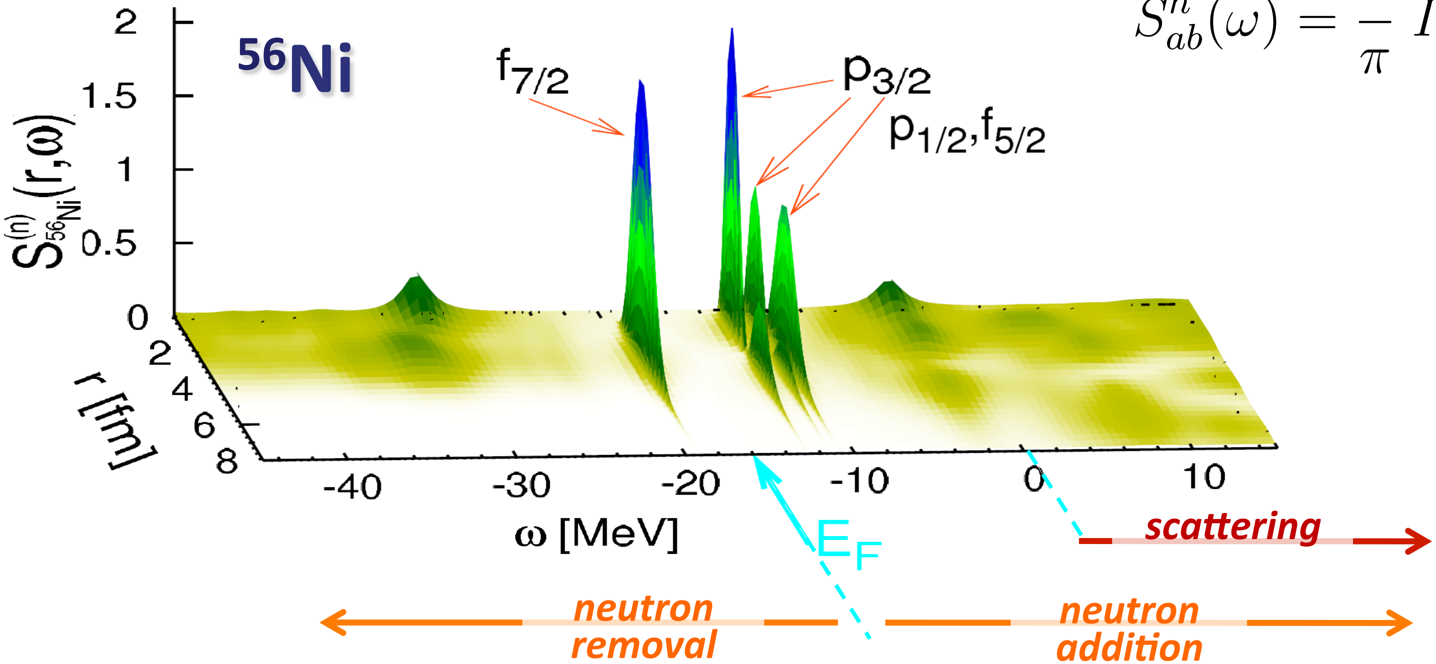
Example of spectral function ^{56}Ni

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):

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



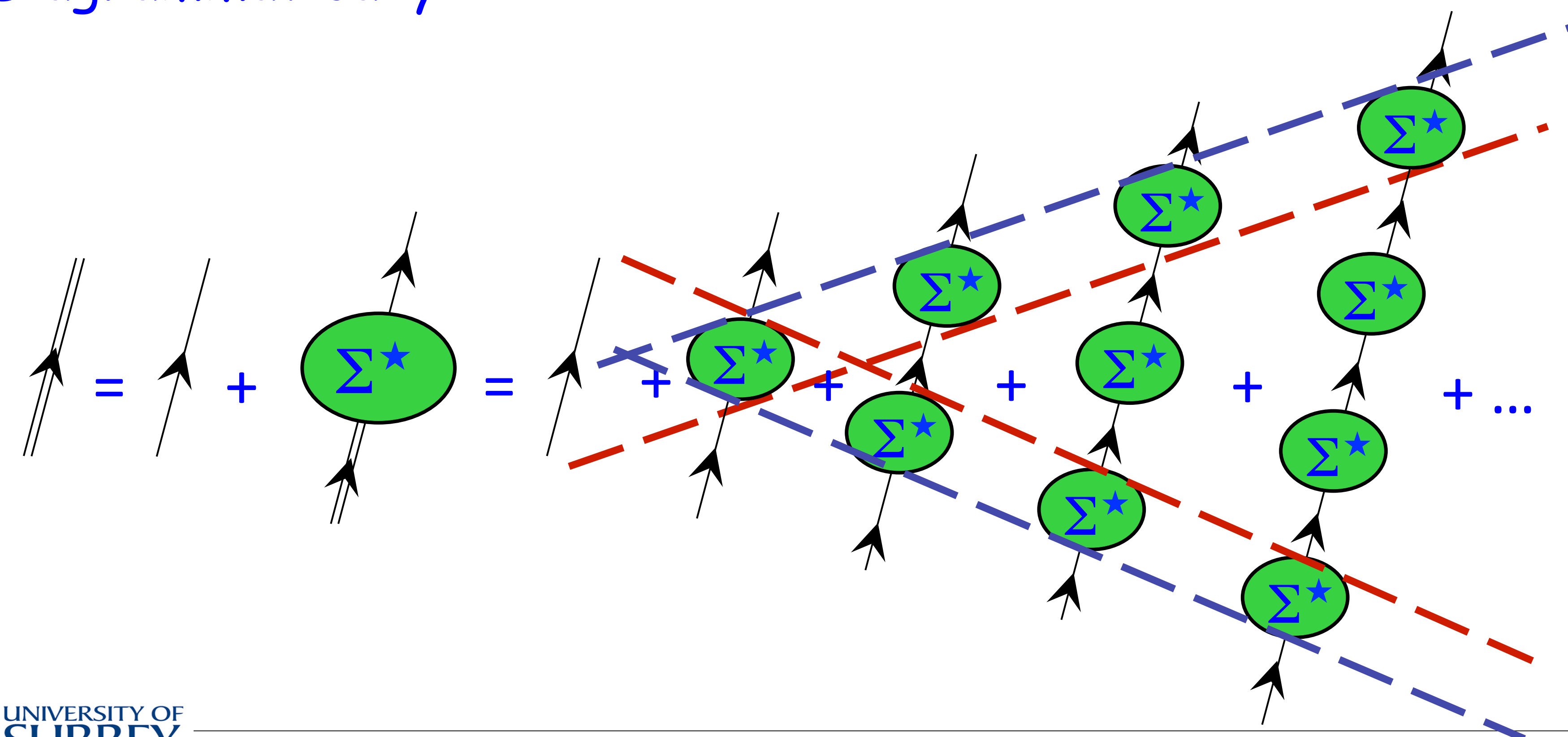
[CB, M.Hjorth-Jensen, Pys. Rev. C**79**, 064313 (2009); CB, Phys. Rev. Lett. **103**, 202502 (2009)]

Dyson equation

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:



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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

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*.

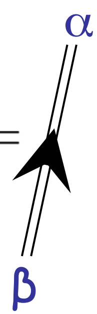
The complete propagator requires the Heisenberg evolution for the full H:

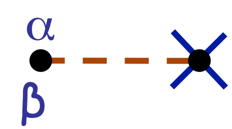
$$g_{\alpha\beta}(t,t') = -\frac{i}{\hbar}\langle\Psi_0^N|T[c_\alpha(t)c_\beta^\dagger(t')]|\Psi_0^N\rangle, \quad c_\alpha(t) \;=\; e^{iHt/\hbar}\, c_\alpha\, e^{-iHt/\hbar}$$

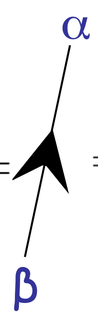
but we can handle only H_0. Thus, evolve operators according to an H_0 mpensate for the missing part (H_1) evolving the wave function → This is the Interaction (or Dirac) picture.

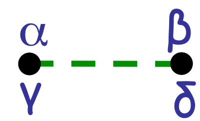
Feynman diagram rules

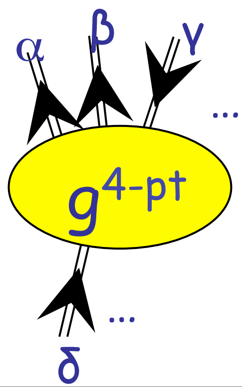
Graphic conventions:

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

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

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

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

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

Feynman diagram rules

Rules in *time* representation

1. Write all connected and topologically equivalent diagrams—and only those.
2. Each single line w/ an arrow, contributes running from β to α
3. Each closed circle contributes a density matrix (no factor!)
4. Each two-body interaction line contributes
5. Each external field line contributes
6. Add an extra -1 factor for each closed circuit (the density matrix loops excluded)
7. Sum (integrate) over all coordinate and integrate over all internal times
8. IF are *antisymmtrized* matrix elements, and extra factor ½ is required for each pair of equivalent lines, starting from the common interaction and ending on common interaction (not necessarily the same).
9. Add final factor is to get G(t-t`) .

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Feynman diagram rules

On can transform any propagator in frequency space. This is done by:

$$g_{\alpha\beta\ldots;\mu\nu\ldots}(\omega_\alpha, \omega_\beta, \ldots) = \int dt_\alpha \int dt_\beta \cdots \int dt_\mu \int dt_\nu \cdots$$

$$\times e^{i\omega_\alpha t_\alpha} \, e^{i\omega_\beta t_\beta} \cdots \; g_{\alpha\beta\ldots;\mu\nu\ldots}(t_\alpha, t_\beta, \ldots; t_\mu, t_\nu, \ldots) \, e^{-i\omega_\mu t_\mu} e^{-i\omega_\nu t_\nu} \cdots$$

Note that:

$$g_{\alpha\beta}(\omega, \omega') = \delta(\omega - \omega') \, g_{\alpha\beta}(\omega)$$

usual transformation for the 2-time propagators.

For the interactions: after Fourier transformation the delta terms in $t_{\alpha\beta}\delta(t_\alpha - t_\beta)$ and $v_{\alpha\beta,\gamma\delta}\delta(t_\alpha - t_\beta)\delta(t_\gamma - t_\delta)\delta(t_\alpha - t_\gamma)$ give the conservation of incoming and outgoing energy.

Feynman diagram rules

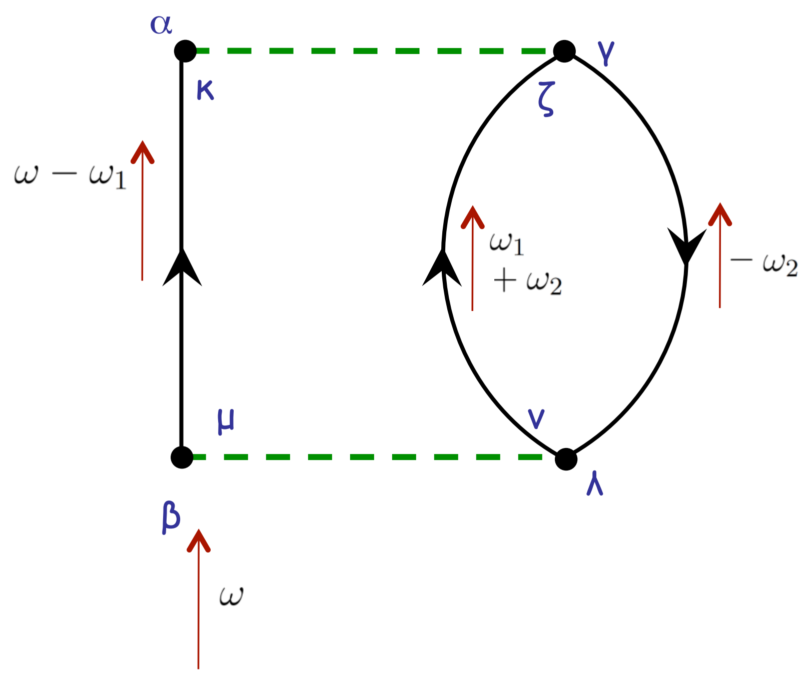
Rules in *frequency* representation

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

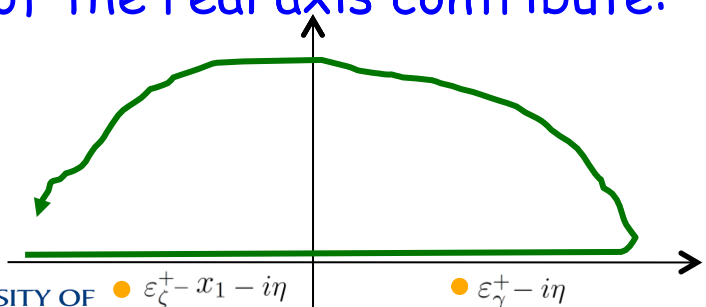
Example of using Feynman diagram rules

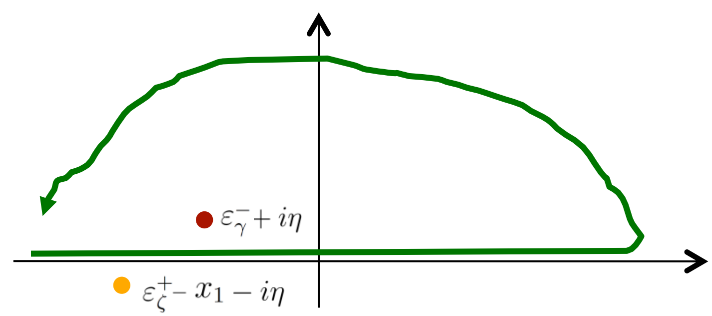
Calculating the *second order* self-energy:

$\boxed{x_i \equiv \hbar\omega_i}$

$$
\begin{aligned}
\Sigma^{2nd}_{\alpha\beta}(\omega) &= i\hbar\,(i\hbar)^3\left(\frac{-i}{\hbar}\right)^2\frac{(-1)^2}{2}v_{\alpha\gamma,\kappa\zeta}v_{\mu\nu,\beta\lambda}\int\frac{d\omega_1}{2\pi}\int\frac{d\omega_2}{2\pi}g_{\kappa\mu}(\omega-\omega_1)g_{\zeta\nu}(\omega_1+\omega_2)g_{\lambda\gamma}(\omega_2)\\
&= -\frac{1}{2}v_{\alpha\gamma,\kappa\zeta}v_{\mu\nu,\beta\lambda}\int\frac{dx_1}{2\pi i}\int\frac{dx_2}{2\pi i}g_{\kappa\mu}(\omega-\omega_1)g_{\zeta\nu}(\omega_1+\omega_2)g_{\lambda\gamma}(\omega_2)\\
&= -\frac{1}{2}v_{\alpha\gamma,\kappa\zeta}v_{\mu\nu,\beta\lambda}\int\frac{dx_1}{2\pi i}g_{\kappa\mu}(\omega-\omega_1)\int\frac{dx_2}{2\pi i}\\
&\quad\times\delta_{\zeta\nu}\left\{\underset{x_2\downarrow}{\frac{\delta_{\zeta\notin F}}{x_1+x_2-\varepsilon^+_\zeta+i\eta}}+\underset{x_2\uparrow}{\frac{\delta_{\zeta\in F}}{x_1+x_2-\varepsilon^-_\zeta-i\eta}}\right\}\left\{\underset{x_2\downarrow}{\frac{\delta_{\gamma\notin F}}{x_2-\varepsilon^+_\gamma+i\eta}}+\underset{x_2\uparrow}{\frac{\delta_{\gamma\in F}}{x_2-\varepsilon^-_\gamma-i\eta}}\right\}
\end{aligned}
$$

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





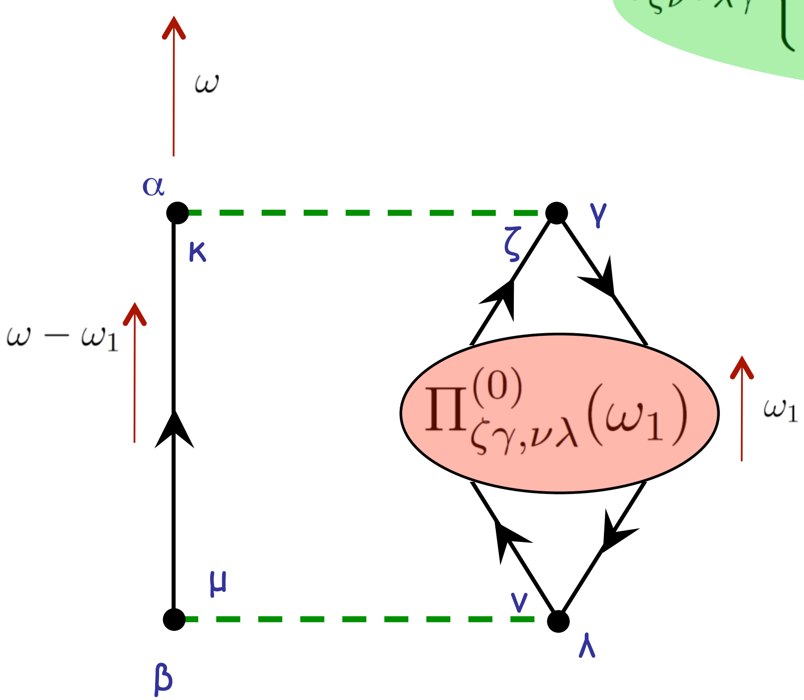
Example of using Feynman diagram rules

Calculating the *second order* self-energy:

$\boxed{x_i \equiv \hbar\omega_i}$

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

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



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

Example of using Feynman diagram rules

Calculating the *second order* self-energy:

$\boxed{x_i \equiv \hbar\omega_i}$

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

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

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

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

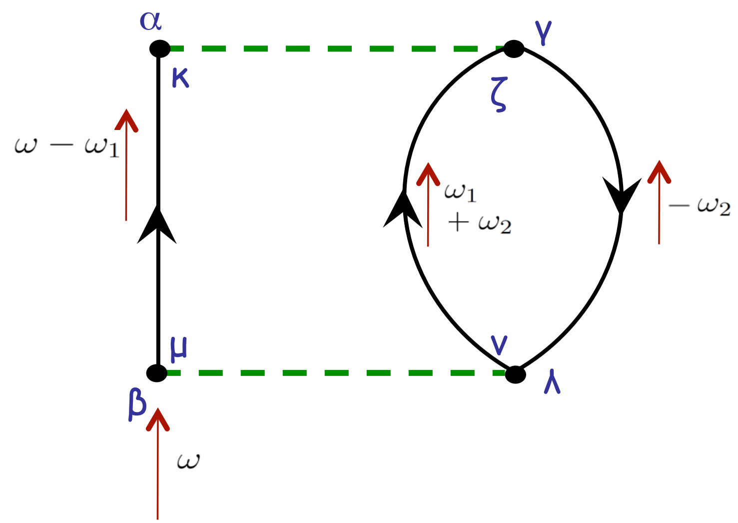
$$\Sigma^{2nd}_{\alpha\beta}(\omega) = \frac{1}{2} v_{\alpha\lambda,\mu\nu}\left\{\frac{\delta_{\mu\notin F}\,\delta_{\nu\notin F}\,\delta_{\lambda\in F}}{\hbar\omega-(\varepsilon^+_\mu+\varepsilon^+_\nu-\varepsilon^-_\lambda)+i\eta} + \frac{\delta_{\mu\in F}\,\delta_{\nu\in F}\,\delta_{\lambda\notin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

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 colls.:

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

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

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

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

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

with

$$\left\{ \begin{array}{lcl} \mathcal{X}^n_\alpha & \equiv & \langle \Psi^{A+1}_n | a^\dagger_\alpha | \Psi^A_0 \rangle \\ \varepsilon^+_n & \equiv & E^{A+1}_n - E^A_0 \\ E^{A+1}_n | \Psi^{A+1}_n \rangle & = & H^{(ref)} | \Psi^{A+1}_n \rangle \end{array} \right. \qquad \left\{ \begin{array}{lcl} \mathcal{Y}^k_\alpha & \equiv & \langle \Psi^{A-1}_k | a_\alpha | \Psi^A_0 \rangle \\ \varepsilon^-_k & \equiv & E^A_k - E^{A-1}_0 \\ E^{A-1}_k | \Psi^{A-1}_k \rangle & = & H^{(ref)} | \Psi^{A-1}_k \rangle \end{array} \right.$$

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 $\;2p1h, \;\; 3p2h, \;\; 4p3h, \; ...\;$ excitations

$r,\ p \longrightarrow$ label $\;2h1p, \;\; 3h2p, \; ...\;$ 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

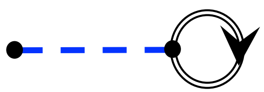
$$(\vec{Z}^{\pm})^{\dagger}\,\vec{Z}^{\pm}\ +\ \vec{W}^{\dagger}\,\vec{W}\ +\ \vec{U}^{\dagger}\,\vec{U}=1$$

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

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

Working eqs. for ADC(2)

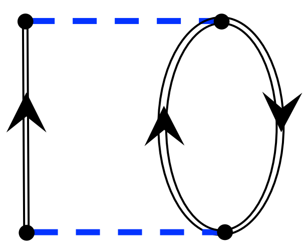
The dressed 1st and 2nd order diagrams are:

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

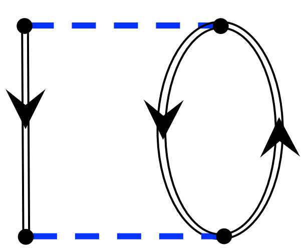
$$\Sigma^{cHF}_{\alpha\beta} = \int_{C\uparrow} \frac{\mathrm{d}\omega}{2\pi i}\, v_{\alpha\gamma,\beta\delta}\, g^{(ref)}_{\delta\gamma}(\omega) = \sum_k v_{\alpha\gamma,\beta\delta}\, \mathcal{Y}^k_\delta (\mathcal{Y}^k_\gamma)^*$$

and

$$\Sigma^{(2)}_{\alpha\beta}(\omega) =$$



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



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

Repeated greek indices are implicitly summed

Working eqs. for ADC(2)

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

$$(\mathbf{H}_0 + \mathbf{\Sigma}^{\infty})_{\alpha\beta} = (\mathbf{T} + \mathbf{U})_{\alpha\beta} + (-\mathbf{U} + \mathbf{\Sigma}^{cHF})_{\alpha\beta}$$

$$= t_{\alpha\beta} + \sum_k v_{\alpha\gamma,\beta\delta}\, \mathcal{Y}^k_\delta (\mathcal{Y}^k_\gamma)^*$$

$$\mathbf{M}_{(n_1,n_2,k),\alpha} = \mathcal{X}^{n_1}_\mu \mathcal{X}^{n_2}_\nu \mathcal{Y}^k_\lambda\, v_{\mu\nu,\alpha\lambda}$$

$$\mathbf{N}_{(k_1,k_2,n),\alpha} = (\mathcal{Y}^{k_1}_\mu \mathcal{Y}^{k_2}_\nu \mathcal{X}^n_\lambda)^*\, v_{\mu\nu,\alpha\lambda}$$

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

$$\mathbf{E}^{bk}_{k_1,k_2,n} = \varepsilon^-_{k_1} + \varepsilon^-_{k_2} - \varepsilon^-_n$$

$$\mathbf{C} = 0$$

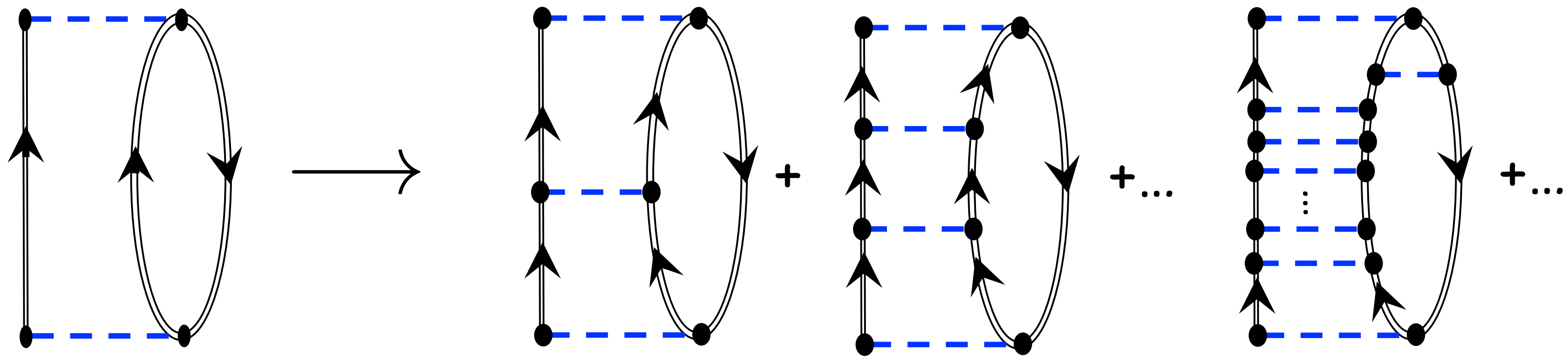
$$\mathbf{D} = 0$$

Repeated greek 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:

$$
\begin{aligned}
\longrightarrow V\frac{1}{\omega - E_{2p1h}}V \;+\; & V\frac{1}{\omega - E_{2p1h}}V\frac{1}{\omega - E_{2p1h}}V \\
+\; & V\frac{1}{\omega - E_{2p1h}}V\frac{1}{\omega - E_{2p1h}}V\frac{1}{\omega - E_{2p1h}}V \\
+\; & V\frac{1}{\omega - E_{2p1h}}V\frac{1}{\omega - E_{2p1h}}V\frac{1}{\omega - E_{2p1h}}V\frac{1}{\omega - E_{2p1h}}V + \dots
\end{aligned}
$$

Working eqs. for ext-ADC(2)

Expand the self-energy in the interparticle 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, D, E are only at 1st order. This leads to contributions of the form:

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

➔from here one reads out 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:

$$\mathbf{C}_{(n_1,n_2,k_3),(n_4,n_5,k_6)} = \langle n_1 n_2 | v | n_4 n_5 \rangle \delta_{k_3,k_6} + \langle n_1 k_3 | v^{ph} | n_4 k_6 \rangle \delta_{n_2,n_6} + \langle n_2 k_3 | v^{ph} | n_5 k_6 \rangle \delta_{n_1,n_4}$$

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

where:

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

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

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

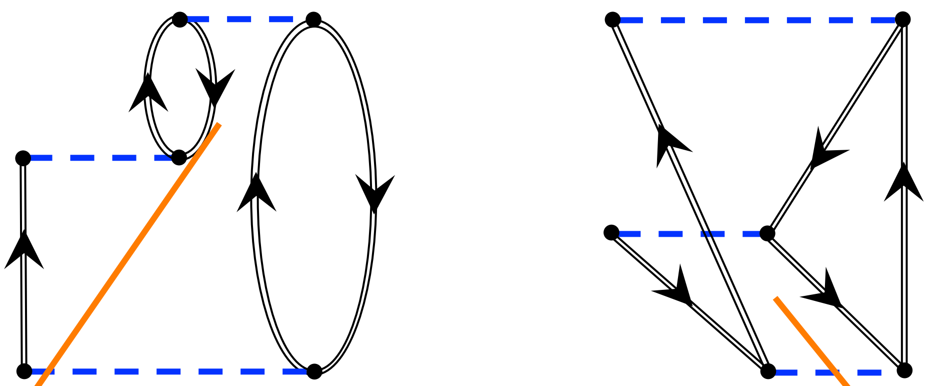
$$\langle k_1 n_3 | v^{ph} | k_4 n_6 \rangle \equiv (\mathcal{Y}_\alpha^{k_1} \mathcal{X}_\beta^{n_3})^* v_{\alpha\delta,\beta\gamma} \, \mathcal{Y}_\gamma^{k_4} \mathcal{X}_\delta^{n_6}$$

Repeated greek indices are implicitly summed

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

Working eqs. For ADC(3)

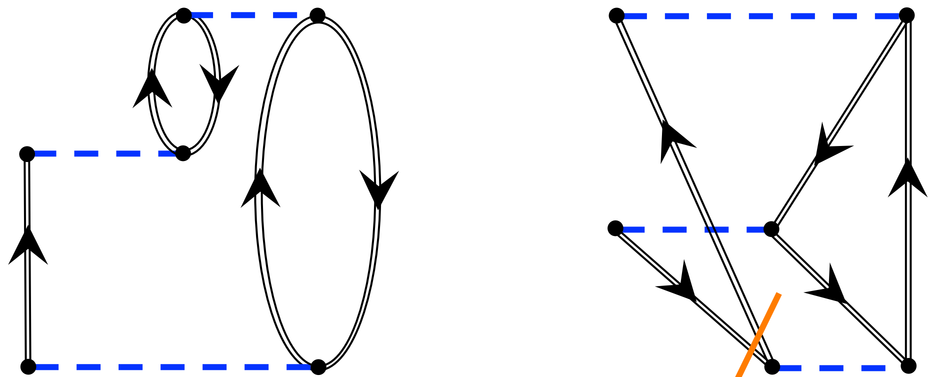
Requiting that ALL 3rd order Goldstone diagrams are included requires to also extending the coupling matrices:



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

Working eqs. For ADC(3)

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



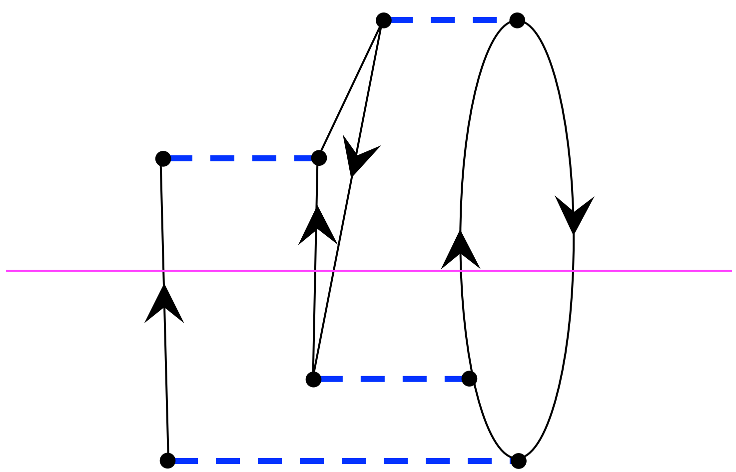
$$\mathbf{M}_{(n_1,n_2,k),\alpha} = \mathcal{X}_\mu^{n_1}\mathcal{X}_\nu^{n_2}\mathcal{Y}_\lambda^{k}\, v_{\mu\nu,\alpha\lambda} + \frac{\mathcal{X}_\sigma^{n_1}\mathcal{X}_\rho^{n_2} v_{\sigma\rho,\gamma\delta}(\mathcal{Y}_\gamma^{k_7}\mathcal{Y}_\delta^{k_8})^*}{2(\varepsilon_{k_7}^- + \varepsilon_{k_8}^-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

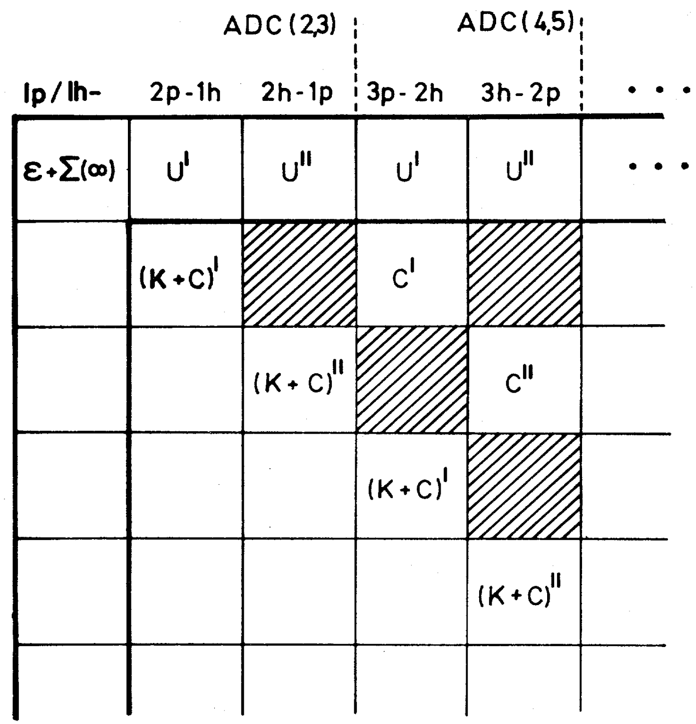
$$\mathbf{N}_{(k_1,k_2,n),\alpha} = (\mathcal{Y}_\mu^{k_1}\mathcal{Y}_\nu^{k_2}\mathcal{X}_\lambda^{n})^*\, v_{\mu\nu,\alpha\lambda} + \frac{(\mathcal{Y}_\sigma^{k_1}\mathcal{Y}_\rho^{k_2})^* v_{\sigma\rho,\gamma\delta}\mathcal{X}_\gamma^{n_7}\mathcal{X}_\delta^{n_8}}{2(\varepsilon_{k_1}^- + \varepsilon_{k_2}^-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

Beyond ADC(3)...

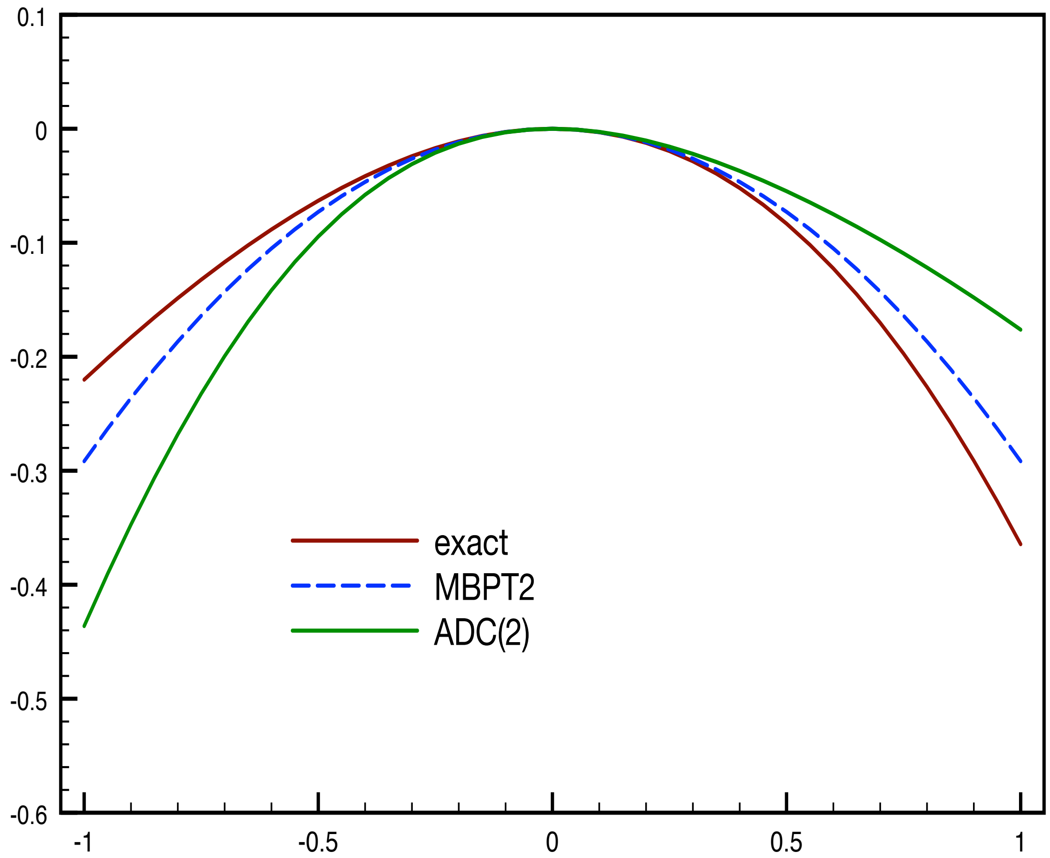
The general strategy is: expand the self-energy in Feynman/ Goldstone diagrams up to order *n* and the compare to the minimal expansion in terms of matrices C, D and M, N.

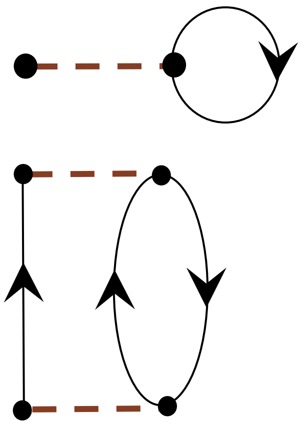
For ADC(4), also 3p2h/3h2p intermediate states appear:



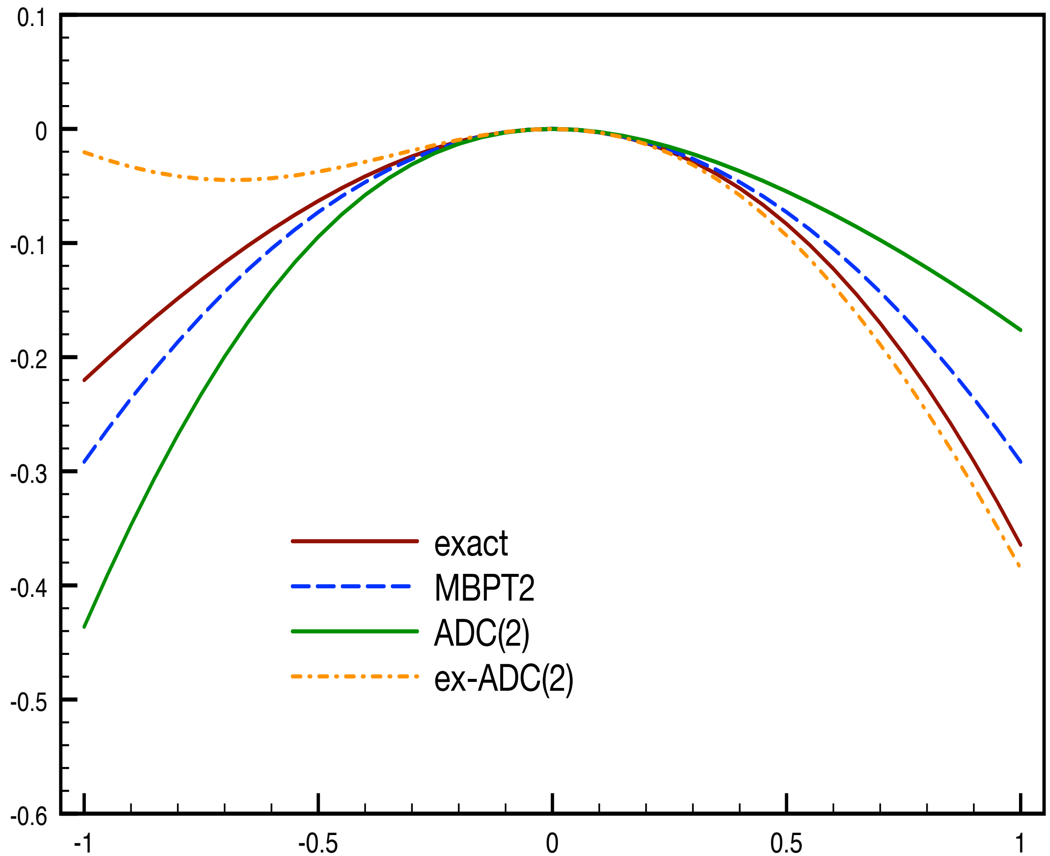


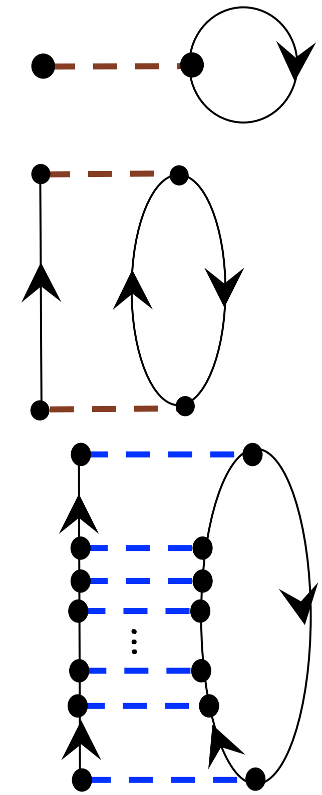
Results for the pairing model

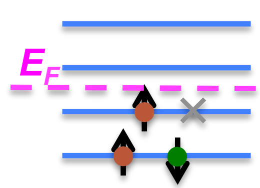
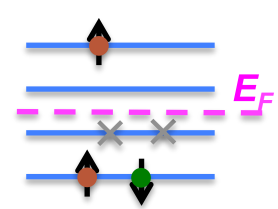




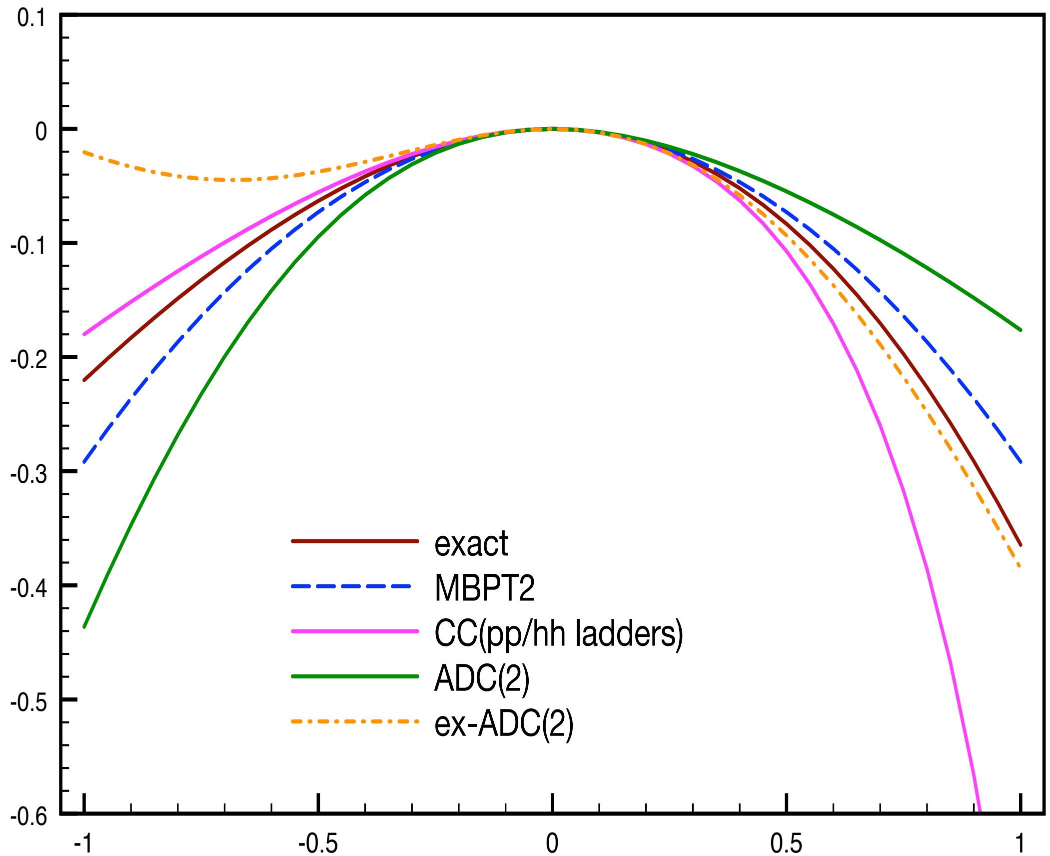
Results for the pairing model

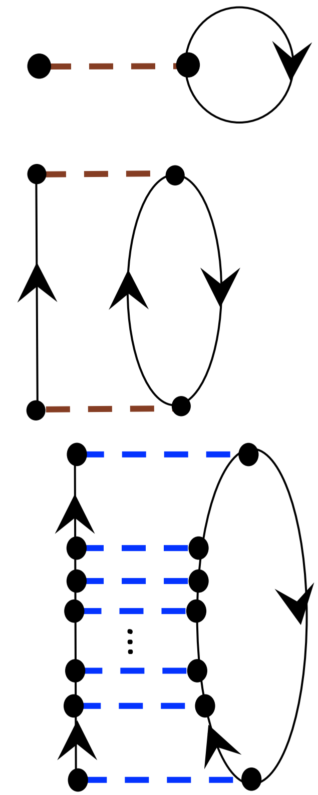




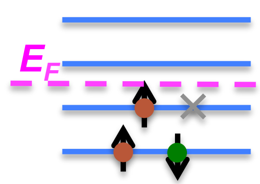
$\langle\, \Phi_k; 1h \;|H_1|\; \Phi^n_{k1,k2}; 2h1p \,\rangle = \;\langle$  $\;|\sum_{p.q} P_p^\dagger P_q|\;$  $\rangle = 0$

Results for the pairing model

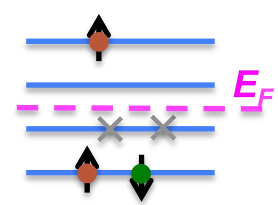




$\langle\ \Phi_k; 1h\ |H_1|\ \Phi^n_{k1,k2}; 2h1p\ \rangle =\ \langle$



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



$\rangle = 0$

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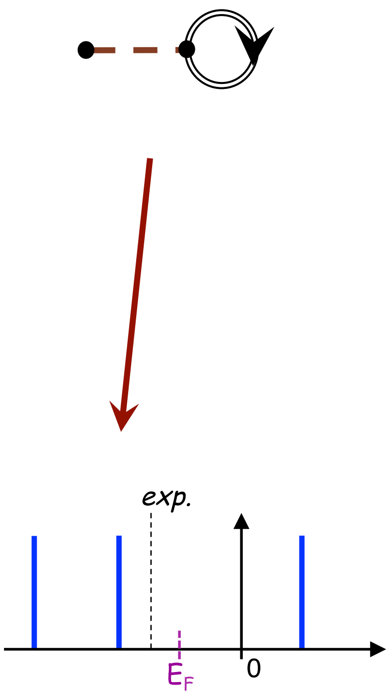
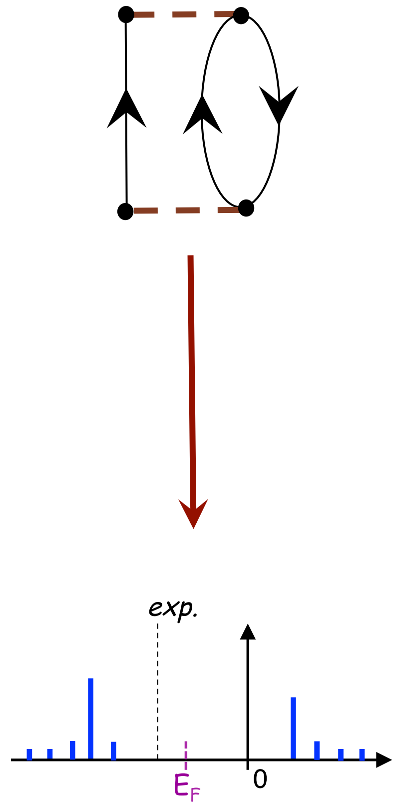
Accuracy of ADC(n) - simple atoms/molecules

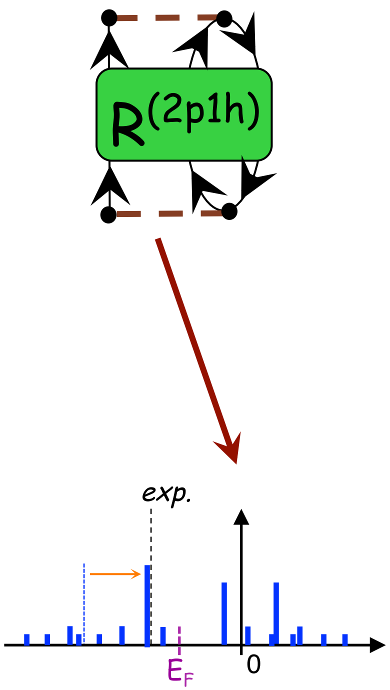
ADC(1) ≡ HF



ADC(2) ≡ 2^{nd} ord.



ADC(3) ≡ FTDA
FRPA

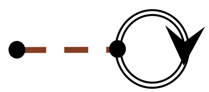


98-99% of correlation energy is recovered

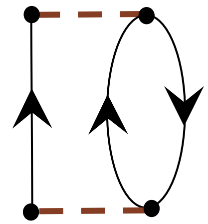
binding, eq. bond distances, →
ionization energies (molecules)

Accuracy of ADC(n) – simple atoms/molecules

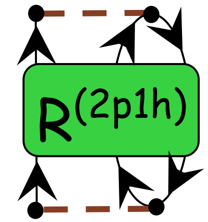
ADC(1) ≡ HF



ADC(2) ≡ 2nd ord.



ADC(3) ≡ FTDA
FRPA



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

← ionization energies (atoms)

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

NB: energies in Hartree
errors in mHartree

Accuracy of FRPA for atoms

- Diatomic molecules

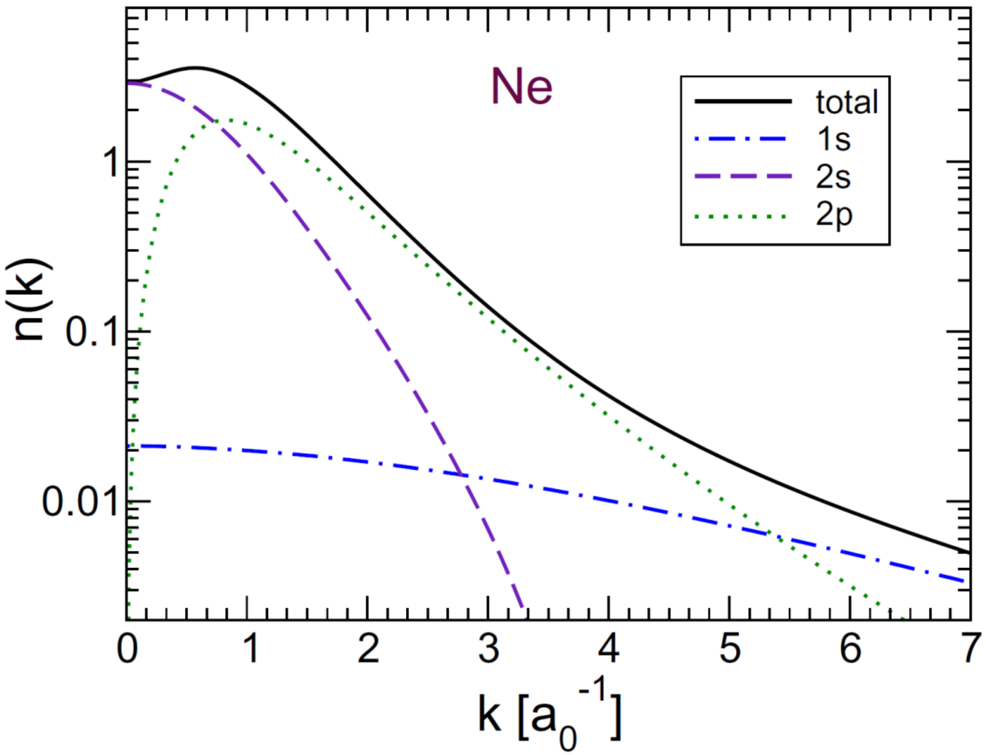
		FTDAc	FRPAc	CCSD(T)	Expt.
N_2					
	E_0	-109.258	-109.272	-109.276	-
	r_0	1.104	1.106	1.119	1.098
	I	0.565	0.544	0.602[a]	0.573
BF					
	E_0	-124.365	-124.368	-124.380	-
	r_0	1.284	1.285	1.295	1.267
	I	0.395	0.402	0.406	-
CO					
	E_0	-113.037	-113.048	-113.055	-
	r_0	1.130	1.123	1.145	1.128
	I	0.503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

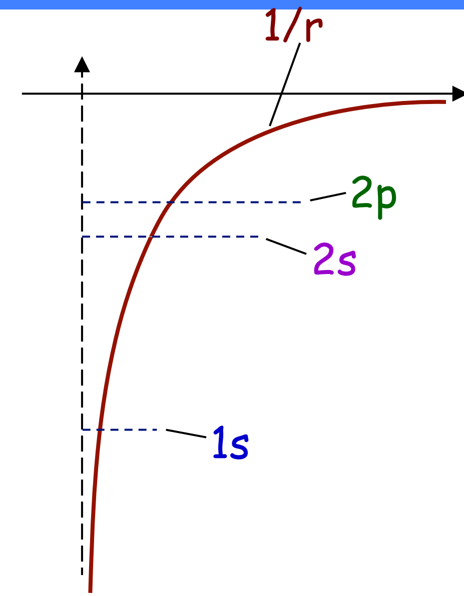
[a] Only up to CCD

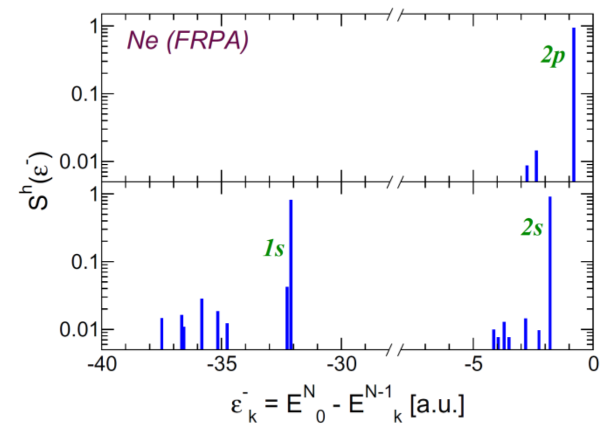
[M. Degroote, D. van Neck, C. B. Phys. Rev. A **83**, 042517 (2011); **85**, 012501 (2012)]

Spectral strength of Neon

Momentum distribution:





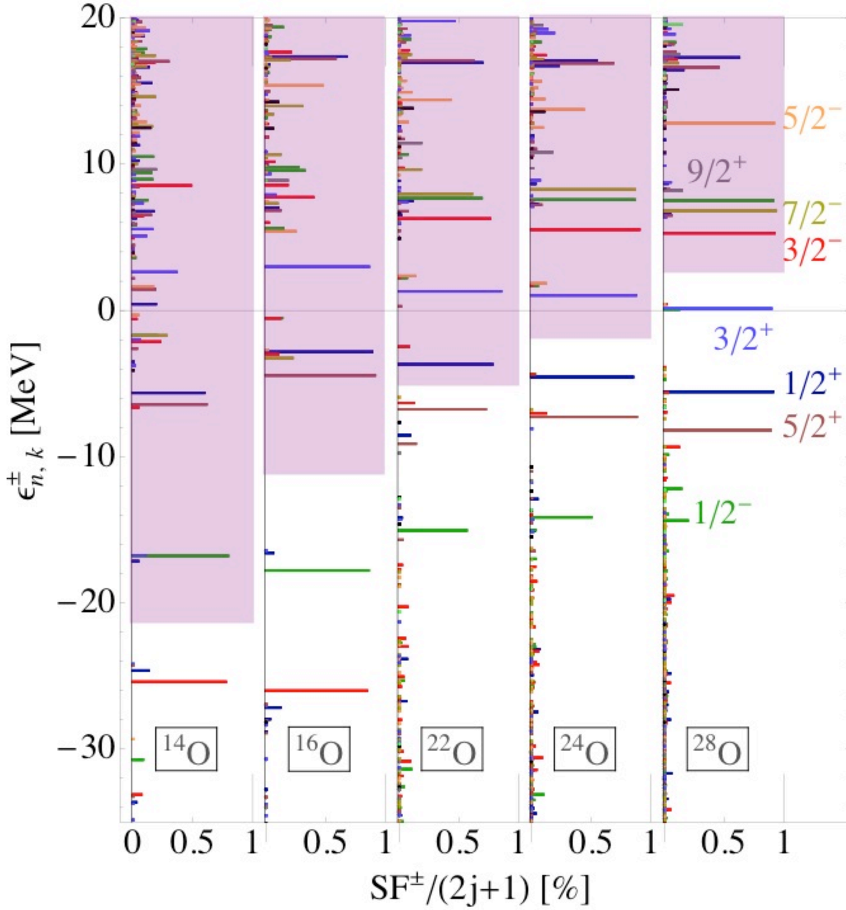


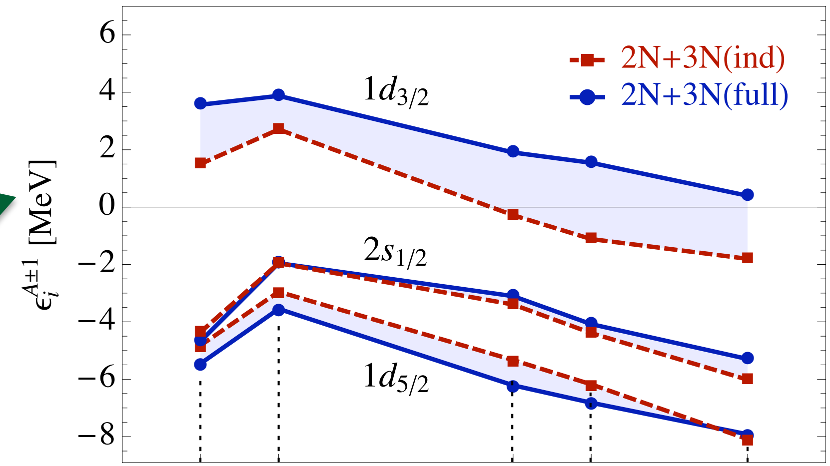
[CB, Van Neck, AIP Conf.Proc.1120, 104 ('09)]

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

Results for the N-O-F chains

A. Cipollone, CB, P. Navrátil, Phys. Rev. Lett. **111**, 062501 (2013)
and arXiv:1412.3002 [nucl-th] (2014)





→ *$d_{3/2}$ raised* by genuine 3NF

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

Results for the N-O-F chains

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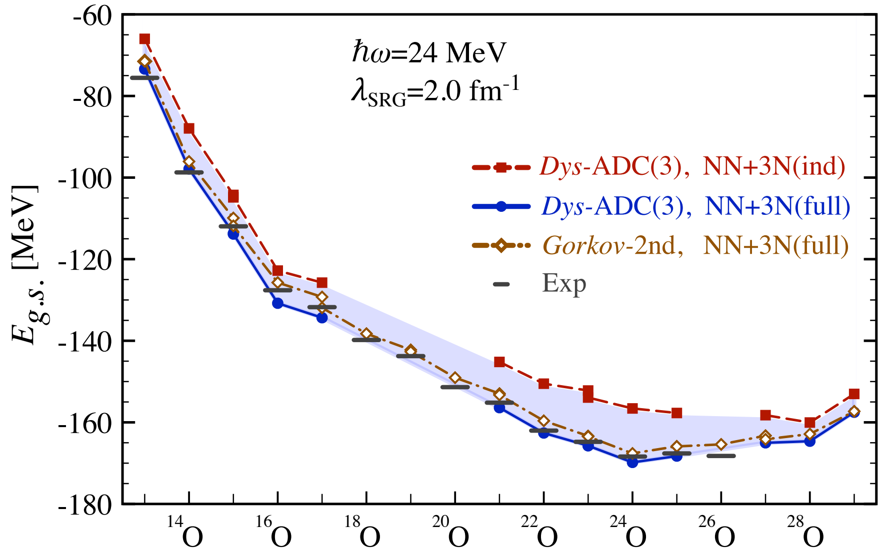

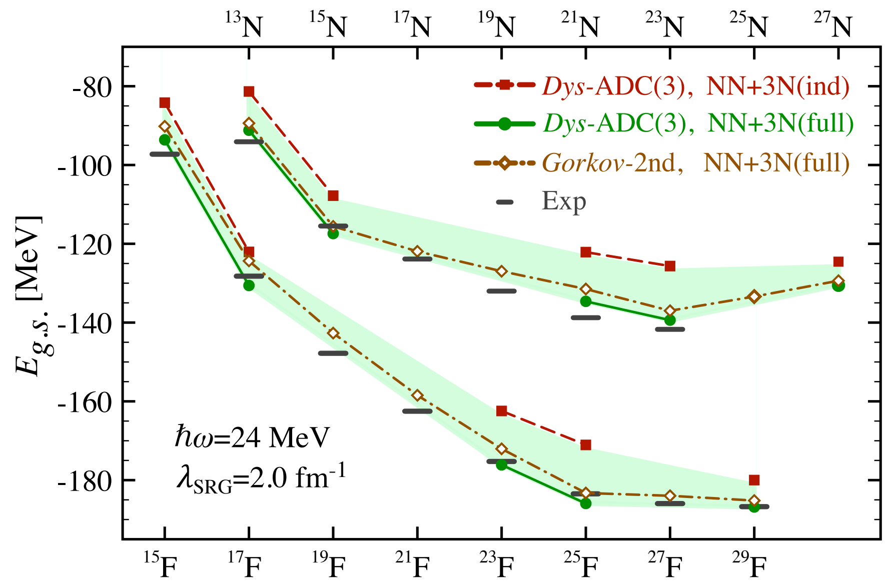

→ 3NF crucial for reproducing binding energies and driplines around oxygen

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

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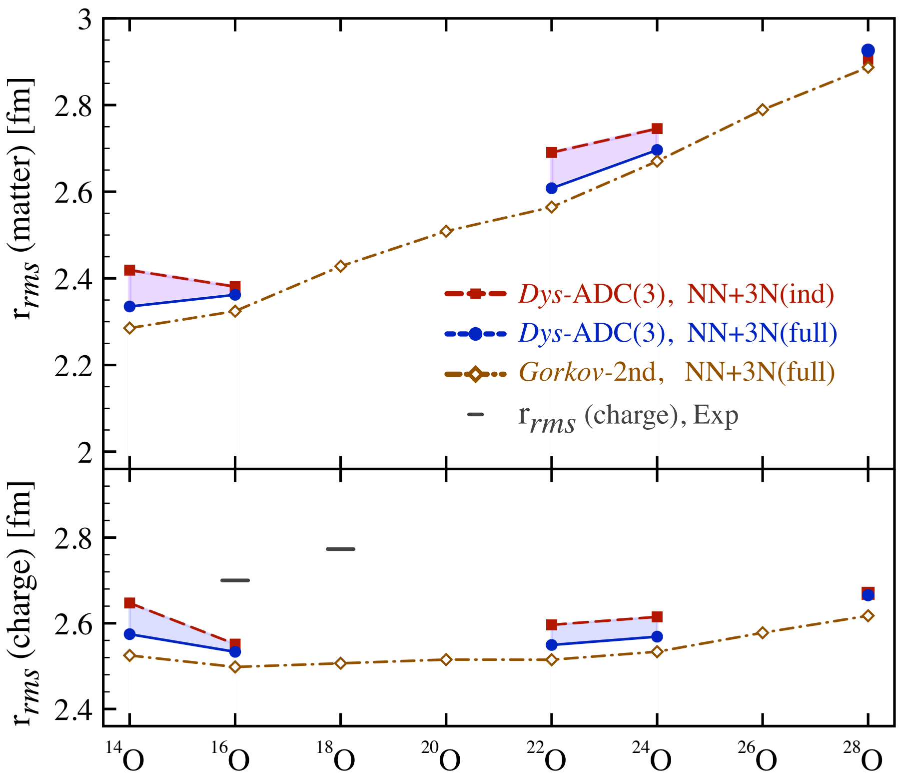
N3LO (Λ = 500Mev/c) chiral NN interaction evolved to 2N + 3N forces (2.0fm^{-1})
N2LO (Λ = 400Mev/c) chiral 3N interaction evolved (2.0fm^{-1})

Results for the oxygen chain

A. Cipollone, CB, P. Navrátil, arXiv:1412.3002 [nucl-th] (2014)



→ Single particle spectra slightly to spread and

→ systematic underestimation of radii

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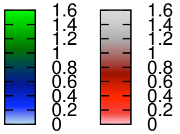
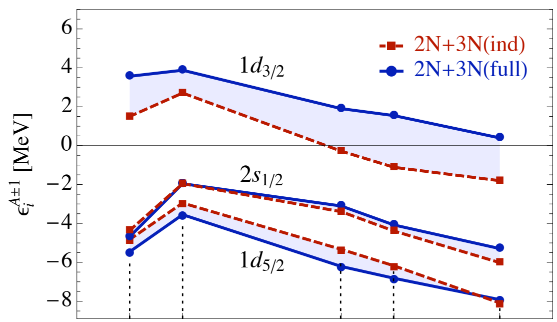
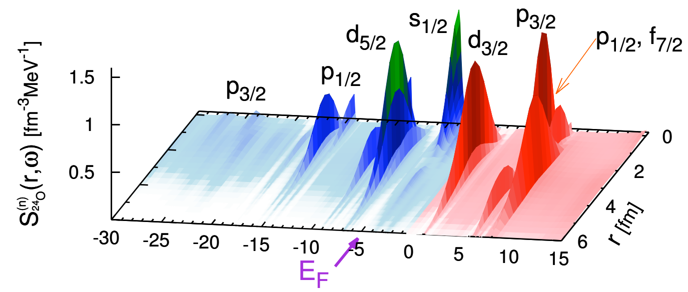
Neutron spectral function of Oxygens

A. Cipollone, CB P. Navrátil, *PRC submitted* (2014)

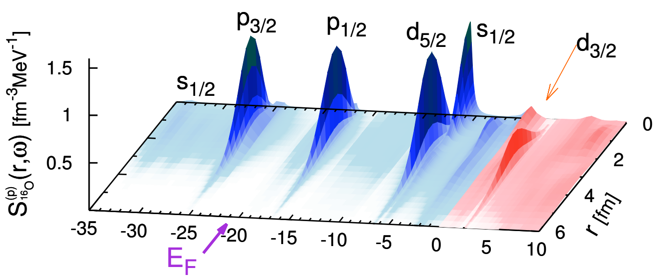




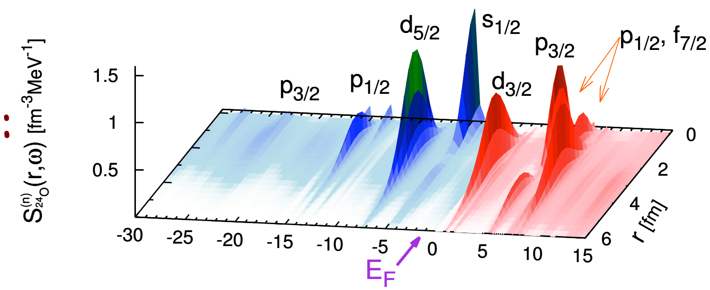
^{22}O:



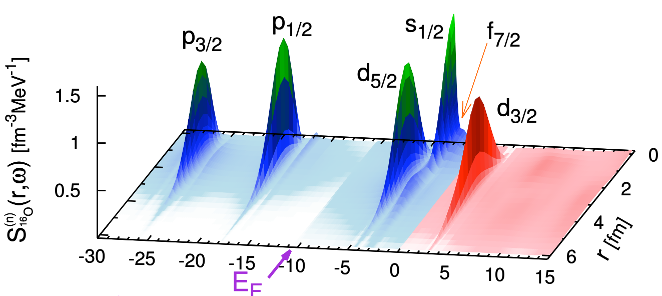
^{14}O:



^{24}O:

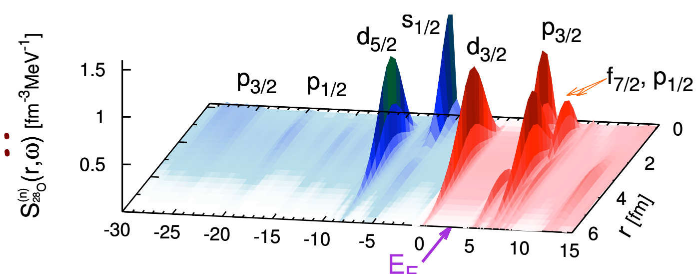


^{16}O:



^{15}O ← → ^{17}O

^{28}O:



^{27}O ← → ^{29}O

Nuclear matter project with Green's function and coupled cluster

This week we will start looking into how to calculate nuclear matter with the same methods introduced last week. Some short comments on this:

- We will discretize the continuous momentum space by using a box with periodic boundary conditions (PBC). This will be discussed in much detail by Gaute in the next lecture.

- The setup of the basis and the calculation of the reference HF state is the same for all methods (MBPT, CCM, SCGF…) and so next talk will apply to all projects.

- So set up you code with a general basis infrastructure, that will be separate from the solver…

- Some more comments specific to GF:
    - Once the HF is set up, we will need to build bases for pp and hh configurations (as for CC) but also 2p1h and 2h1p. These are are all built very similarly.
    - We will use the ADC(2) approach and later move to extended ADC(2), which requires a relatively small extra effort.
    - The self-energy is diagonal in k-space, which is a great simplification: for each value of momentum, we can diagonalize a part of the Dyson equations independently.
    - The approach is very similar to last week pairing model. However, we will have to deal with technical complications (the more sophisticated basis to handle, with more quantum numbers, the dimension of the Dyson sub-matrices, ecc…). All of this will be discussed little by little.