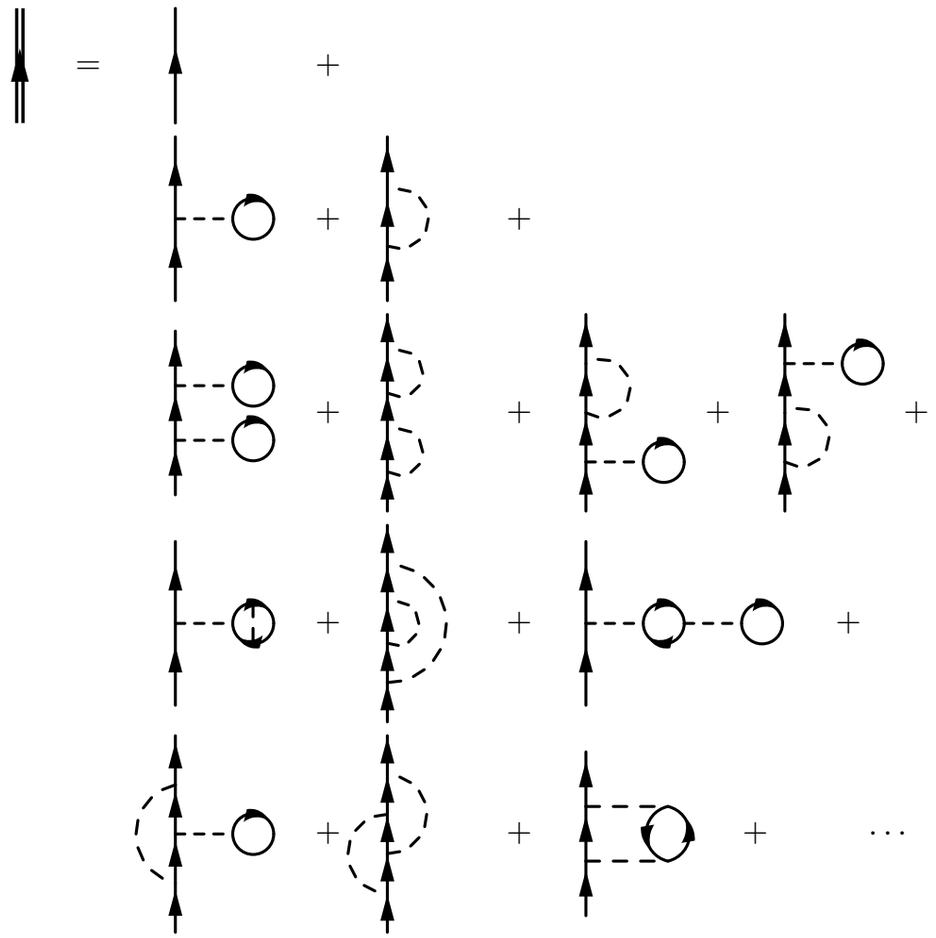
Self-consistent Green's function approach

Introduction to many-body GF theory and applications to nuclear systems



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Indian summer school "*Ab initio methods in nuclear physics*"

Prague, 29 August-2 September 2016

Ab initio vs effective approach to *A*-nucleon problem

Ab initio approaches

$$H|\Psi\rangle = E|\Psi\rangle$$

- H describes NN system in vacuum
  - **Fit to NN scattering data & deuteron**
- Link to QCD is usually **present**
- Systematically improvable, predictive
- Requires sophisticated many-body scheme
  - **Limited applicability (A<100)**

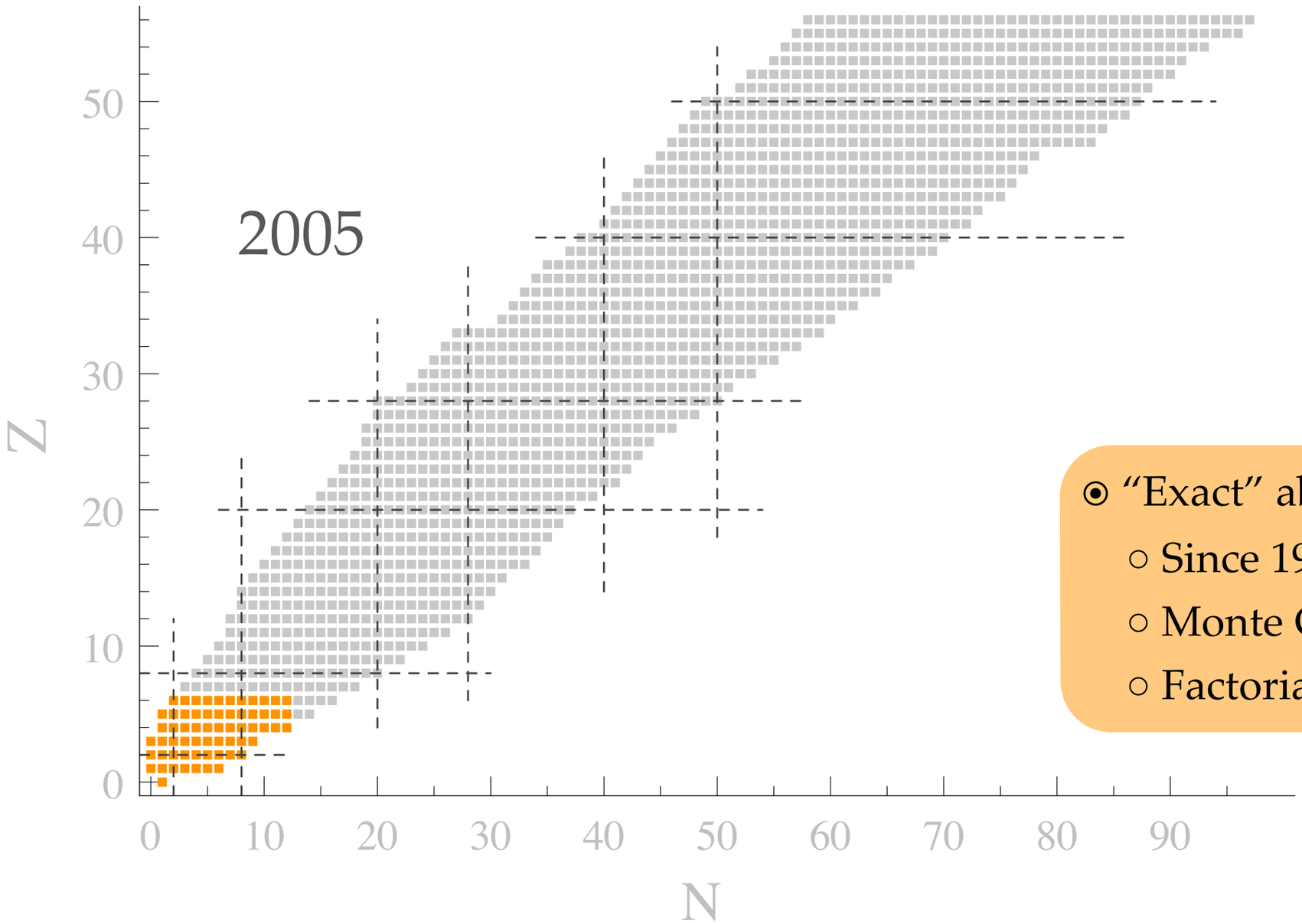
Effective approaches

$$H^{\rm eff}|\Psi^{\rm eff}\rangle = E|\Psi^{\rm eff}\rangle$$

- $H^{\rm eff}$ incorporates in-medium correlations
  - **Fit to many-body observables**
- Link to QCD is usually **lost**
- Model dependence to be assessed
- Allows use of simple many-body scheme
  - **Applicable to whole nuclear chart**

How far can this strategy be pushed? ⟷ Can we derive $H^{\rm eff}$ from H?

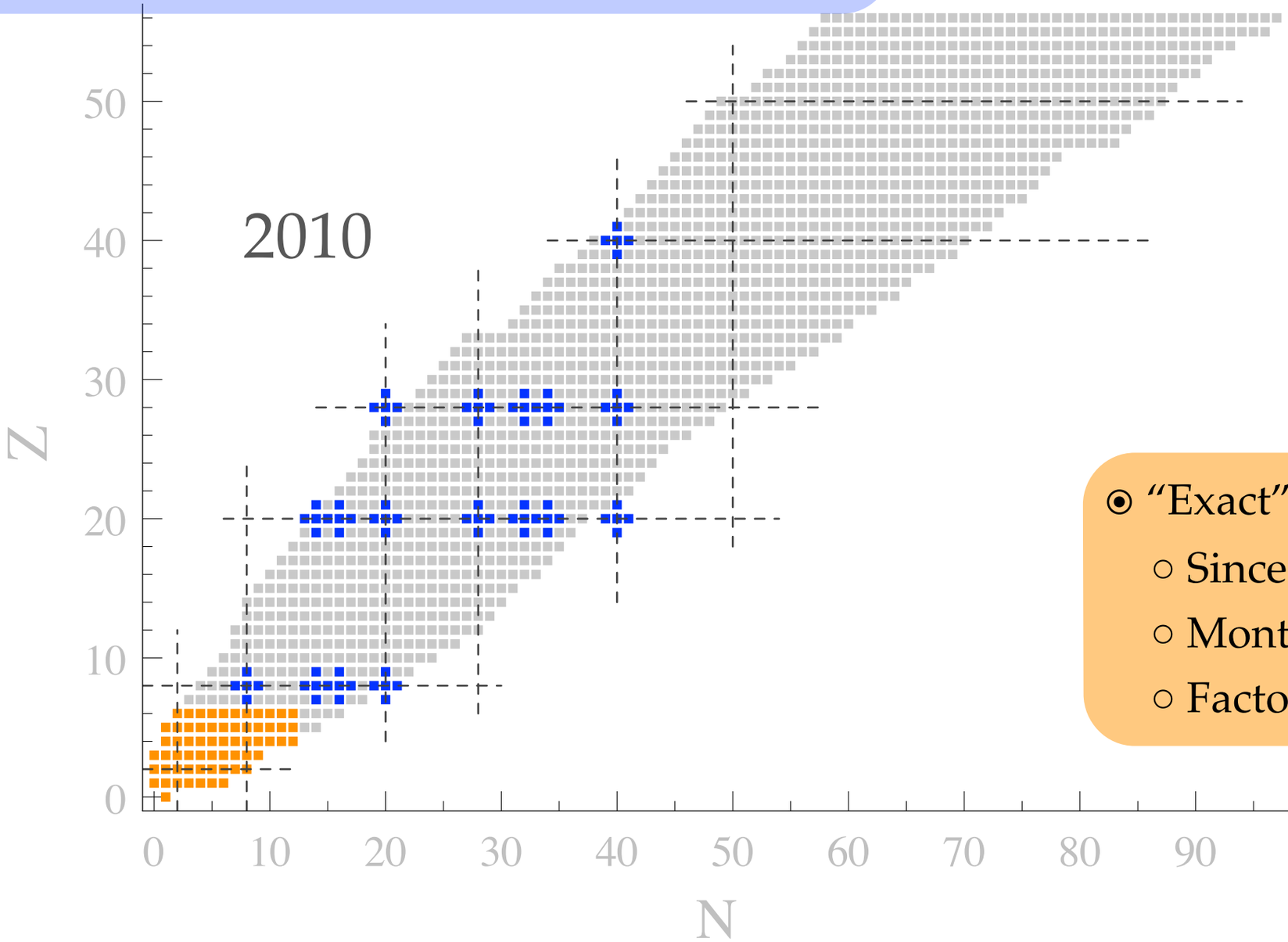
Evolution of ab initio nuclear chart



- “Exact” ab initio approaches
  - Since 1980’s
  - Monte Carlo, CI, …
  - Factorial scaling

Evolution of ab initio nuclear chart

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



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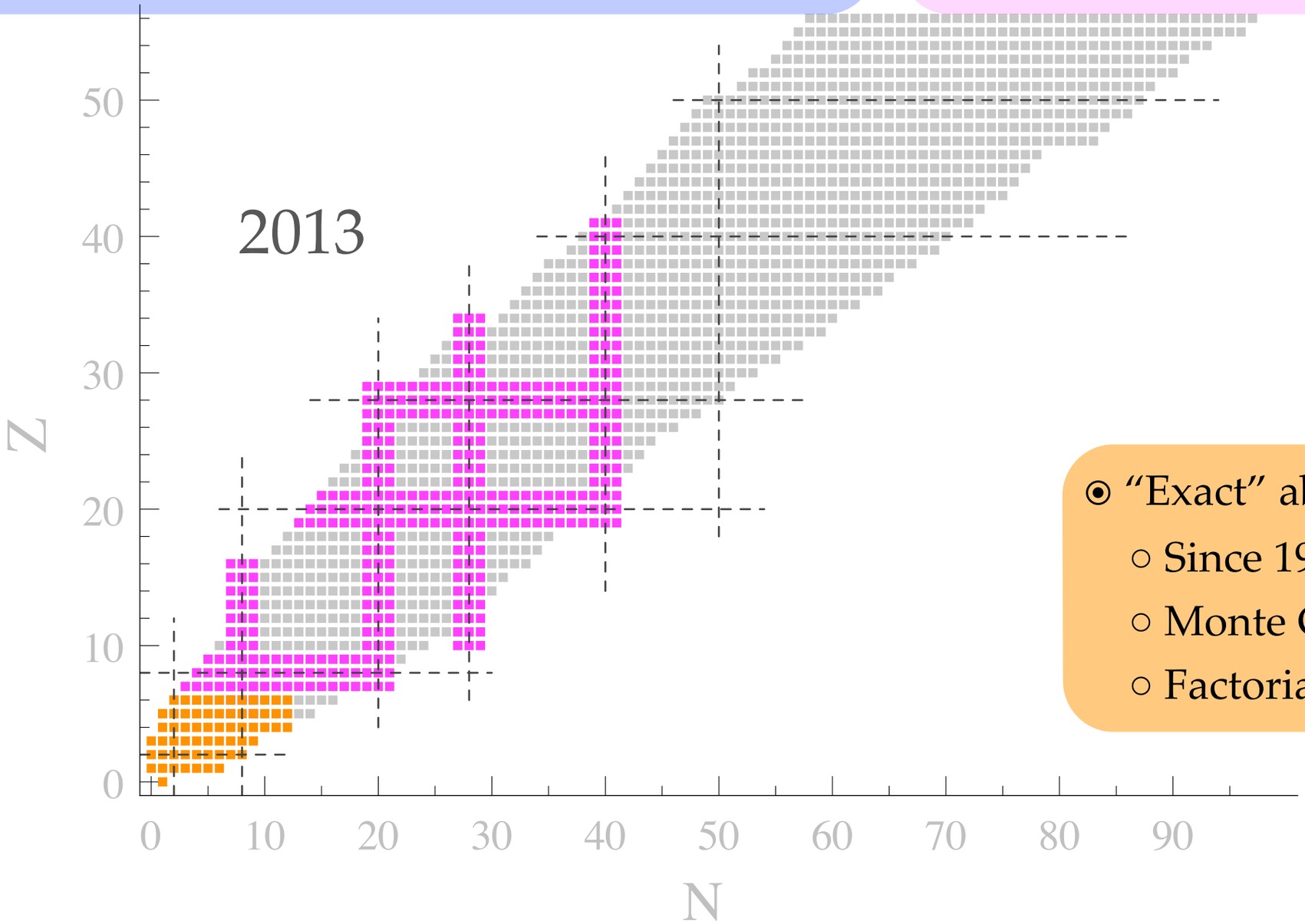

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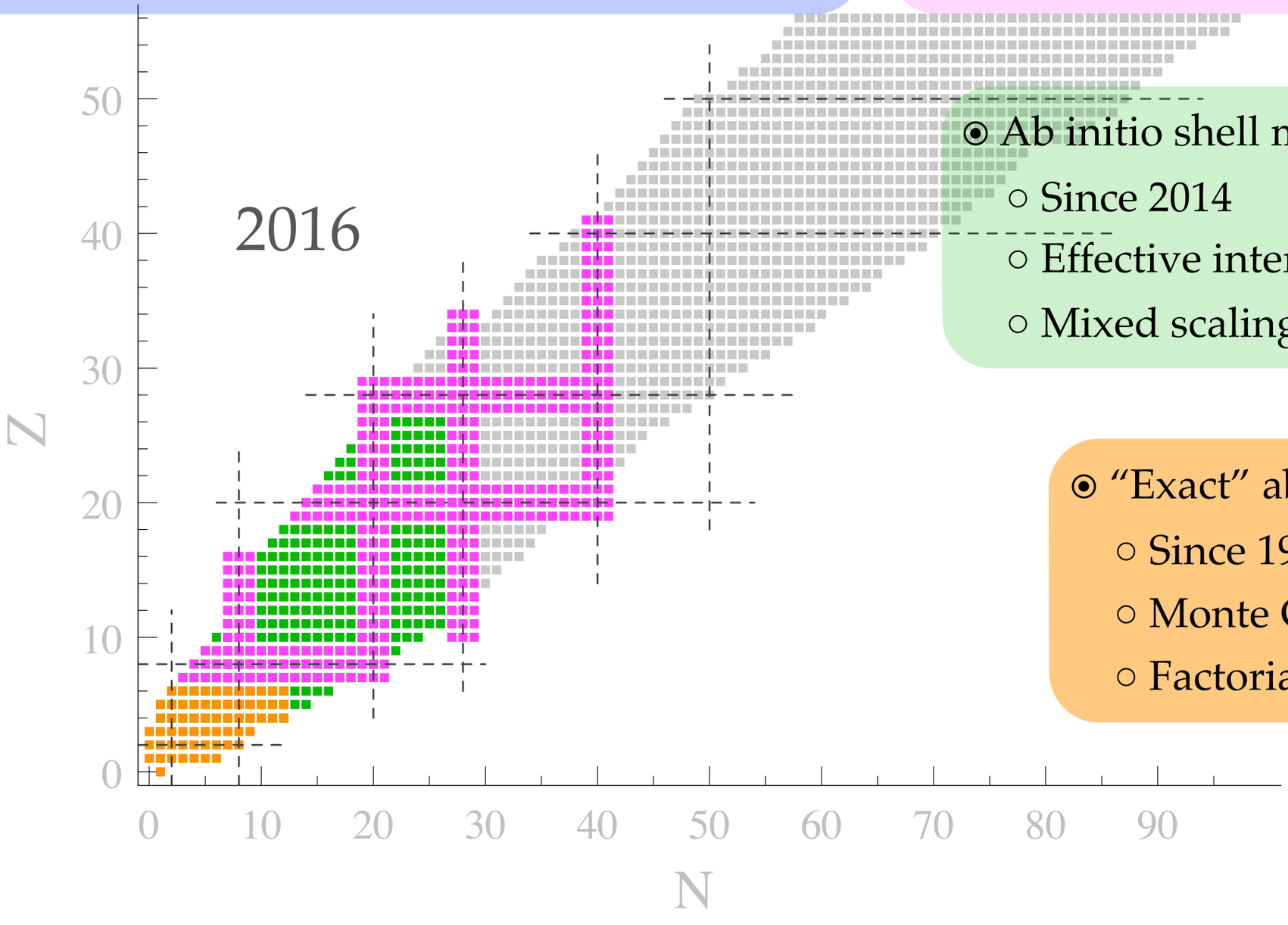

- Ab initio shell model
  - Since 2014
  - Effective interaction via CC/IMSRG
  - Mixed scaling

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

Plan of the lectures

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1. Introduction and basic concepts

2. Dyson equation

- Derivation from equation of motion
- Derivation from diagrammatic expansion
- Approximations for the self-energy

3. Spectral representation

- Spectral content of the Green's function
- Connection with experiment

4. Solving Dyson equation in practise: Dyson eigenvalue problem

- Feynman rules and calculation of self-energy diagrams
- Energy-independent Dyson equation
- Krylov projection
- Examples of results in closed-shell nuclei

Plan of the lectures

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5. Three-body forces

6. Green's functions for open-shell nuclei

- Degenerate systems and symmetry breaking
- Gorkov theory
- Examples of results in open-shell nuclei

7. Public Green's function code

8. Extras

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Semantics & history

- Many-body Green's function theory: set of techniques that originated in quantum field theory and have then been imported to the many-body problem

- Few names for the same thing
  - ***Green's function***
  - ***Propagator***
  - ***Correlation function***

- Many-body Green's functions are applicable to different many-body systems: crystals, molecules, atoms, atomic nuclei, …

- **Self-consistent** Green's functions: many-body Green's functions with dressed propagators (see later)

- *Many-body Green's functions* are **not** *Green's function Monte Carlo*

- Few decades of developments
  - Late 1950s, 1960s: import of ideas from QFT and development of formalism
  - 1970s → today: technical developments and applications in several fields of physics
  - 1990s → today: implementation as an *ab initio* method in nuclear physics

Green's functions in one slide

⊙ The goal is to solve the ***A*-body Schrödinger equation**

$$H|\Psi_k^A\rangle = E_k^A|\Psi_k^A\rangle$$

⊙ Instead of working with the full A-body wave function $|\Psi_k^A\rangle$, rewrite the Schrödinger equation in terms of **1-, 2-, …. *A*-body objects** G_1=G, G_2, … G_A (**Green's functions**)

➟ A-1 coupled equations

⊙ 1-, 2-, …. A-body Green's functions yield **expectation values of 1-, 2-, …. *A*-body operators**

➟ In practise, one usually needs 1- and/or 2-body objects

⊙ One-body Green's function obtained by solving **Dyson equation** (derived from Schrödinger eq.)

$$G = G^{(0)} + G^{(0)}\,\Sigma\,G$$

unperturbed Green's function

many-body effects contained in the **self-energy** Σ

⊙ Bonus: one-body Green's function contains information about ***A*±1 excitation energy spectra**

➟ Spectral or **Lehmann representation** of the Green's function

Green's functions in maths

⊙ In *mathematics*: **solution** of an inhomogeneous **differential equation**

$$[z - L(\boldsymbol{r})]\, G\,(\boldsymbol{r}, \boldsymbol{r}'; z) = \delta\,(\boldsymbol{r} - \boldsymbol{r}')$$

Hermitian operator

$$L(\boldsymbol{r})\phi_n(\boldsymbol{r}) = \lambda_n \phi_n(\boldsymbol{r})$$

Green's function

⊙ *GF* contains information about **eigenstates** & **eigenvalues** of L

$$G(\boldsymbol{r}, \boldsymbol{r}'; z) = \langle \boldsymbol{r}| \frac{1}{z - L} \left[\sum_n |\phi_n\rangle\langle\phi_n| \right] |\boldsymbol{r}'\rangle = \sum_n \langle \boldsymbol{r}| \frac{1}{z - L} |\phi_n\rangle\langle\phi_n \,|\, \boldsymbol{r}'\rangle = \sum_n \frac{\langle \boldsymbol{r} \,|\, \phi_n\rangle\langle\phi_n \,|\, \boldsymbol{r}'\rangle}{z - \lambda_n}$$

more generally

$$G\,(\boldsymbol{r}, \boldsymbol{r}'; z) = \sum_n{}' \frac{\phi_n(\boldsymbol{r})\phi_n^*\,(\boldsymbol{r}')}{z - \lambda_n} + \int \mathrm{d}c\, \frac{\phi_c(\boldsymbol{r})\phi_c^*\,(\boldsymbol{r}')}{z - \lambda_c}$$

discrete spectrum

continuous spectrum

⊙ Substituting $L(\boldsymbol{r}) \to \mathcal{H}(\boldsymbol{r}),\ z \to E$ with $\mathcal{H}(\boldsymbol{r})$ a one-particle Hamiltonian

$$[E - \mathcal{H}(\boldsymbol{r})] G(\boldsymbol{r}, \boldsymbol{r}'; E) = \delta(\boldsymbol{r} - \boldsymbol{r}')$$

From one to many

⊙ By introducing *second-quantised* **annihilation** & **creation** operators one can express

$$G(\boldsymbol{r},\boldsymbol{r}';z) = \sum_n \frac{\langle \boldsymbol{r} \,|\, \phi_n\rangle\langle\phi_n \,|\, \boldsymbol{r}'\rangle}{z-E_n} = \sum_n \frac{\langle 0|a_{\boldsymbol{r}} \,|\, \phi_n\rangle\langle\phi_n \,|\, a^\dagger_{\boldsymbol{r}'}|0\rangle}{z-E_n} \qquad \textbf{one-body}$$

$$G(\boldsymbol{r},\boldsymbol{r}';z) = \sum_\mu \frac{\langle \Psi^N_0|a_{\boldsymbol{r}} \,|\, \Psi^{N+1}_\mu\rangle\langle\Psi^{N+1}_\mu \,|\, a^\dagger_{\boldsymbol{r}'}|\Psi^N_0\rangle}{z-E^+_\mu} + \sum_\nu \frac{\langle \Psi^N_0|a^\dagger_{\boldsymbol{r}'} \,|\, \Psi^{N-1}_\nu\rangle\langle\Psi^{N-1}_\nu \,|\, a_{\boldsymbol{r}}|\Psi^N_0\rangle}{z-E^-_\nu} \qquad \textbf{many-body}$$

➠ two terms: **addition**, but also **removal** of a particle

with

$|\Psi^N_0\rangle$ ⟶ (Exact) ground state of N-body system

$|\Psi^{N\pm1}_\kappa\rangle$ ⟶ κ-excited state of (N±1)-body system

$E^+_\mu \equiv E^{N+1}_\mu - E^N_0$ ⟶ one-particle (addition) separation energy

$E^-_\nu \equiv E^N_0 - E^{N-1}_\nu$ ⟶ one-particle (removal) separation energy

Propagator

⊙ General definition

$$G_{ab}(t,t') \equiv -i\langle \Psi_0^N | \mathcal{T}\left[a_a(t)\, a_b^\dagger(t')\right] | \Psi_0^N \rangle$$

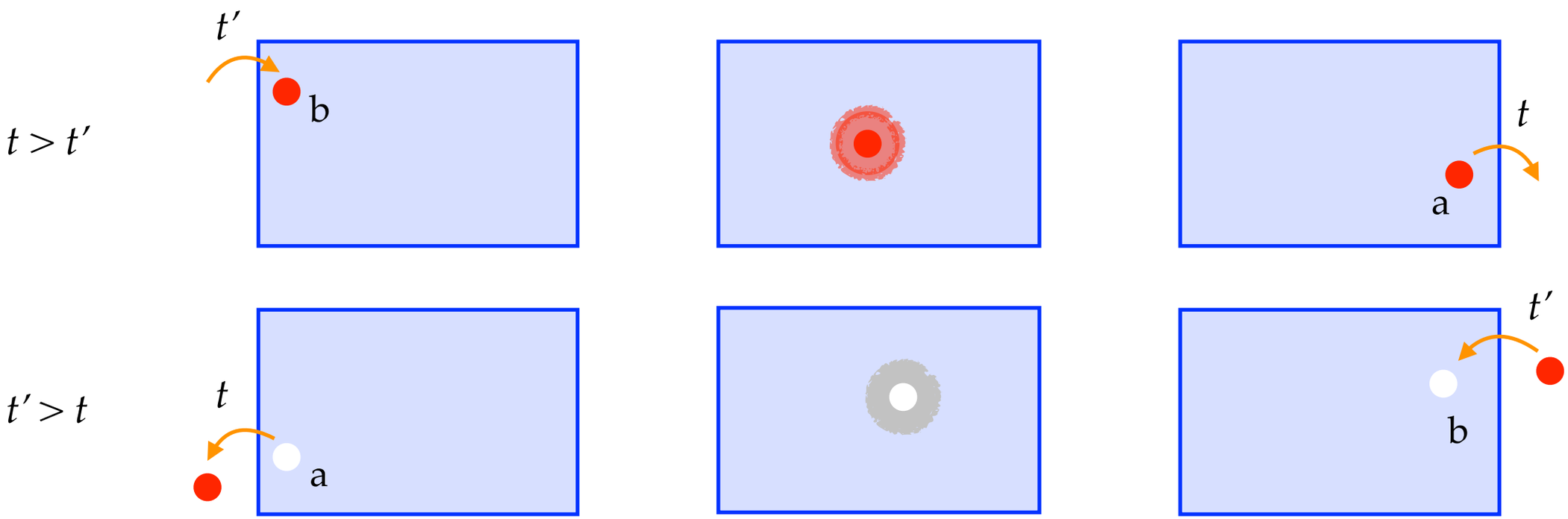
single-particle labels

time-ordering operator

(Exact) ground state of N-body system

➟ It describes the process of **adding** a particle at time t' and **removing** it at time t (or viceversa if $t'>t$)

➟ Hence the equivalent name of **single-particle propagator**



Lehmann (or *spectral*) representation

⊙ Start from general definition

$$G_{ab}(t,t') \equiv -i\langle \Psi_0^A | \mathcal{T}\left[a_a(t)\, a_b^\dagger(t')\right] | \Psi_0^A \rangle$$

For a time-independent Hamiltonian

$$G_{ab}(t,t') = G_{ab}(t-t') \quad \xrightarrow[\text{Fourier transform}]{} \quad G_{ab}(z)$$

derivation in lecture 2

$$G_{ab}(z) = \sum_\mu \frac{\langle \Psi_0^A | a_a \mid \Psi_\mu^{A+1}\rangle\langle \Psi_\mu^{A+1} \mid a_b^\dagger | \Psi_0^A\rangle}{z - E_\mu^+ + i\eta} + \sum_\nu \frac{\langle \Psi_0^A | a_b^\dagger \mid \Psi_\nu^{A-1}\rangle\langle \Psi_\nu^{A-1} \mid a_a | \Psi_0^A\rangle}{z - E_\nu^- - i\eta}$$

Lehmann representation

[Lehmann 1954]

Observables

⊙ Any **one-body** observable can be computed from the **one-body** Green function G

$$\langle \Psi_0^N \,|\, \mathcal{O} \,|\, \Psi_0^N \rangle = \sum_{ab} \int \frac{dz}{2\pi i} \, G_{ba}(z) \, o_{ab} \qquad \text{with} \qquad o_{ab} = \langle a \,|\, \mathcal{O} | b \rangle$$

⊙ In addition, one particular **two-body** observable (the **total energy**) can be computed from G

$$E_0 = \langle \Psi_0^N \,|\, \mathcal{H} \,|\, \Psi_0^N \rangle = \frac{1}{2} \sum_{ab} \int \frac{dz}{2\pi i} \, G_{ba}(z) \; [t_{ab} + z \, \delta_{ab}]$$

Galitskii-Migdal-Koltun sum rule [Galitskii & Migdal 1958; Koltun 1972]

➟ t_{ab} are matrix elements of the kinetic energy operator

➟ It can be proven using (anti)commutation relations of creation/annihilation operators

➟ Exact if a two-body Hamiltonian is employed

➟ Additional term(s) needed if higher-body operator(s) present

⊙ All other two-body observables necessitate the two-body GF.

⊙ In general, N-body observables necessitate N-body GFs.

Many-particle Green's functions

⊙ One can define up to A-body Green's functions (GFs).

⊙ The two-body GF reads

$$G_{2\,abcd}(t_a,t_b,t_c,t_d) \equiv -i\langle\Psi_0^N|\mathcal{T}\left[a_b(t_b)\,a_a(t_a)\,a_c^\dagger(t_c)\,a_d^\dagger(t_d)\right]|\Psi_0^N\rangle$$

➟ This is also called the **4-point GF**.

➟ Depending on the ordering of the 4 times one can then define the two-particle (or two-hole) GF

$$G^{pp/hh}_{abcd}(t,t') \equiv -i\langle\Psi_0^N|\mathcal{T}\left[a_b(t)\,a_a(t)\,a_c^\dagger(t')\,a_d^\dagger(t')\right]|\Psi_0^N\rangle$$

or the particle-hole (~polarisation) propagator

$$G^{ph}_{abcd}(t,t') \equiv -i\langle\Psi_0^N|\mathcal{T}\left[a_b^\dagger(t)\,a_a(t)\,a_c^\dagger(t')\,a_d(t')\right]|\Psi_0^N\rangle$$

⊙ Similarly, one can introduce up to $2A$-point GFs.

Single-particle Green's function ⇿ Schrödinger equation

⊙ Single-particle GF: matches (psychological & practical) needs of handling one-body objects

⊙ For certain (typically one-body) properties, the **exact single-particle GF** contains the same information as the **exact many-body wave function**

➟ E.g. expectation values of a one-body operator in the ground state

➟ Ground-state energy is an exception

⊙ For others (typically many-body) it does not, and one need to resort to higher-body GFs.

➟ E.g. expectation values of a many-body operator in the ground state

⊙ The knowledge of the (A-body) ground state gives us information about ($A\pm1$-body) excited states in a **single calculation** (the magic of Green's functions!).

➟ *Pro*: consistent one-shot calculation of neighbouring systems

➟ *Con*: calculations computationally heavier

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1. Introduction and basic concepts
2. **Dyson equation**
   - **Derivation from equation of motion**
   - Derivation from diagrammatic expansion
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   - Spectral content of the Green's function
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Dyson equation

I. Equation of motion method

⊙ In an interacting many-body system, Green's functions obey a hierarchy of equations

➟ Hierarchy = integro-differential system of coupled equations

➟ It can be derived starting from the eq. of motion of annihilation/creation operators

⊙ The first equation reads [$1 \equiv (\boldsymbol{r}_1, t_1)$ and $(1, 2^+) \equiv (\boldsymbol{r}_1, t_1, \boldsymbol{r}_2, t_1 + 0^+)$]

$$\left(i\frac{\partial}{\partial t_1} + \frac{\nabla^2_{r_1}}{2m} \right) G(1,2) = \delta(1,2) - \int d\,3\, v(1^+,3)\, G_2(1,3;2,3^+)$$

➟ The second one connects G_2 and G_3 (and so on)

➟ If three-body forces are present, one more G is coupled (and so on)

⊙ First option: approximate directly G_2

➟ Simple example: Hartree approximation $\quad G_2(1,2;1',2') \approx G(1,1')\, G(2,2')$

➡ $$\left[i\frac{\partial}{\partial t_1} + \frac{\nabla^2_{r_1}}{2m} + V_H(1) \right] G(1,2) = \delta(1,2) \qquad \text{with} \qquad V_H(1) \equiv \int d\,2\, v(1,2)\, G(2,2^+)$$

i.e. a particle that moves independently in the potential V_H

Dyson equation

⊙ Second option: introduce a new object, the **self-energy** Σ

$$\int d\,3v(1^+,3)G_2(1,3;2,3^+) \quad \longrightarrow \quad i\int d\,3\,\Sigma(1,3)\,G(3,2)$$

➟ Higher-body correlations all contained in the self-energy

➟ Can be seen as a (non-local energy-dependent) effective potential

➟ Advantage is that it is a "one-body" object

⊙ Equation of motion is rewritten into **Dyson equation**

$$G(1,2) = G_0(1,2) + \int d3\,G_0(1,3)\,V_{\mathrm{H}}(3)G(3,2) + \int d4d3\,G_0(1,3)\,\Sigma(3,4)G(4,2)$$

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Dyson equation

II. Diagrammatic method

⊙ Basic idea:

1) Separate full Hamiltonian into unperturbed part + perturbation

$$\mathcal{H} = \mathcal{H}_0 + \mathcal{H}_1$$

2) Compute unperturbed propagator

$$G_0(z) = (z - \mathcal{H}_0)^{-1}$$

3) Express full propagator in terms of G_0 and $\mathcal{H}_1$

⊙ Simple in the case of **one-particle** system:

$$\begin{aligned} G(z) = (z - \mathcal{H}_0 - \mathcal{H}_1)^{-1} &= \left\{ (z - \mathcal{H}_0) \left[1 - (z - \mathcal{H}_0)^{-1} \mathcal{H}_1 \right] \right\}^{-1} \\ &= \left[1 - (z - \mathcal{H}_0)^{-1} \mathcal{H}_1 \right]^{-1} (z - \mathcal{H}_0)^{-1} \\ &= \left[1 - G_0(z) \mathcal{H}_1 \right]^{-1} G_0(z) \, . \end{aligned}$$

⬇ expand $(1 - G_0 \mathcal{H}_1)^{-1}$ in power series

$$G = G_0 + G_0 \mathcal{H}_1 \left(G_0 + G_0 \mathcal{H}_1 G_0 + \cdots \right) = G_0 + G_0 \mathcal{H}_1 G$$

Dyson equation

- **Many-body** case more complicated:

  - Separation $\mathcal{H} = \mathcal{H}_0 + \mathcal{H}_1$ exploited by working in *interaction representation*

  - One-body Green's function is expanded as (now $\mathcal{H}_1 = v$)

$$G(1,1') = \frac{\sum_n \cdots \int\int \cdots G^{(0)}_{2n+1}(\overbrace{1,1';2,2';3,3';\cdots}^{4n+2 \text{ variables}}) \overbrace{v\cdots v\cdots}^{n \text{ terms}}}{\sum_n \cdots \int\int \cdots G^{(0)}_{2n}(\underbrace{2,2';3,3';\cdots}_{4n \text{ variables}}) \underbrace{v\cdots v\cdots}_{n \text{ terms}}}$$

  - *Unperturbed* many-body GFs can be written just as *products* of one-body GFs

$$G^{(0)}_{2n}(\underbrace{1,1';2,2';3,3';\cdots}_{4n \text{ variables}}) = \sum_{\text{permutations}} (-1)^P \underbrace{G^{(0)}(1,\tilde{1}')\cdots G^{(0)}(2n,\tilde{2n}')}_{2n \text{ one-body GFs}} \qquad \textbf{(Wick theorem)}$$

  - Several terms cancel out (all disconnected combinations of variables), at the end:

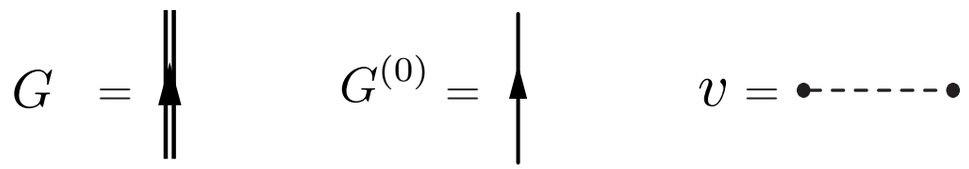
$$G = \sum_n \sum_{\text{connected}} \underbrace{G^{(0)}\cdots G^{(0)}\cdots}_{2n+1 \text{ propagators}} \underbrace{v\cdots v\cdots}_{n \text{ interactions}}$$

- In practise: introduce **Feynman diagrams** and work out the expansion diagrammatically

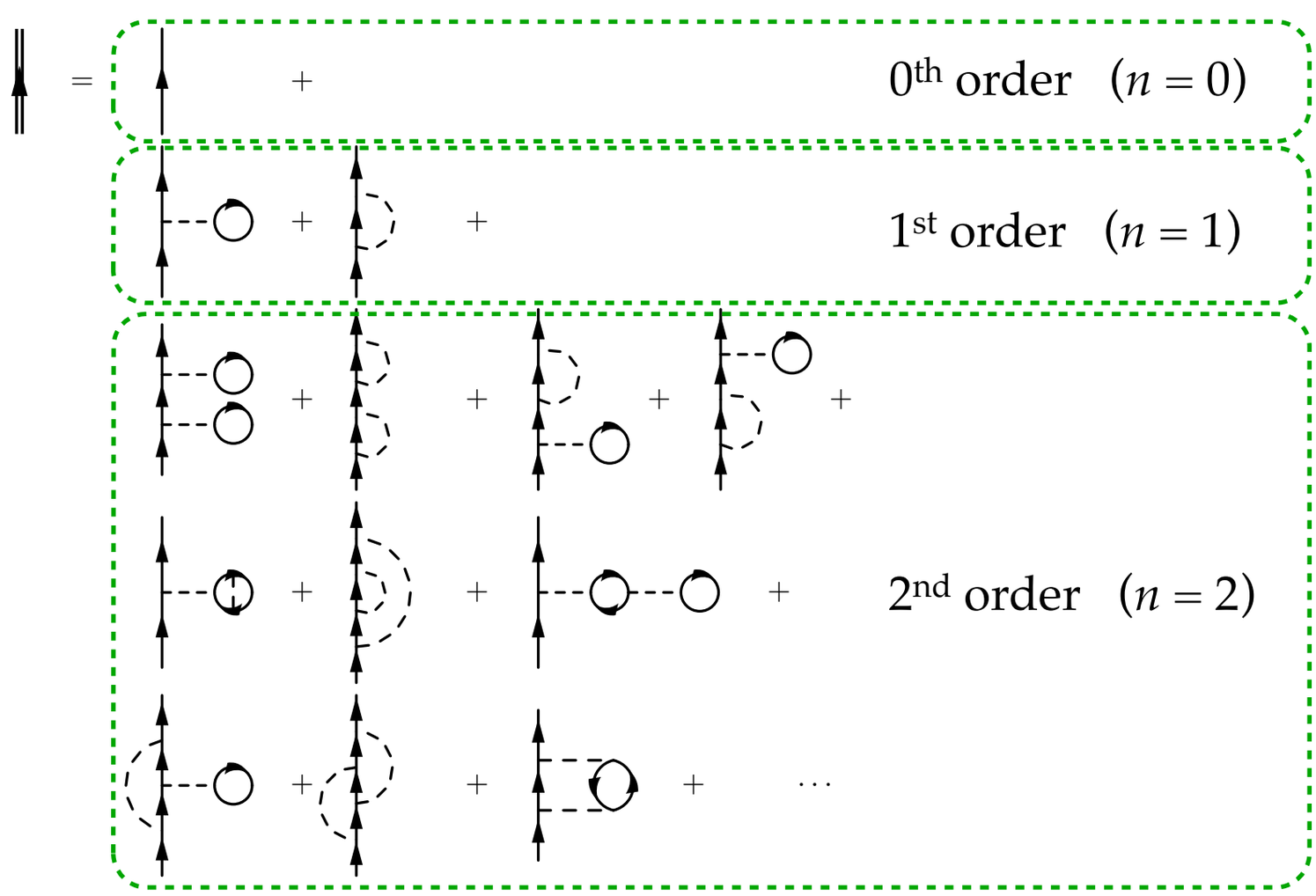
  - Approximations devised in terms of (sets of) diagrams

Diagrammatic expansion

⊙ Depict **exact** & **unperturbed propagators** and **interaction lines** as

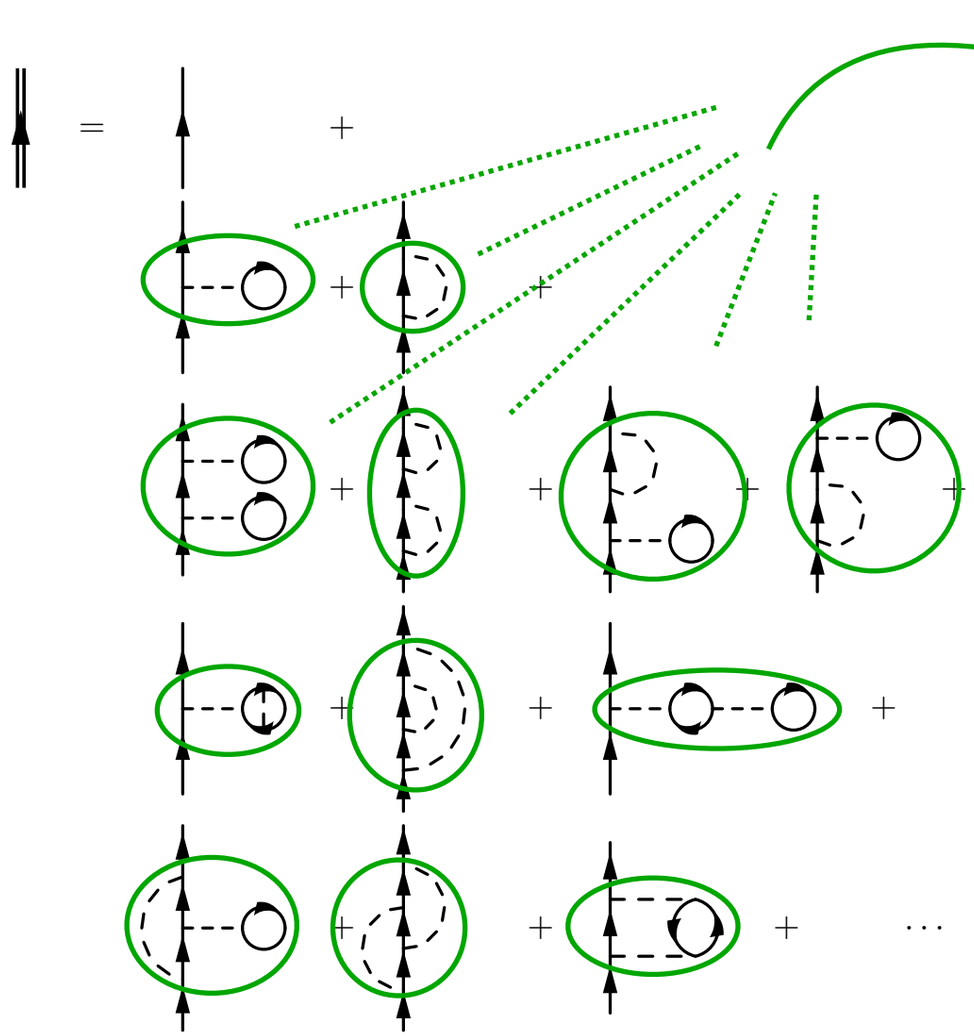


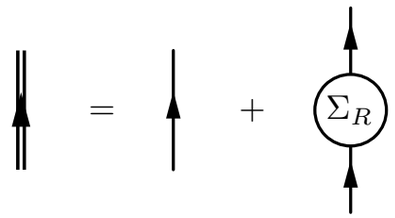
⊙ Write down the expansion for $G = \sum_{n} \sum_{\text{connected}} \underbrace{G^{(0)} \cdots G^{(0)} \cdots}_{2n+1 \text{ propagators}} \underbrace{v \cdots v \cdots}_{n \text{ interactions}}$



Diagrammatic expansion

- Introduce (**reducible**) self-energy
  - ➟ All diagrams without external legs

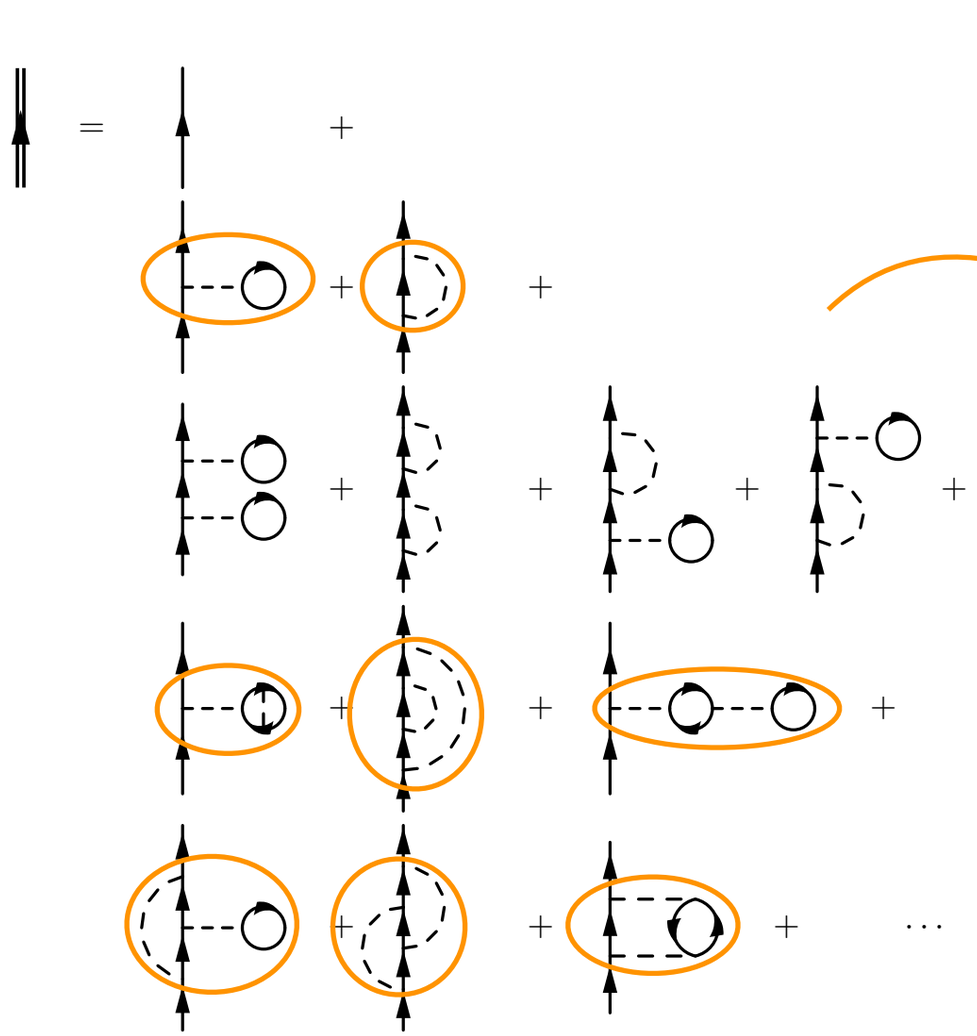


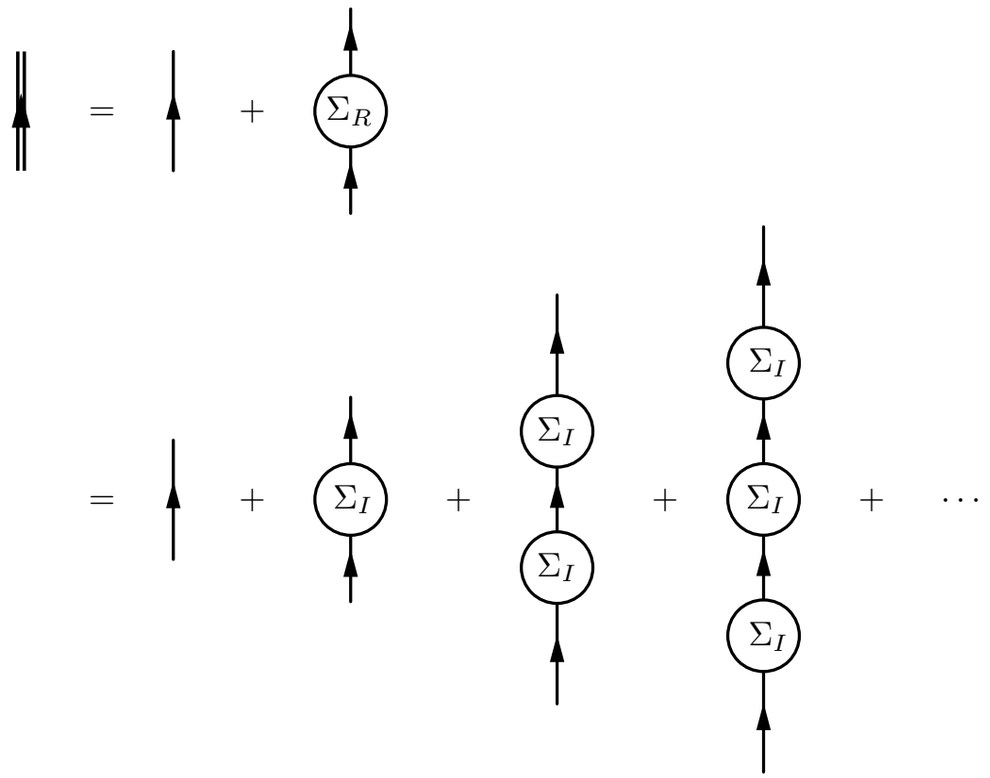


Diagrammatic expansion

⊙ Select **irreducible** self-energy diagrams

➟ All self-energy contributions that cannot be separated in two parts by cutting a propagation line





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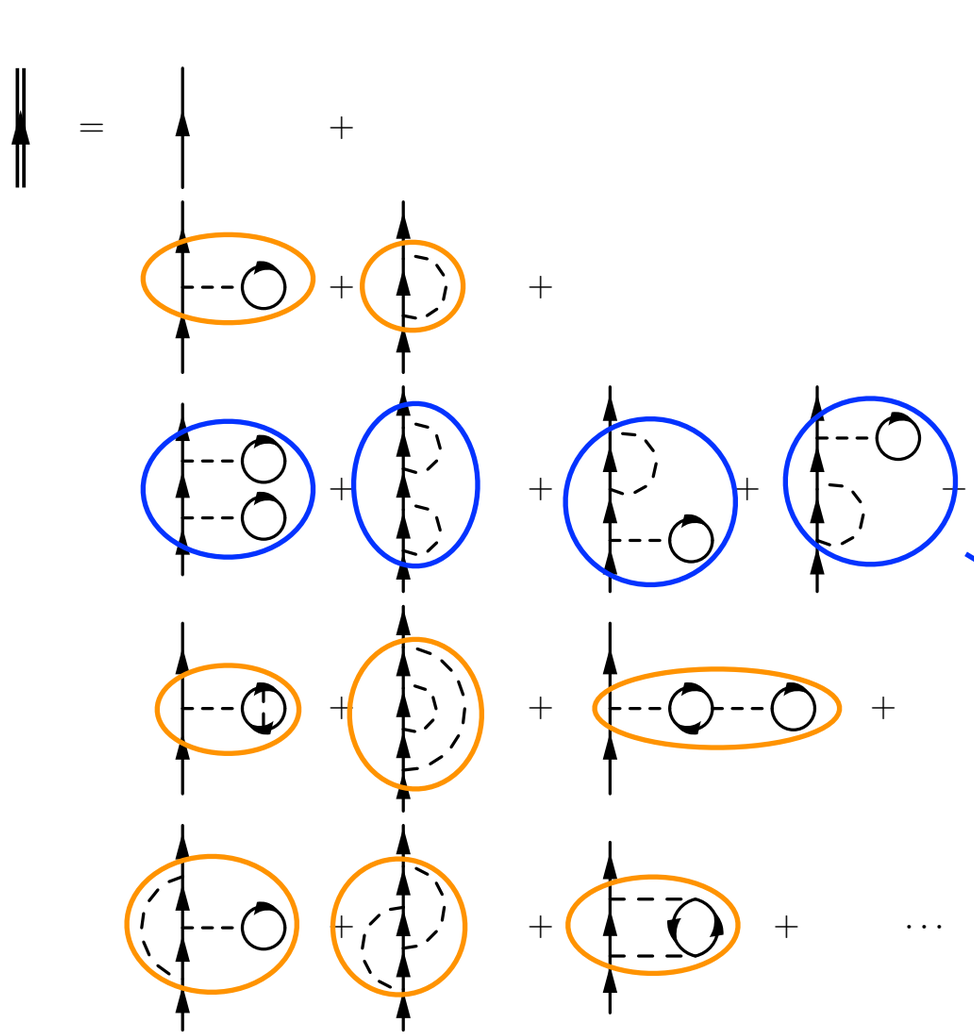
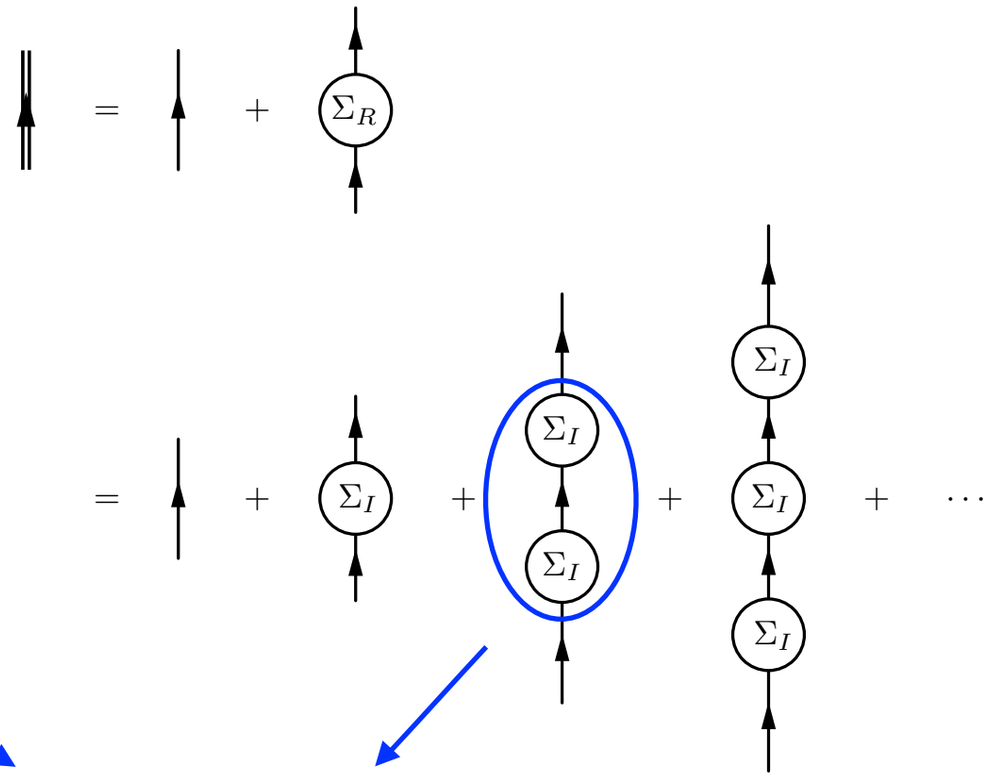
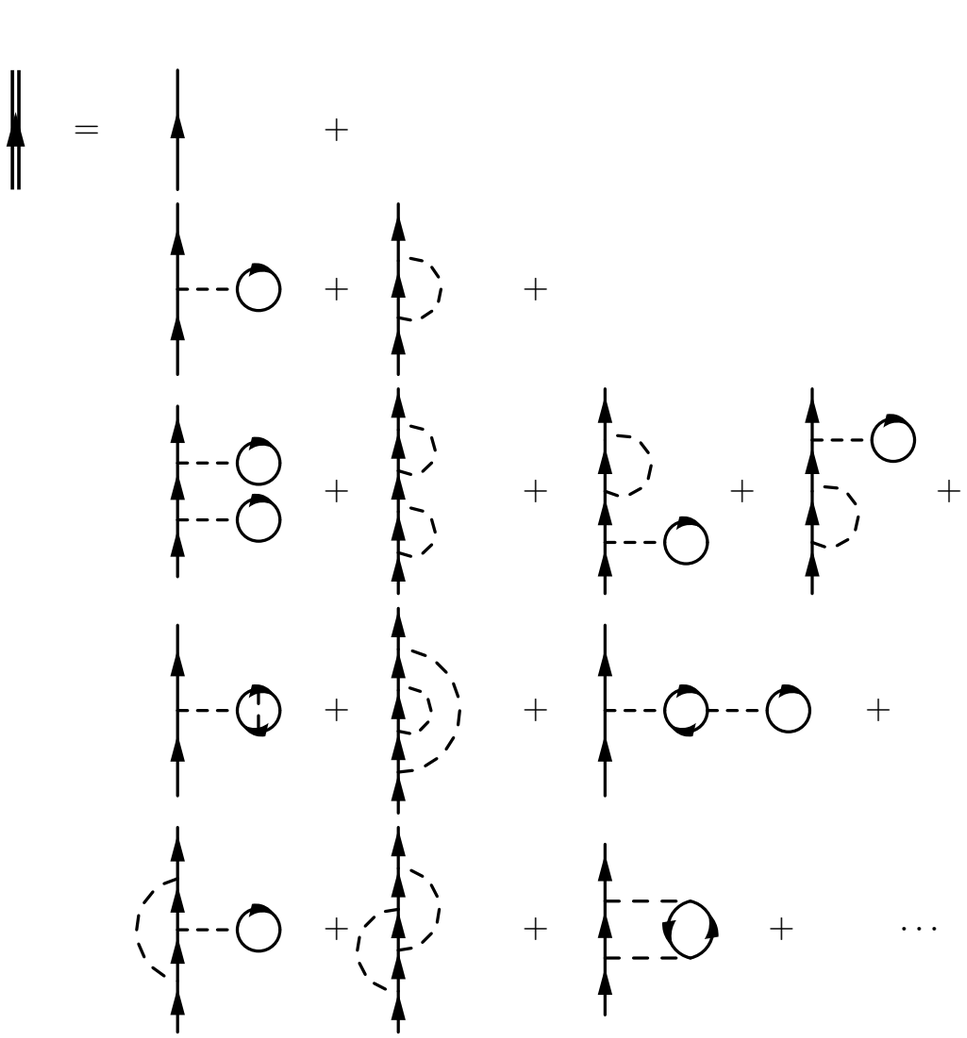


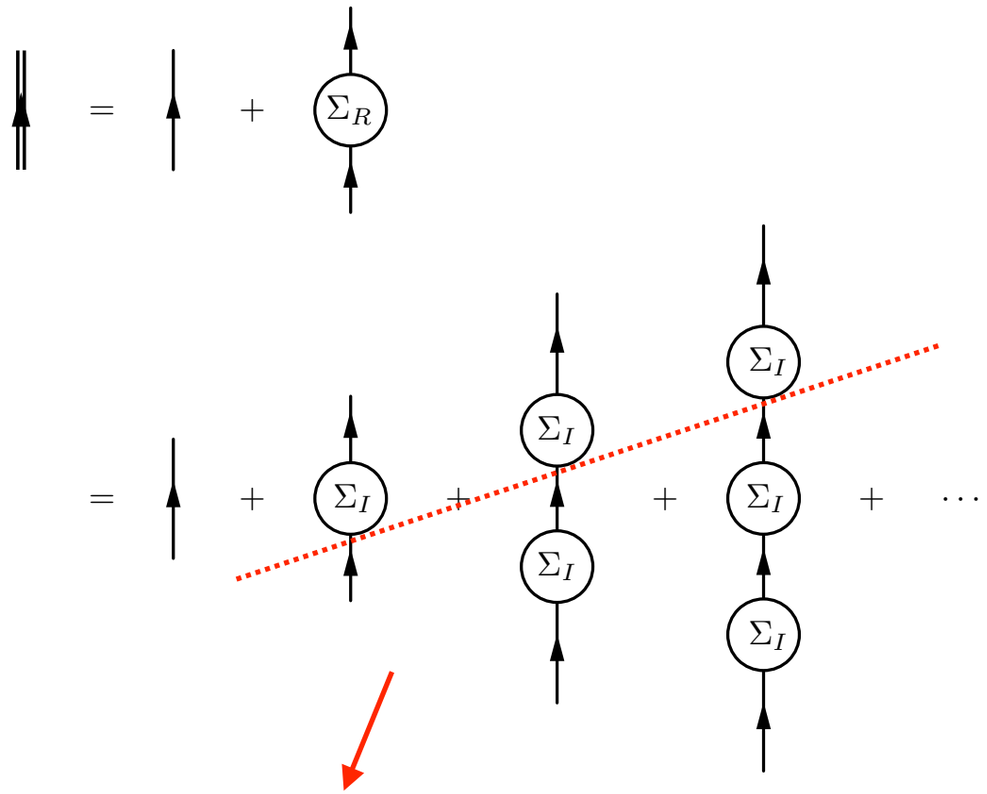


Remaining diagrams generated
by successive self-energy insertions

Diagrammatic expansion

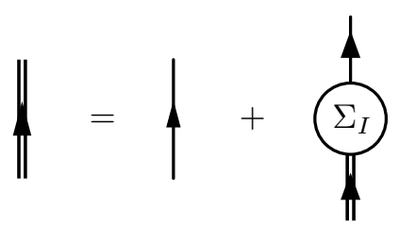
⊙ Rewrite the expansion in the form of an iterative equation





This is itself the expansion for the dressed propagator

$$G = G^{(0)} + G^{(0)}\,\Sigma\,G$$

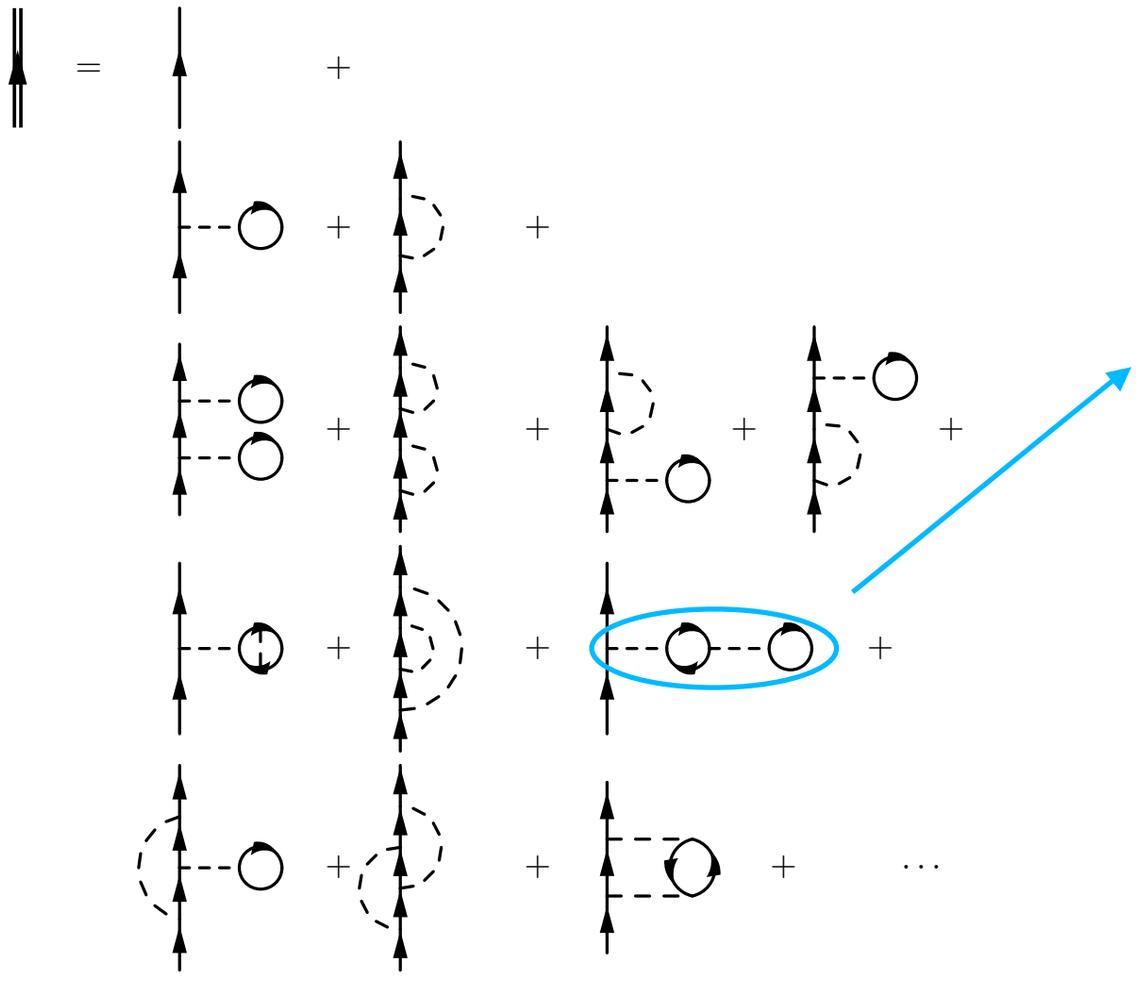


Dyson equation

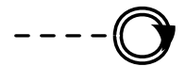
Diagrammatic expansion

⊙ One can further select irreducible **skeleton** diagrams

➟ Contributions that cannot be generated from *lower-order* diagrams with *dressed* propagators



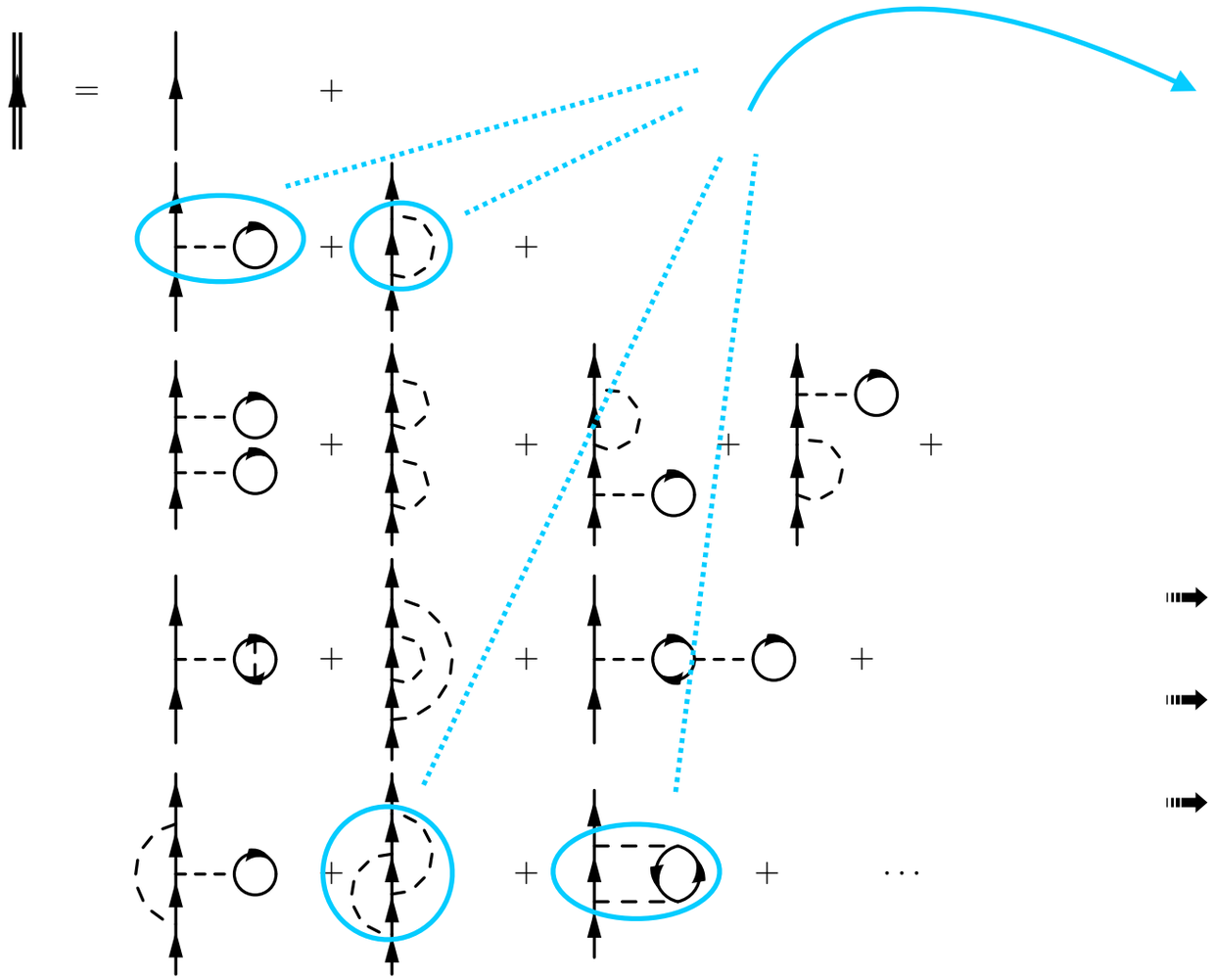
E.g. this can be generated by the self-energy term



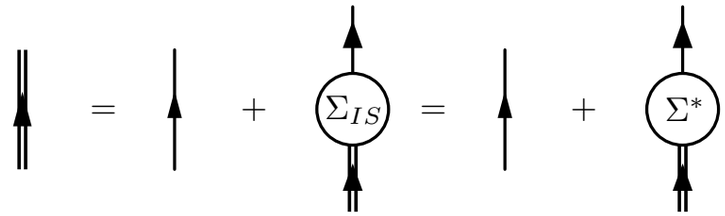
Diagrammatic expansion

⊙ One can further select irreducible **skeleton** diagrams

➟ Contributions that cannot be generated from *lower-order* diagrams with *dressed* propagators



Dyson equation



➟ All propagators in Σ_{IS} are **dressed**

➟ This characterises **self-consistent** schemes

➟ Selected PT terms iterated to all orders

⬇

Intrinsically **non-perturbative** method

Diagrammatic expansion

- In general, not only propagation lines but also interaction lines and vertices can get dressed
- Classes of diagrams can be selected

1) **Self-energy** parts inserted in propagator lines

➟ *dressed* or *renormalised* propagators

2) **Polarisation** parts inserted in interaction lines

➟ *dressed* or *effective* or *renormalised* interactions

3) (**Irreducible) vertex** parts inserted in place of a vertex

➟ *dressed* vertices

- Each class identifies a **subset of diagrams** in the full expansion
- The choice of one of these options generally depends on the problem under study
- Only if the three parts are treated (= truncated) consistently one maintains **Ward identity**

Plan of the lectures

1. Introduction and basic concepts

2. Dyson equation

- Derivation from equation of motion
- Derivation from diagrammatic expansion
- **Approximations for the self-energy**

3. Spectral representation

- Spectral content of the Green's function
- Connection with experiment

4. Solving Dyson equation in practise: Dyson eigenvalue problem

- Feynman rules and calculation of self-energy diagrams
- Energy-independent Dyson equation
- Krylov projection
- Examples of results in closed-shell nuclei

Φ-functional

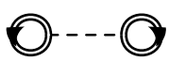
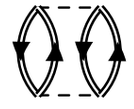
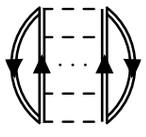
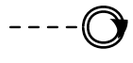
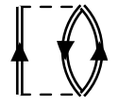
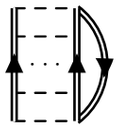
- If the whole expansion is kept, Dyson equation is exact and conservation laws are fulfilled
- What if we approximate the solution, i.e. select only a subset of diagrams?
- There exist a class of self-energy approximations that *by construction* fulfils basic conservation laws
  - The condition is the existence of a functional Φ of G and v, such that

$$\Sigma(1,2) = \frac{\delta\,\Phi[G,v]}{\delta\,G(1,2)}$$

[Baym & Kadanoff 1961, 1962]

  - ➟ Conserved quantities (number of particles, momentum, energy…) don't change (*time-dependent*)
  - ➟ Thermodynamic relations are fulfilled (*finite temperature*)

- Common approximations are **Φ-derivable**

	Hartree	Fock	2nd order	T-matrix
Φ	1/2 	1/2 	1/4 	1/2n 
Σ				

First and second order

⊙ **First-order** diagrams in the self-energy expansion correspond to Hartree and Fock terms

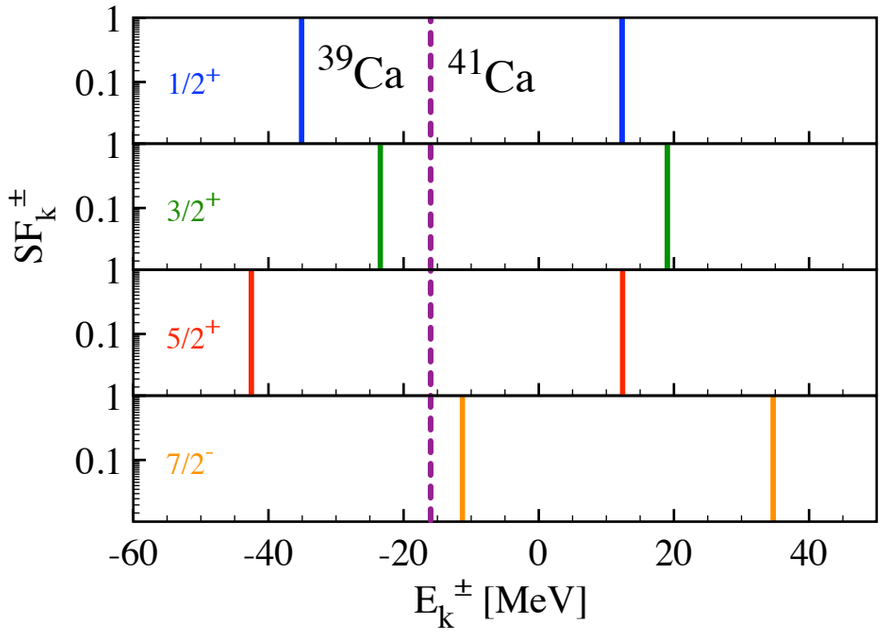
Hartree **Fock**

○ *Hartree*: particles in a common potential, contains unphysical self-interaction

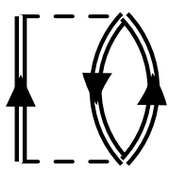
○ *Fock*: removes self-interaction

○ Account for **static** correlations

[Somà *et al.* unpublished]



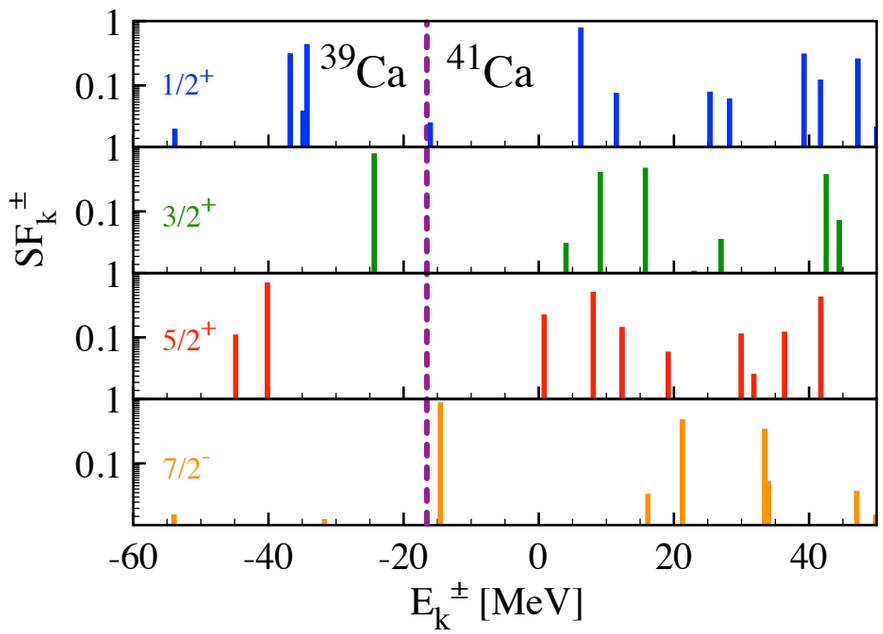
⊙ **Second-order** diagrams often referred to as Born approximation



+ exchange

➟ Analogous to CCD (2p-1h & 2h-1p)

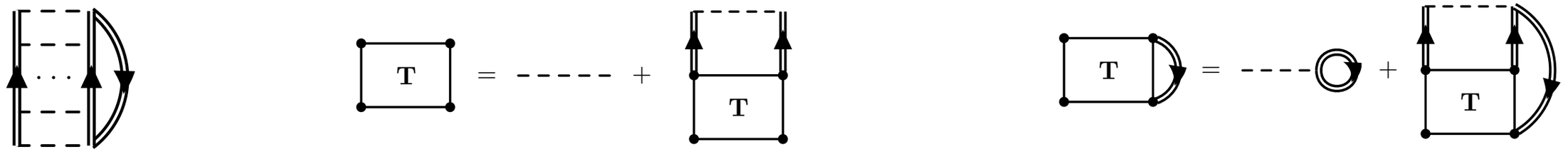
➟ Introduces leading **dynamical** correlation



Ladder

⊙ **Ladder**-type or T-matrix diagrams account for repeated two-particle scattering

Ladder self-energy *or* Introduce T-matrix → T-matrix self-energy



+ exchanges

[Galitskii 1958; …]

○ Contains an infinite number of skeleton diagrams (second iterative layer!)

○ Resums contributions relevant at low-density and in strongly-interacting systems

○ Quality decreases at high density as screening becomes important

⊙ ***Electronic systems***

○ Works well at low densities, i.e. close to completely filled or empty bands

○ Extensively used in Hubbard models

⊙ ***Nuclear systems***

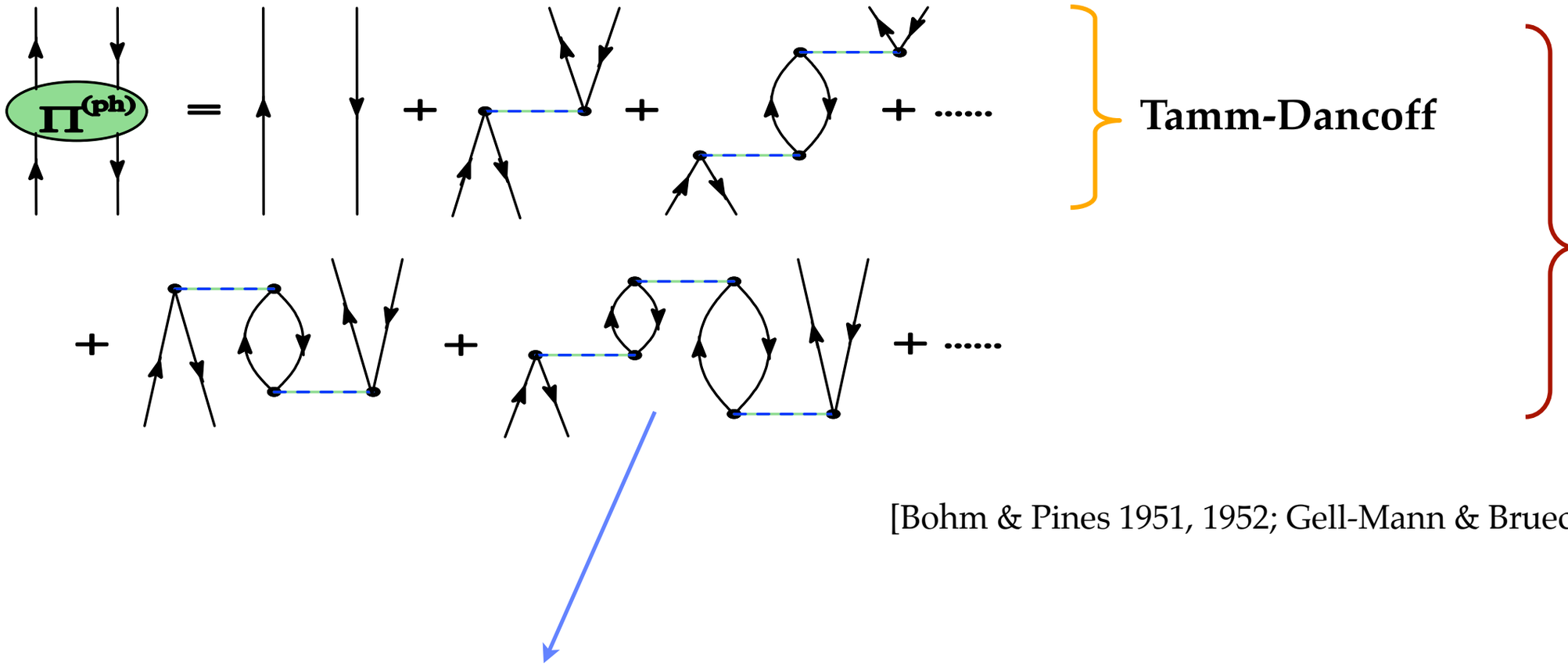
○ Treats the repulsive short-range part of nuclear interactions

○ Method of choice for nuclear matter (self-consistency obligatory for high densities)

○ Applications to finite nuclei computationally demanding

Rings

- Resummation of particle-hole excitations (*bubbles* or *rings*) leads to a screened interaction
  - **Random Phase Approximation (RPA)** or ring ladder or ph ladder
  - Can be seen as an expansion for the **polarisation propagator** $\Pi^{(ph)}$

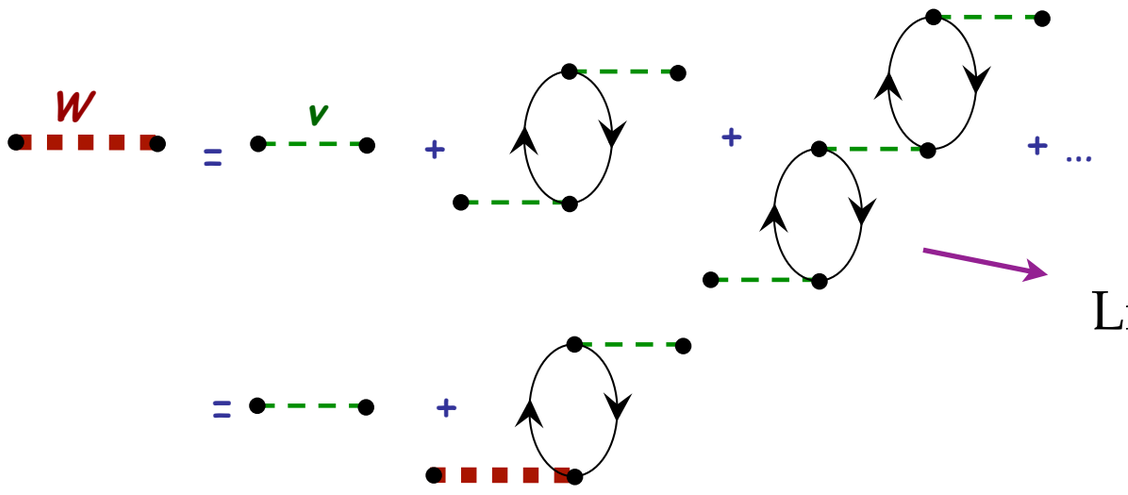


[Bohm & Pines 1951, 1952; Gell-Mann & Brueckner 1957; …]

The name comes from the fact that Pauli correlations are partially **neglected**,
but one assumes that missing corrections cancel each other **randomly**.

GW

⊙ RPA can be applied to resum an interaction (typically **electron-electron**) in the medium



[Hedin 1965]

Lindhard function $\Pi^{(0)}(\mathbf{q},\omega)$

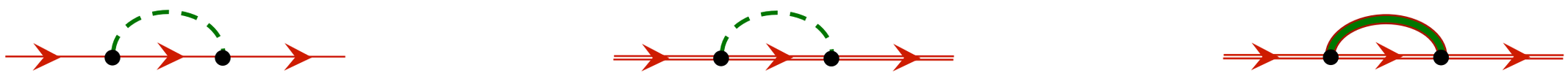
$$W(\mathbf{q},\omega) = v(\mathbf{q}) + v(\mathbf{q})\,\Pi^{(0)}(\mathbf{q},\omega)\,W(\mathbf{q},\omega) \quad \Rightarrow \quad \Sigma^{GW}(\mathbf{k},\omega) = i\int \frac{d\omega'}{2\pi}\int \frac{d\mathbf{k}'}{(2\pi)^3}\,G(\mathbf{k}-\mathbf{k}',\omega-\omega')\,W(\mathbf{k}',\omega')$$

➟ Accounts for screening effects

➟ For electrons only Fock term in *GW* (Hartree → constant electrostatic repulsion)

➟ Different degrees of self-consistency possible (and debated)

G⁰W⁰ *GW⁰* *GW*



Plan of the lectures

1. Introduction and basic concepts
2. Dyson equation
   - Derivation from equation of motion
   - Derivation from diagrammatic expansion
   - Approximations for the self-energy
3. **Spectral representation**
   - **Spectral content of the Green's function**
   - Connection with experiment
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Lehmann (or *spectral*) representation

⊙ Start from general definition

$$G_{ab}(t,t') \equiv -i\langle \Psi_0^A | \mathcal{T}\left[a_a(t)\, a_b^\dagger(t')\right] | \Psi_0^A \rangle$$

For a time-independent Hamiltonian

$$G_{ab}(t,t') = G_{ab}(t-t') \quad \xrightarrow[\text{Fourier transform}]{} \quad G_{ab}(z)$$

Use integral representation of Heaviside function

$$\Theta(t) = \lim_{\eta\to 0^+} \frac{1}{2\pi i} \int_{-\infty}^{+\infty} dz\, \frac{e^{itz}}{z - i\eta}$$

$$G_{ab}(z) = \sum_\mu \frac{\langle \Psi_0^A | a_a \,|\, \Psi_\mu^{A+1}\rangle\langle \Psi_\mu^{A+1} \,|\, a_b^\dagger | \Psi_0^A\rangle}{z - E_\mu^+ + i\eta} + \sum_\nu \frac{\langle \Psi_0^A | a_b^\dagger \,|\, \Psi_\nu^{A-1}\rangle\langle \Psi_\nu^{A-1} \,|\, a_a | \Psi_0^A\rangle}{z - E_\nu^- - i\eta}$$

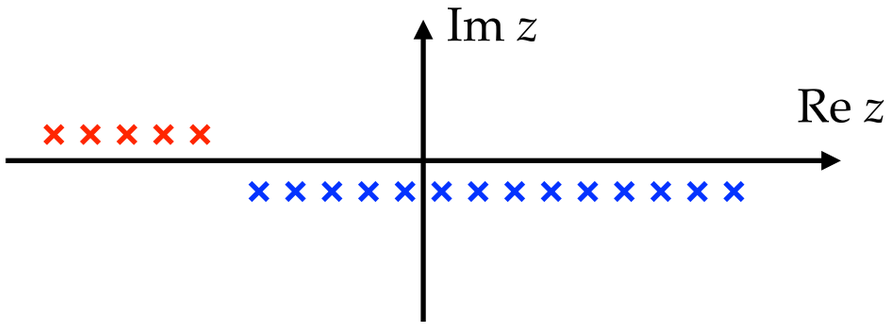
Lehmann representation [Lehmann 1954]

Spectral representation: *finite* vs *infinite* systems

⊙ Poles of the propagator represent one-particle excitation energies

i.e. energies of the ***A*±1-body** system w.r.t. the ground state of the ***A*-body** system

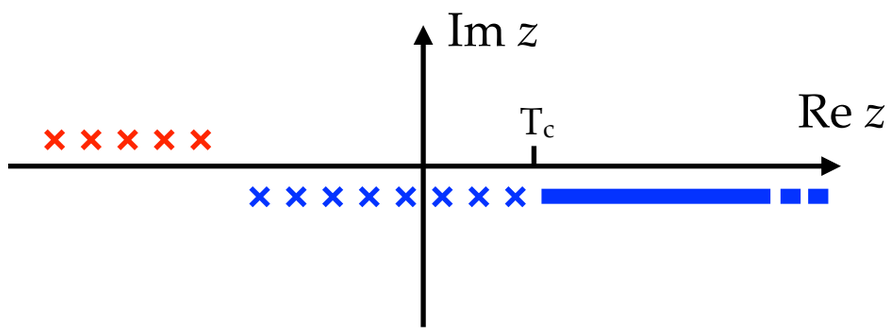
$$G_{ab}(z) = \sum_\mu \frac{\langle \Psi_0^A | a_a \,|\, \Psi_\mu^{A+1}\rangle\langle \Psi_\mu^{A+1} \,|\, a_b^\dagger | \Psi_0^A\rangle}{z - E_\mu^+ + i\eta} + \sum_\nu \frac{\langle \Psi_0^A | a_b^\dagger \,|\, \Psi_\nu^{A-1}\rangle\langle \Psi_\nu^{A-1} \,|\, a_a | \Psi_0^A\rangle}{z - E_\nu^- - i\eta}$$



with

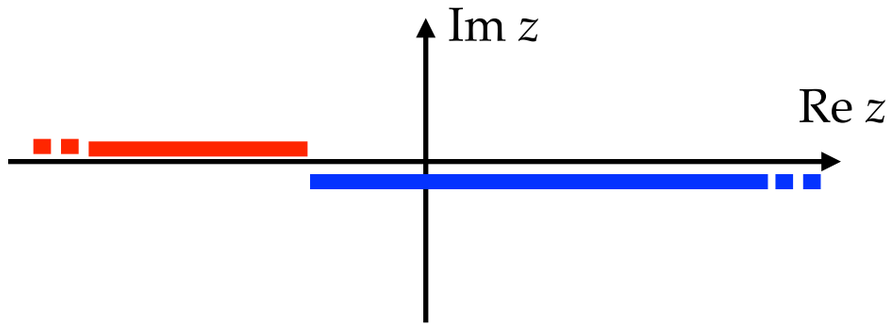
$$E_\mu^+ \equiv E_\mu^{A+1} - E_0^A$$

$$E_\nu^- \equiv E_0^A - E_\nu^{A-1}$$



➟ A continuum contribution can be added

$$+ \sum_\gamma \int_{T_c}^{+\infty} dE \, \frac{\langle \Psi_0^A | a_a \,|\, \Psi_{\gamma E}^{A+1}\rangle\langle \Psi_{\gamma E}^{A+1} \,|\, a_b^\dagger | \Psi_0^A\rangle}{z - E + i\eta}$$



➟ For extended systems (large N) spectrum is degenerate

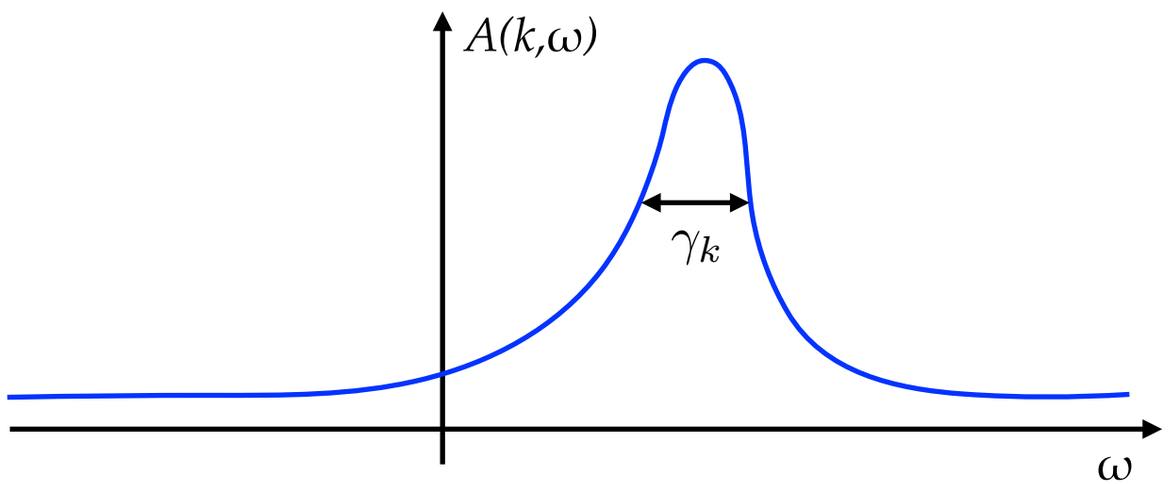
➟ Isolated poles no longer meaningful

$$G_{R/A}(k,z) = \int \frac{d\omega}{2\pi} \frac{\mathcal{A}(k,\omega)}{z - \omega \pm i\eta}$$

Spectral representation and quasiparticles

- The spectral function describes the dispersion in energy of modes with a given momentum
- Excitation of the system would then show up as peaks in A

$$G_{R/A}(k,z) = \int \frac{d\omega}{2\pi} \frac{\mathcal{A}(k,\omega)}{z - \omega \pm i\eta}$$



➟ Idea: associate a well-defined peak with a **quasiparticle.**

- Quasiparticles will have, in general
  - Modified or *renormalised* "single-particle" properties (e.g. an effective mass)
  - A **finite lifetime**, physically associated with the damping of the excitation
  - The lifetime is given by the width of the quasiparticle peak $\tau \sim \gamma_k^{-1}$
  - Quasiparticle properties computed from the GF pole

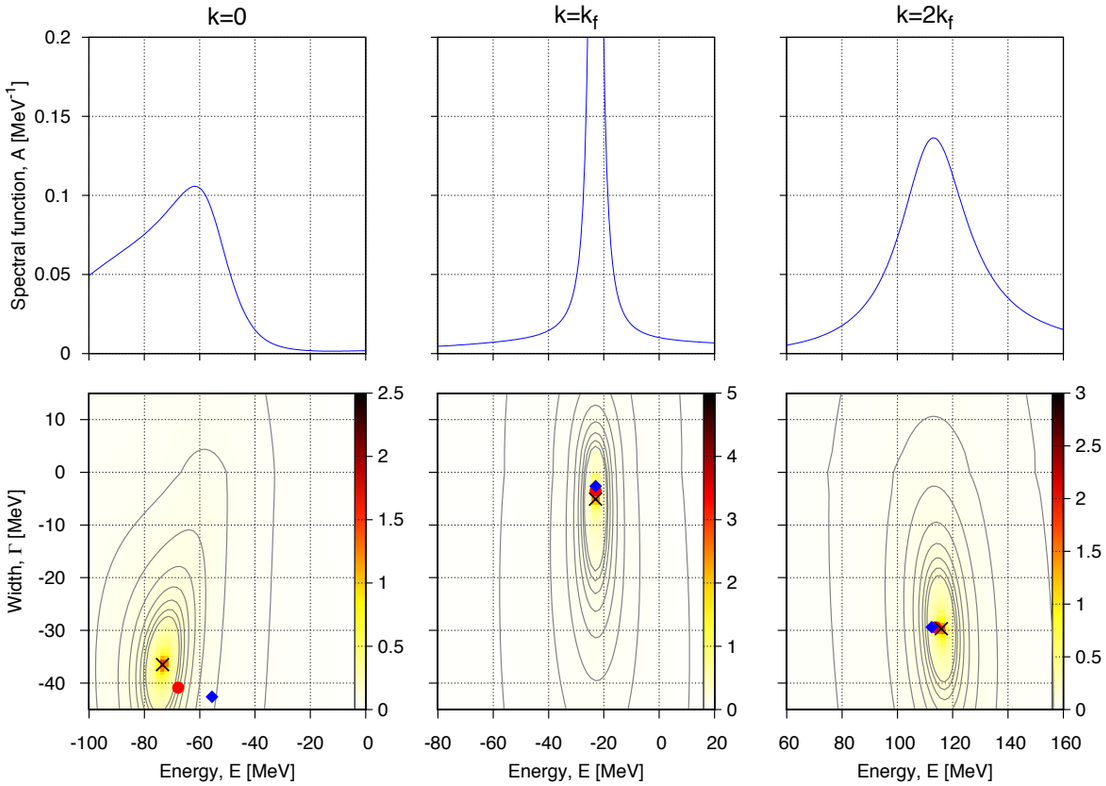
$$G^{-1}(k,z) = z - \frac{k^2}{2m} - \Sigma(k,z) \longrightarrow z_k = \varepsilon_k + i\gamma_k$$

Quasiparticle pole

- Quasiparticle pole can be extracted

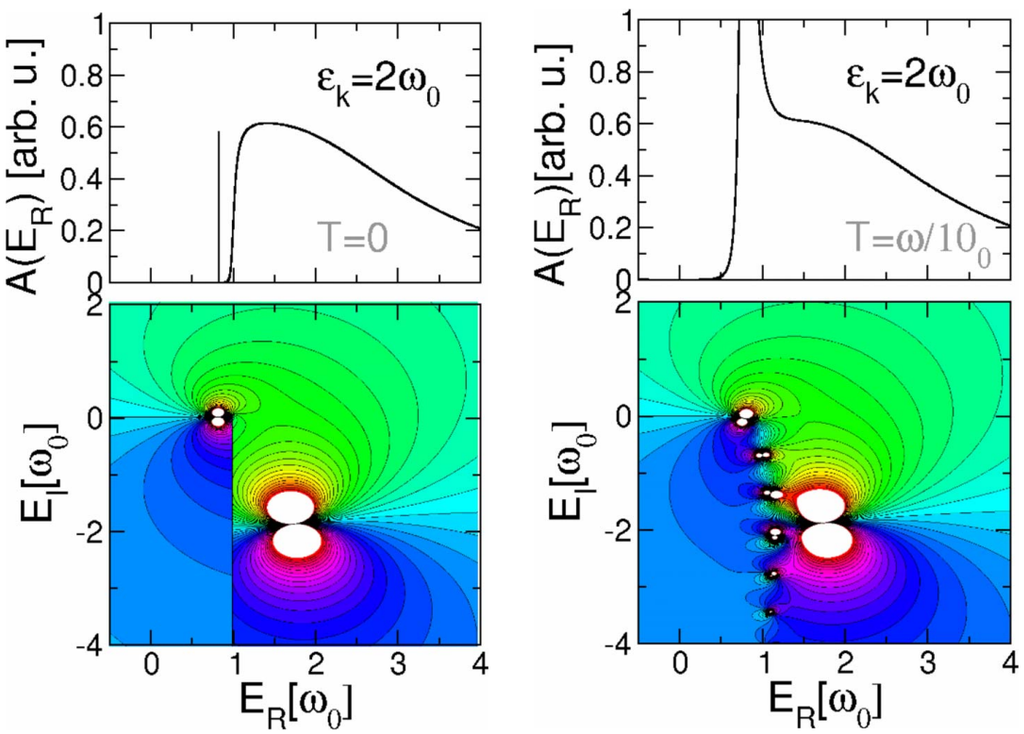
$$z(k) = \frac{k^2}{2m} + \mathrm{Re}\tilde{\Sigma}(k, z(k)) + i\mathrm{Im}\ \tilde{\Sigma}(k, z(k))$$

Symmetric nuclear matter



[Rios & Somà 2012]

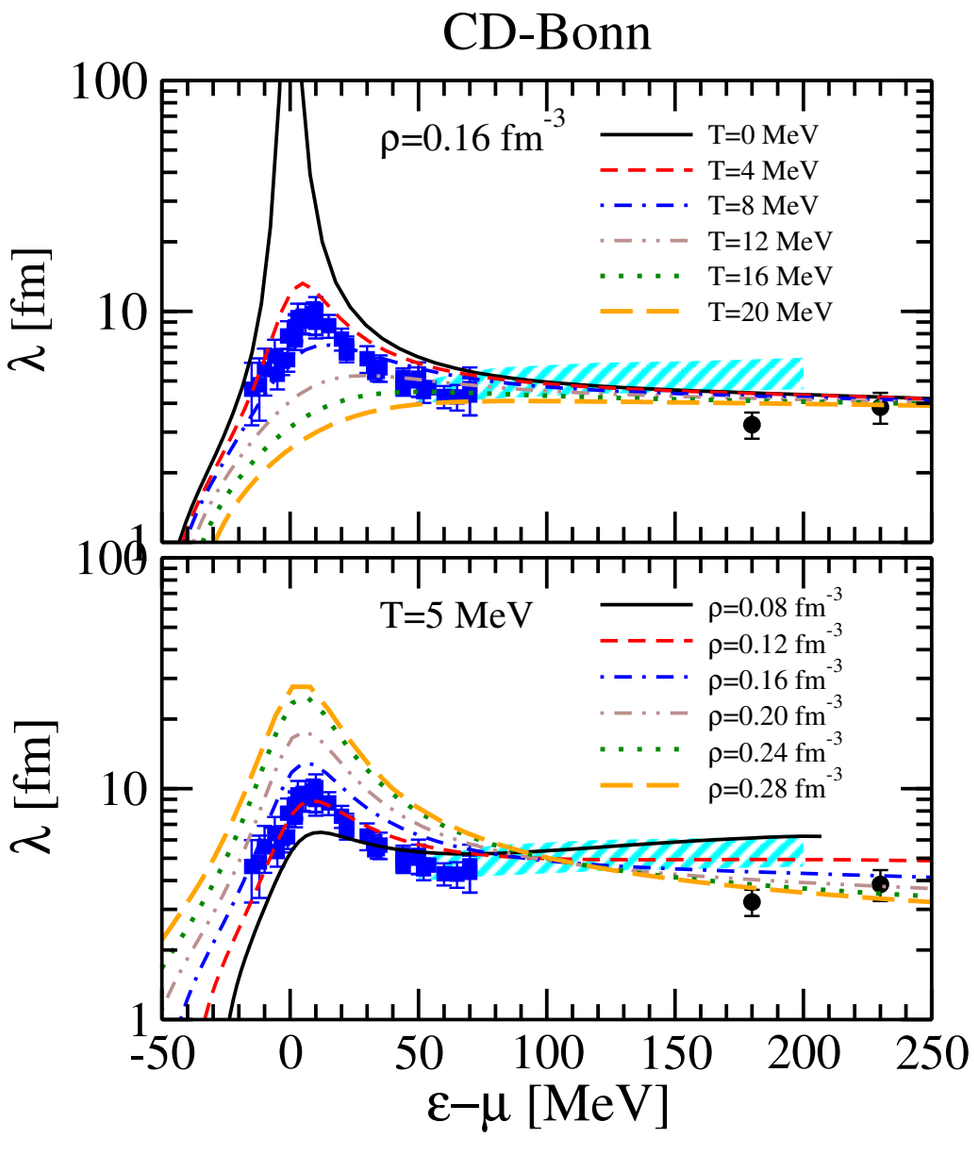
Electron-phonon Einstein model



[Eiguren, Ambrosch-Draxl & Echenique 2009]

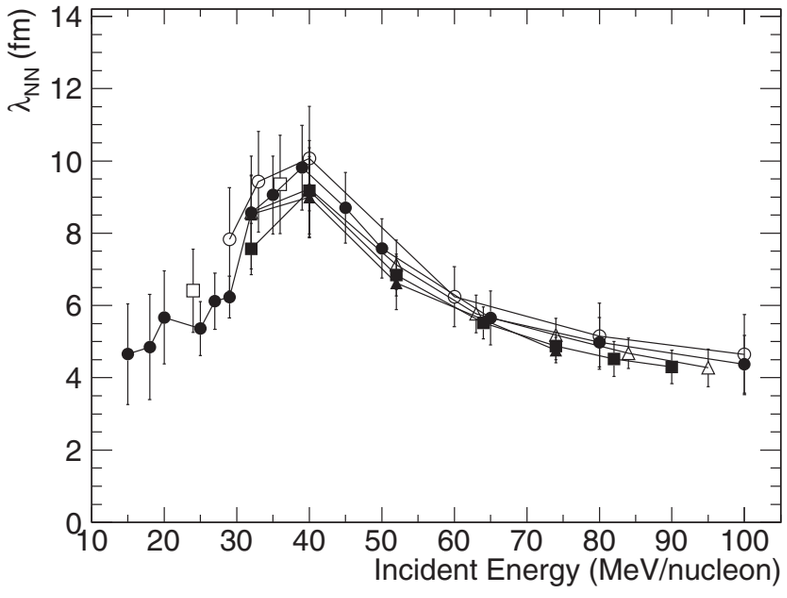
Nucleon mean free path

- Mean free path computed from quasiparticle lifetime and (group) velocity $\lambda_k = \dfrac{v_k}{\gamma_k} = \dfrac{\partial_k \varepsilon_k}{\gamma_k}$
- Crucial ingredient in transport codes



[Rios & Somà 2012 + in preparation]

- Mean-free path extracted from "nuclear stopping"
- Heavy-ion collisions
- INDRA collaboration at GANIL



[Lopez *et al.* 2014]

Spectral representation: *finite* systems

⊙ Numerator contains spectroscopic information

$$G_{ab}(z) = \sum_{\mu} \frac{\langle \Psi_0^A | a_a \,|\, \Psi_\mu^{A+1} \rangle \langle \Psi_\mu^{A+1} \,|\, a_b^\dagger | \Psi_0^A \rangle}{z - E_\mu^+ + i\eta} + \sum_{\nu} \frac{\langle \Psi_0^A | a_b^\dagger \,|\, \Psi_\nu^{A-1} \rangle \langle \Psi_\nu^{A-1} \,|\, a_a | \Psi_0^A \rangle}{z - E_\nu^- - i\eta}$$

spectroscopic amplitudes

$$U_\mu^b \equiv \langle \Psi_0^A | a_b \,|\, \Psi_\mu^{A+1} \rangle$$

$$V_\nu^b \equiv \langle \Psi_0^A | a_b^\dagger \,|\, \Psi_\nu^{A-1} \rangle$$

spectroscopic probabilities matrices

$$S_\mu^{+ab} \equiv \langle \Psi_0^{\mathrm{A}} | a_a | \Psi_\mu^{\mathrm{A+1}} \rangle \langle \Psi_\mu^{\mathrm{A+1}} | a_b^\dagger | \Psi_0^{\mathrm{A}} \rangle$$

$$S_\nu^{-ab} \equiv \langle \Psi_0^{\mathrm{A}} | a_a^\dagger | \Psi_\nu^{\mathrm{A\text{-}1}} \rangle \langle \Psi_\nu^{\mathrm{A\text{-}1}} | a_b | \Psi_0^{\mathrm{A}} \rangle$$

spectroscopic factors

$$SF_\mu^+ \equiv \mathrm{Tr}_{\mathcal{H}_1}\left[\mathbf{S}_\mu^+\right] = \sum_{a \in \mathcal{H}_1} \left| U_\mu^a \right|^2$$

$$SF_\nu^- \equiv \mathrm{Tr}_{\mathcal{H}_1}\left[\mathbf{S}_\nu^-\right] = \sum_{a \in \mathcal{H}_1} \left| V_\nu^a \right|^2$$

spectral function

$$\mathbf{S}(z) \equiv \sum_{\mu \in \mathcal{H}_{A+1}} \mathbf{S}_\mu^+ \, \delta(z - E_\mu^+) + \sum_{\nu \in \mathcal{H}_{A-1}} \mathbf{S}_\nu^- \, \delta(z - E_\nu^-)$$

spectral strength distribution

$$\mathcal{S}(z) \equiv \mathrm{Tr}_{\mathcal{H}_1}[\mathbf{S}(z)]$$

$$= \sum_{\mu \in \mathcal{H}_{A+1}} SF_\mu^+ \, \delta(z - E_\mu^+) + \sum_{\nu \in \mathcal{H}_{A-1}} SF_\nu^- \, \delta(z - E_\nu^-)$$

Spectral representation: *finite* systems

⊙ Combine numerator and denominator of Lehmann representation

$$G_{ab}(z) = \sum_{\mu} \frac{U_a^{\mu}(U_b^{\mu})^*}{z - E_{\mu}^{+} + i\eta} + \sum_{\nu} \frac{(V_a^{\nu})^* V_b^{\nu}}{z - E_{\nu}^{-} - i\eta}$$

denominator

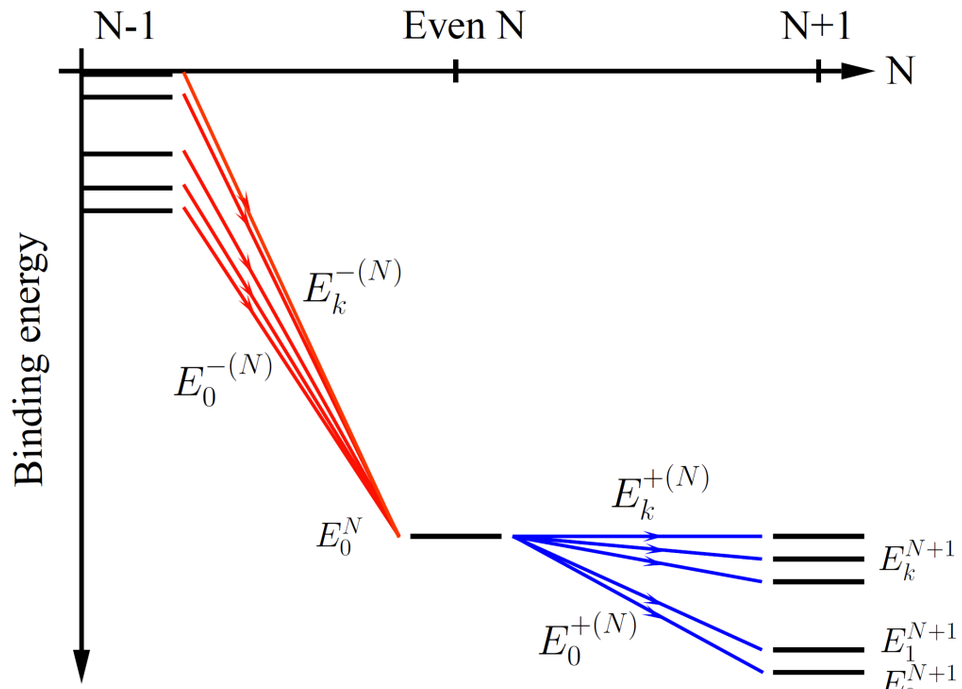
$E_{\mu}^{+} \equiv E_{\mu}^{N+1} - E_0^N$

$E_{\nu}^{-} \equiv E_0^N - E_{\nu}^{N-1}$

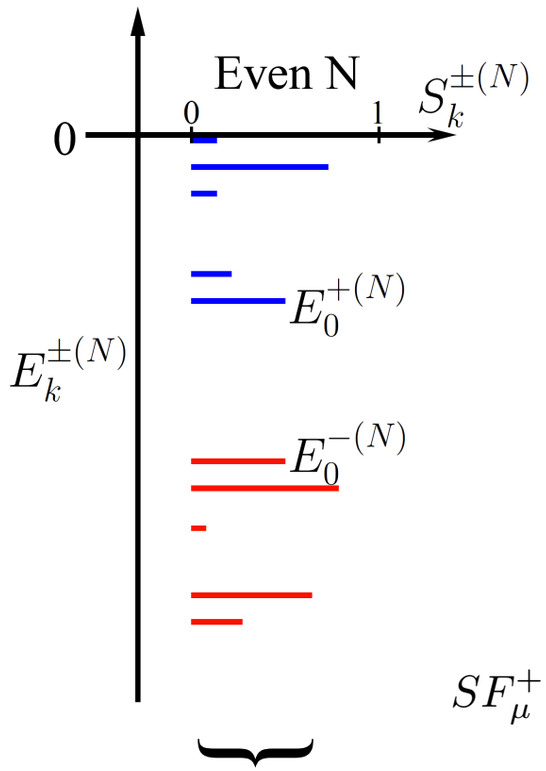
+ numerator →

spectral strength distribution

$$\mathcal{S}(z) = \sum_{\mu \in \mathcal{H}_{A+1}} SF_{\mu}^{+}\, \delta(z - E_{\mu}^{+}) + \sum_{\nu \in \mathcal{H}_{A-1}} SF_{\nu}^{-}\, \delta(z - E_{\nu}^{-})$$



[figures from J. Sadoudi]



spectroscopic factors

$$SF_{\mu}^{+} \equiv \mathrm{Tr}_{\mathcal{H}_1}\left[\mathbf{S}_{\mu}^{+}\right] = \sum_{a \in \mathcal{H}_1} \left|U_{\mu}^{a}\right|^2$$

$$SF_{\nu}^{-} \equiv \mathrm{Tr}_{\mathcal{H}_1}\left[\mathbf{S}_{\nu}^{-}\right] = \sum_{a \in \mathcal{H}_1} \left|V_{\nu}^{a}\right|^2$$

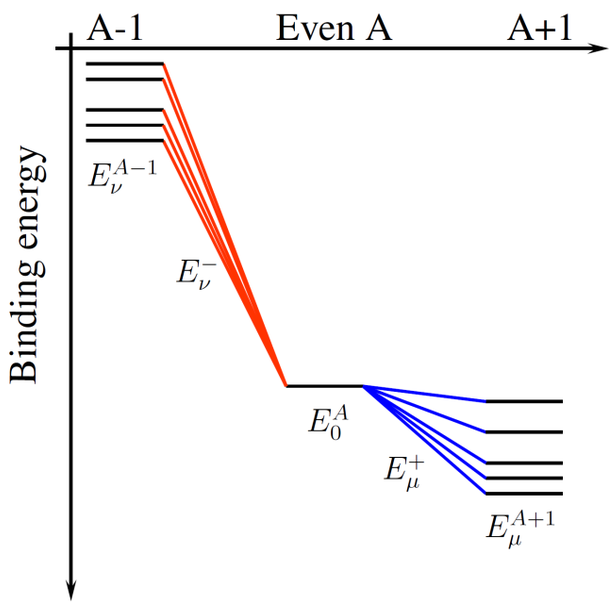
Odd-even systems

- Working equations (see later) typically implemented for $\mathbf{J^{\pi} = 0^{+}}$ **states**
  - Great simplification of the equations: J-coupled scheme, **block-diagonal structure**, ...
  - Critical step for realistic calculations
  - Applicable to **even-even nuclei**

- There are two possibilities to compute g.s. energies of odd-even systems

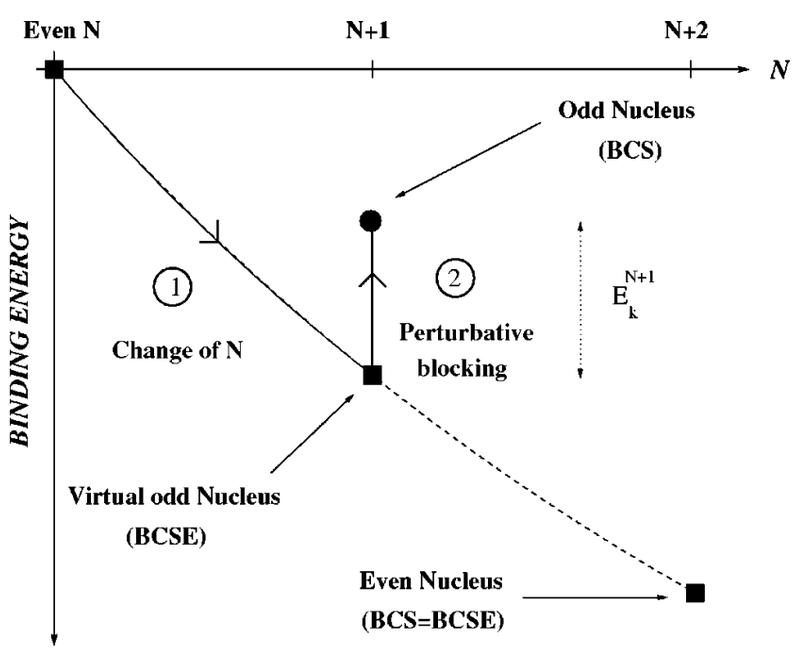
1. From separation energies spectrum

(Either from A-1 or A+1)



2. From fully-paired even number-parity state

("Fake" odd-A plus correction)



[Duguet *et al.* 2001]

➟ Different methods agree (typically within 200-300 hundred keV)

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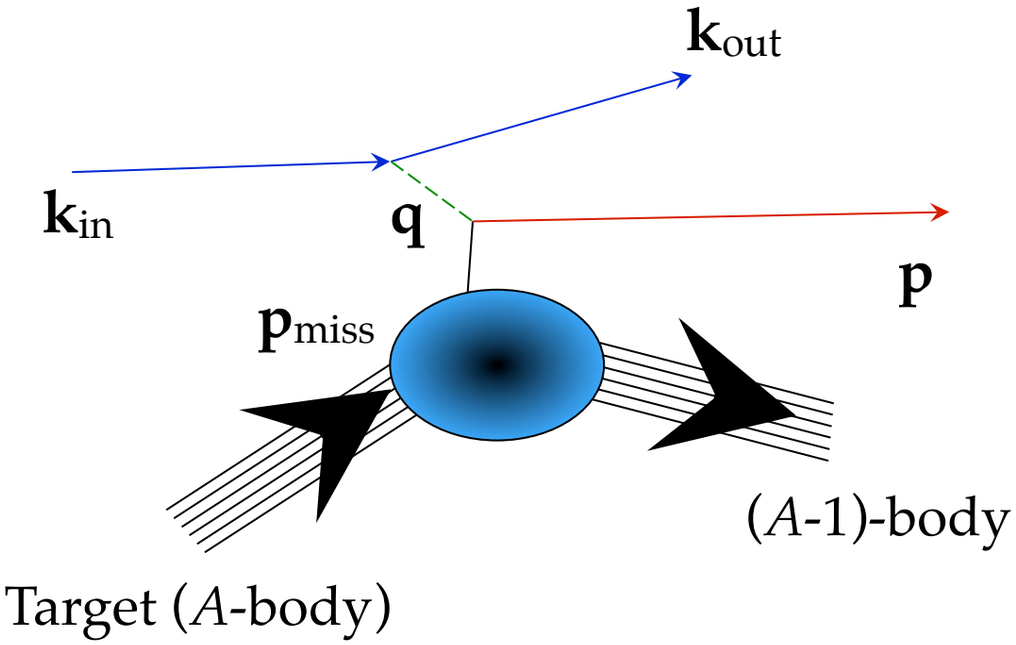
Connection with experiments

- Basic idea: spectroscopy via **knock-out reactions**
  - External probe transferring energy ω and momentum $\mathbf{q}$
  - Cross section $d\sigma \sim \sum_f \delta(\omega + E_i - E_f)\ |\langle \Psi_f | R(\mathbf{q}) | \Psi_i \rangle|^2$ with $R(\mathbf{q}) = \sum_{\mathbf{p}} a^\dagger_{\mathbf{p}}\, a_{\mathbf{p}-\mathbf{q}}$
  - Reconstruct energy and momentum of struck nucleon

$$E_{miss} = \frac{\mathbf{p}^2}{2m} - \omega = E_0^A - E_n^{A-1}$$

$$\mathbf{p}_{miss} = \mathbf{p} - \mathbf{q}$$



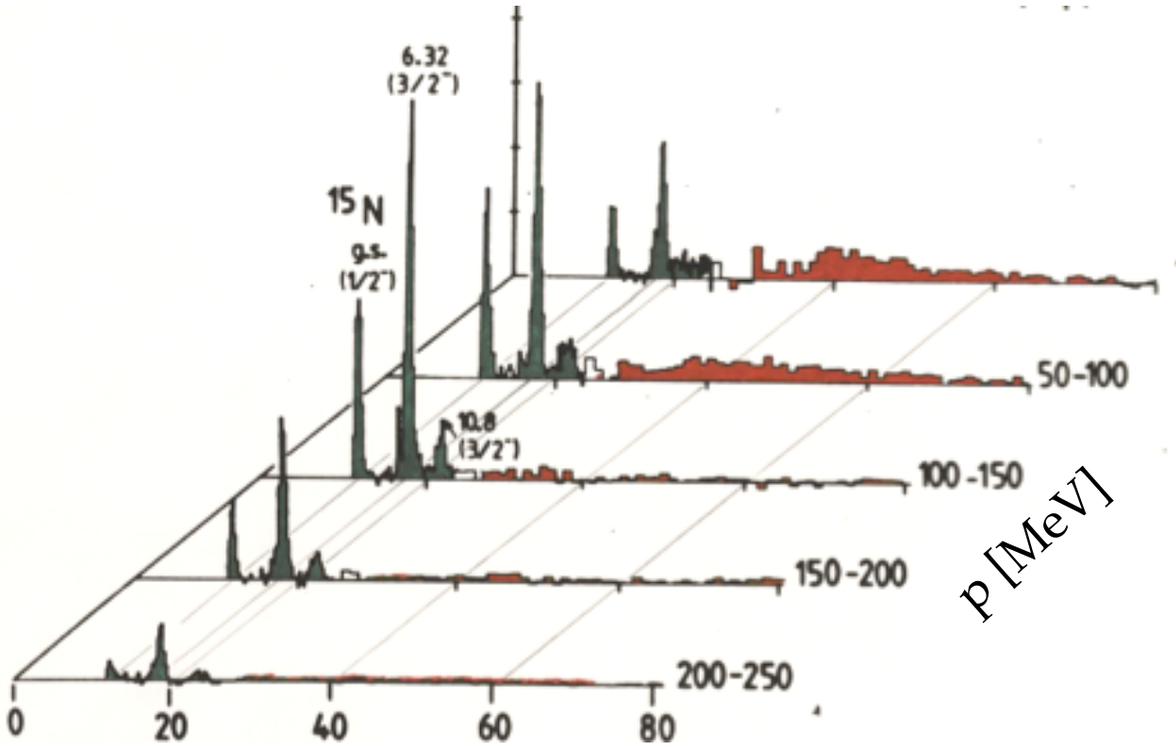
  - Information contained in the spectral function!

$$d\sigma \sim \sum_n \delta(E_{miss} - E_0^A + E_n^{A-1})\ \left|\langle \Psi_n^{A-1} | a_{\mathbf{p}_{miss}} | \Psi_0^A \rangle\right|^2$$
$$= S_{\mathbf{p}_{miss}}(E_{miss})$$

- Two assumptions
  - **Impulse approximation** (all energy transferred to one nucleon)
  - **No final state interactions**

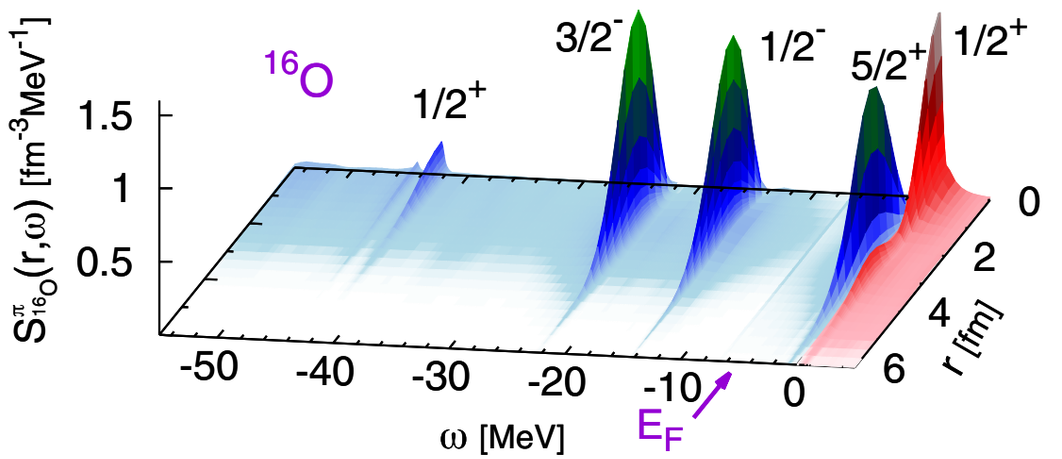
Connection with experiments

⊙ Example: electron scattering



[Mougey *et al.* 1980]

Results from (e,e'p) on ^{16}O (ALS in Saclay)



[Cipollone, Barbieri, Navrátil 2015]

GF calculations with chiral 2N+3N forces

Effective single-particle energies

⊙ To what extent can we extract a single-particle picture from the fragmented spectrum?

$$\underbrace{E_k^{\pm}}_{\text{Outcome of Schr. equation}} = \underbrace{e_p}_{\text{Ind. particles}} + \underbrace{\Delta E_{p\to k}}_{\text{Correlations}}$$

⊙ Baranger centroids (ESPEs) provide a model-independent procedure

➟ Define centroid Hamiltonian

$$\mathbf{h}^{\text{cent}} \equiv \sum_{\mu\in\mathcal{H}_{A+1}} \mathbf{S}_\mu^+ E_\mu^+ + \sum_{\nu\in\mathcal{H}_{A-1}} \mathbf{S}_\nu^- E_\nu^-$$

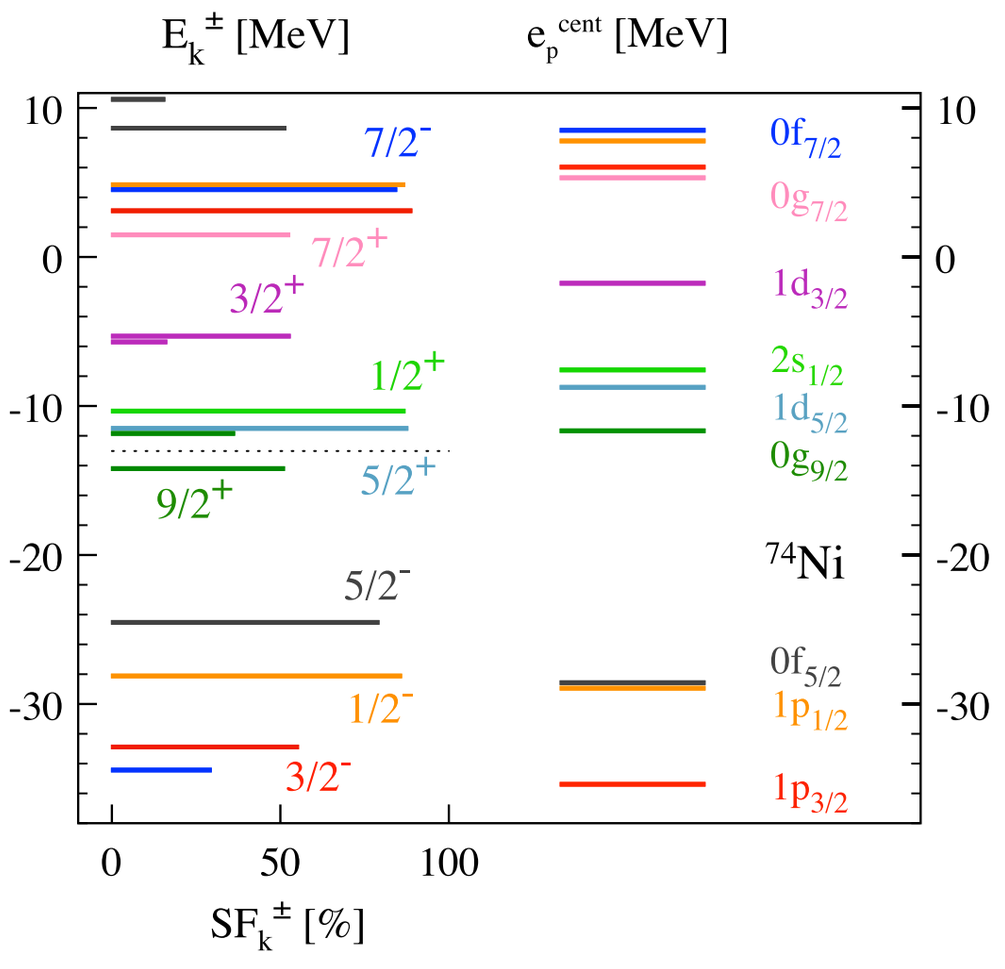
➟ Diagonalise

$$\mathbf{h}^{\text{cent}}\psi_p^{\text{cent}} = e_p^{\text{cent}}\psi_p^{\text{cent}}$$

➟ ESPEs as centroids

$$e_p^{\text{cent}} \equiv \sum_{\mu\in\mathcal{H}_{A+1}} S_\mu^{+pp} E_\mu^+ + \sum_{\nu\in\mathcal{H}_{A-1}} S_\nu^{-pp} E_\nu^-$$

Recollect strength in both removal and addition channels



[Duguet, Hergert, Holt, Somà 2015]

Observables vs non-observables

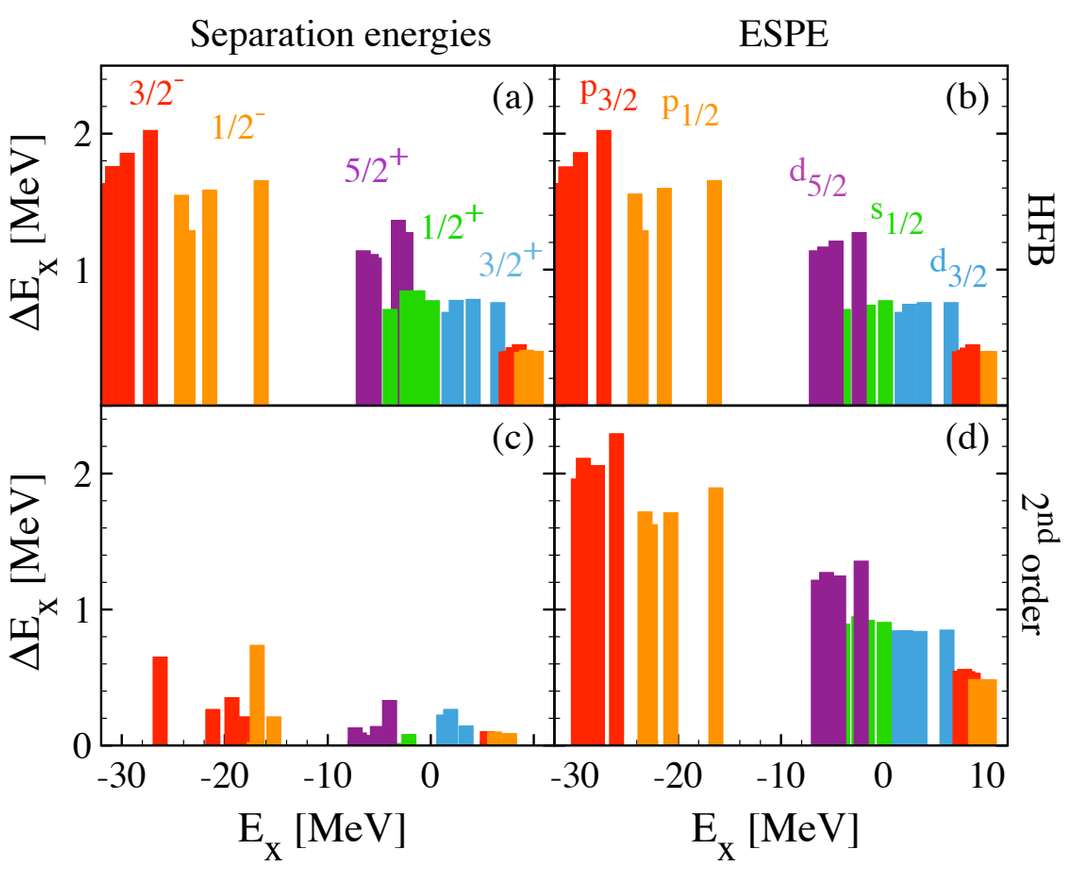
⊙ Spectroscopic factors, hence reconstructed ESPEs are **non-observable** quantities

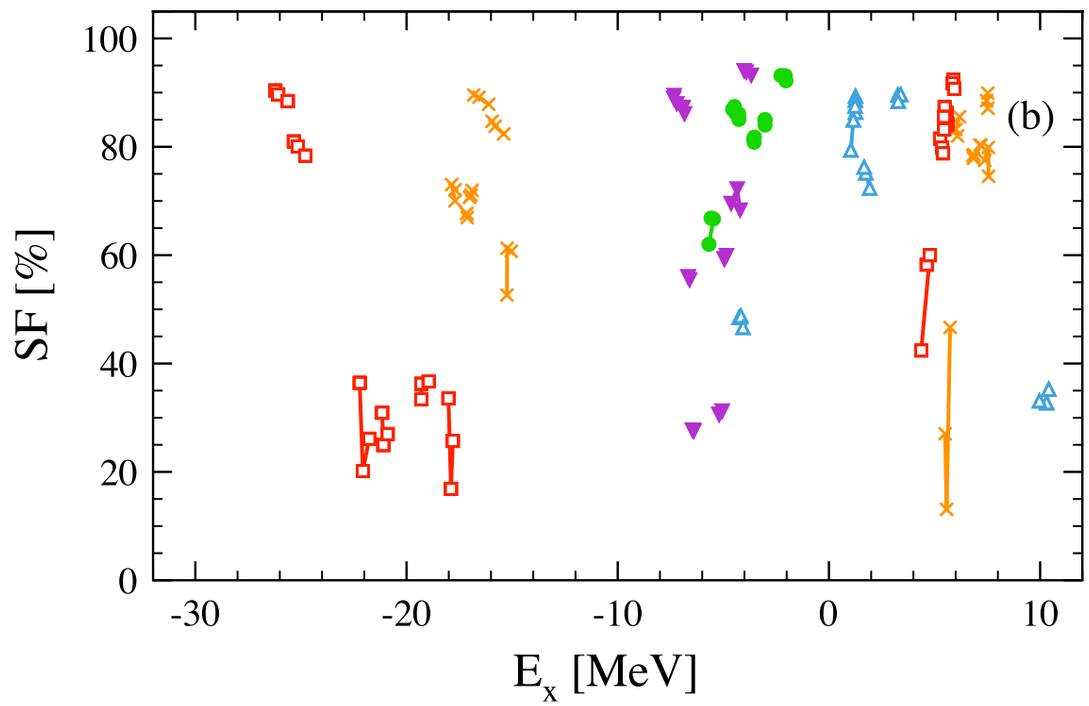
➟ In particular, they depend on the (scale of the) particular Hamiltonian one employs

$$\underbrace{E_\mu^+}_{\text{invariant under } U(\lambda)} \equiv \underbrace{\sum_p s_\mu^{+pp}(\lambda) e_p^{\text{cent}}(\lambda)}_{\text{varies under } U(\lambda)} + \underbrace{\sum_{pq} s_\mu^{+pq}(\lambda) \Sigma_{qp}^{\text{dyn}}(E_\mu^+;\lambda)}_{\text{varies under } U(\lambda)}$$

(single-particle components; correlations)

⊙ Can be shown explicitly for a limited interval of the resolution scale $\lambda \in [1.88, 2.23]$ fm^{-1}





[Duguet, Hergert, Holt, Somà 2015]

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Dyson equation as eigenvalue problem

⊙ Due to energy denominators, solving Dyson equation in this form is problematic

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

⊙ Instead, one can derive an eigenvalue equation by "extracting" the poles of G, i.e.

$$\lim_{\omega \to E^\pm_\nu} (\omega - E^\pm_\nu) \left\{ G_{ab}(\omega) = G^0_{ab}(\omega) + \sum_{cd} G^0_{ac}(\omega)\, \Sigma^*_{cd}(\omega)\, G_{db}(\omega) \right\}$$

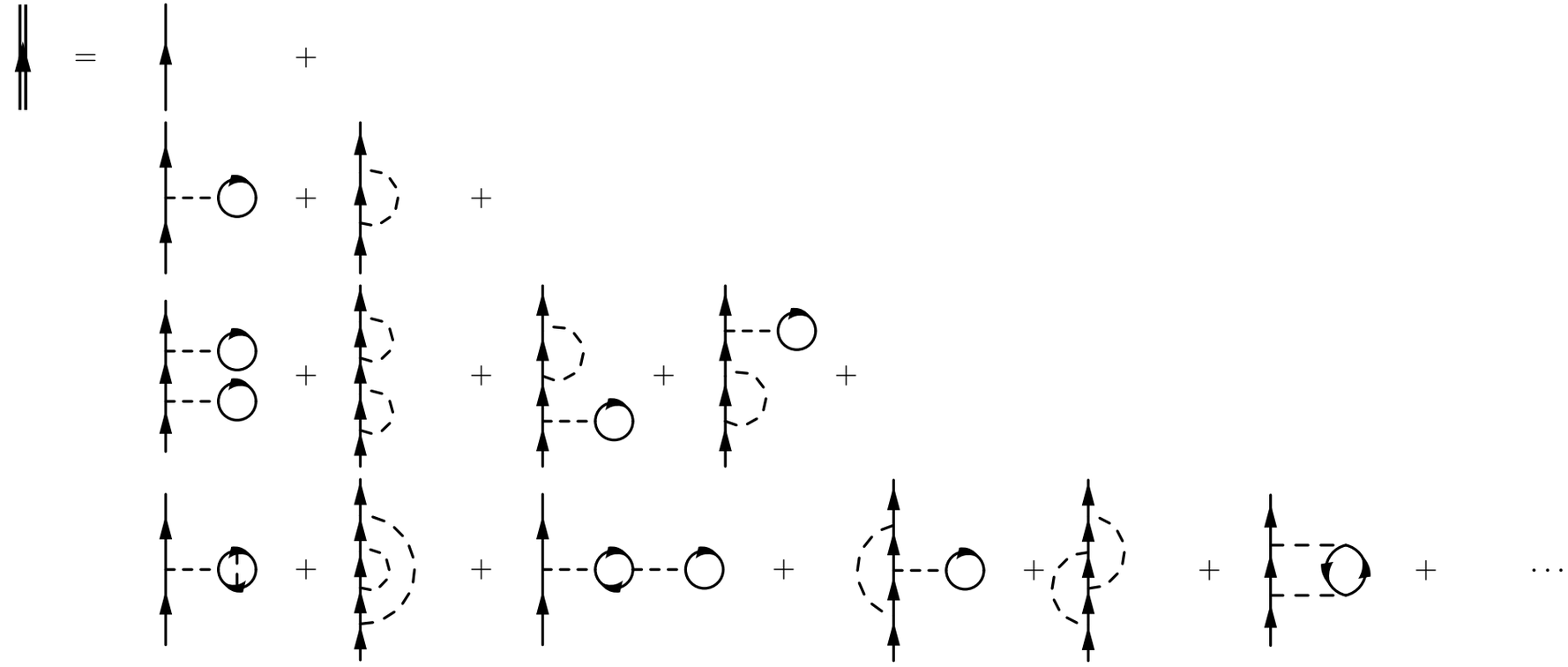
using $\quad G_{ab}(\omega) = \sum_\mu \frac{U^\mu_a (U^\mu_b)^*}{\omega - E^+_\mu + i\eta} + \sum_\nu \frac{(V^\nu_a)^* V^\nu_b}{\omega - E^-_\nu - i\eta}$ $\quad$ and $\quad G^0_{ab}(\omega) = (\omega - T)^{-1}_{ab}$

$$\sum_b \left[t_{ab} + \Sigma^*_{ab}(\omega)|_{\omega = E_k} \right] X^k_b = E_k\, X^k_a$$

with $\quad X^k_a = \left\{ V^{*k}_a, U_a{}^k \right\}$ $\quad$ and $\quad E_k = \left\{ E^-_k, E^+_k \right\}$

Feynman rules

- Diagrammatic rules to derive all m^{th} order terms in the expansion of G
  - Work in energy domain (time domain analogous)
  - Work with an antisymmetrised interaction $\bar{v}_{\alpha\gamma\beta\delta}$ (two-body only)
  - Case of **self-consistent** schemes



1. Draw all **topologically distinct, connected, direct, irreducible, skeleton** diagrams with
   - m interaction lines
   - $2m$+1 propagation lines

Feynman rules

- Diagrammatic rules to derive all m^{th} order terms in the expansion of G
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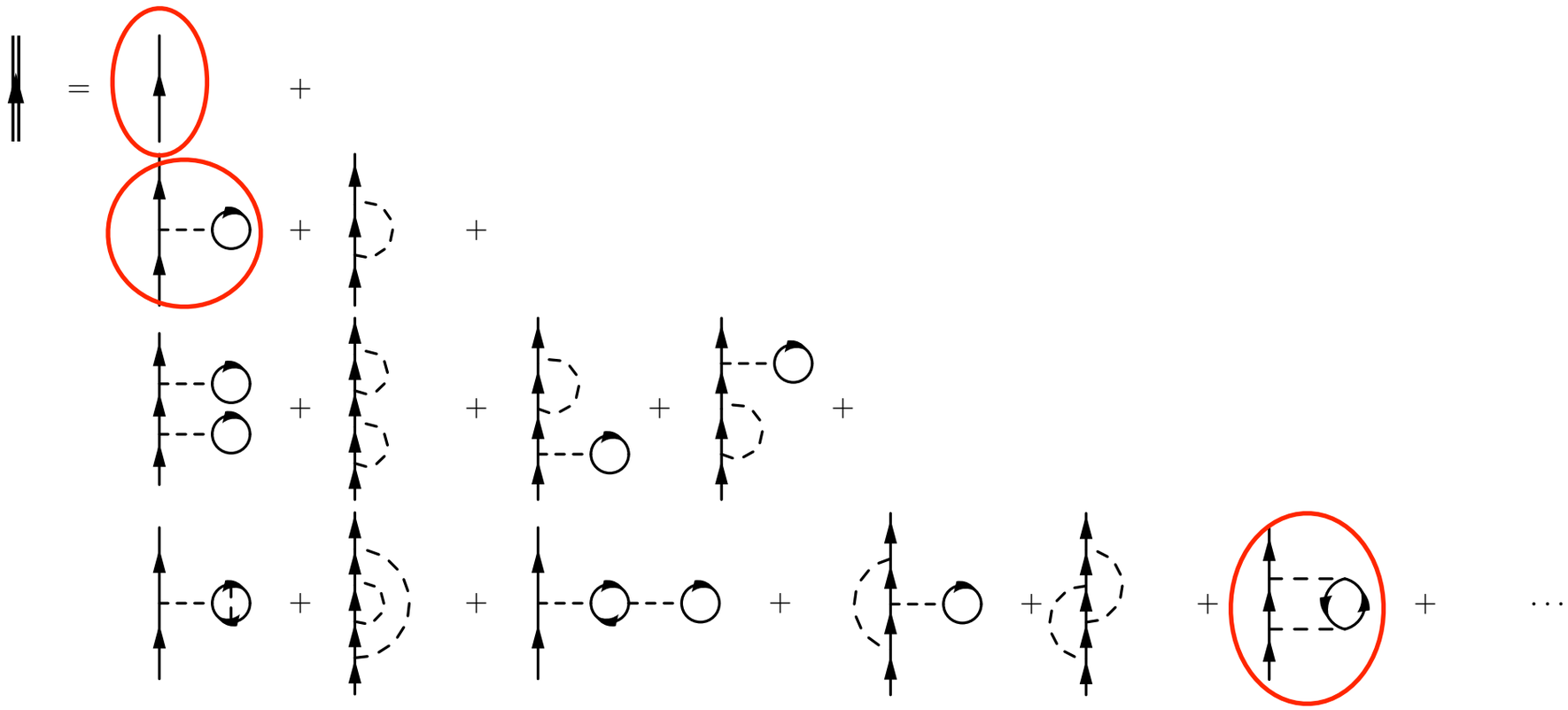


1. Draw all **topologically distinct, connected, direct, irreducible, skeleton** diagrams with
   - m interaction lines
   - $2m$+1 propagation lines

Feynman rules

2. Assign an energy to each propagation line (energy is conserved at each vertex)

3. Assign two indices to each propagation line

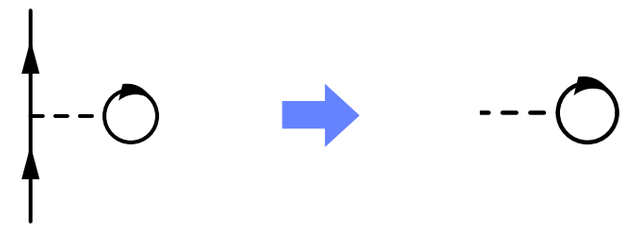
4. Write down $\bar{v}_{\alpha\gamma\beta\delta}$ for each interaction line and $G_{\alpha\beta}(\omega)$ for each propagation line

5. Write down factors

   - i^m
   - 1/2 for each pair of equivalent propagation lines
   - $(-1)^L$ where L is the number of closed sermonic loops

6. Sum over all internal indices and integrate over all internal energies

⊙ Corresponding expressions for **self-energy expansion** obtained by cutting external legs

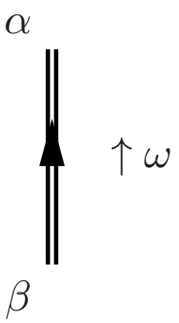


⊙ In self-consistent schemes all propagators in the self-energy are **dressed**

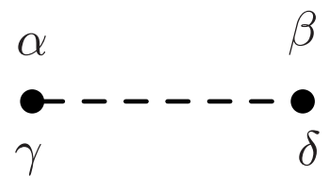
First-order self-energy

⊙ Notation

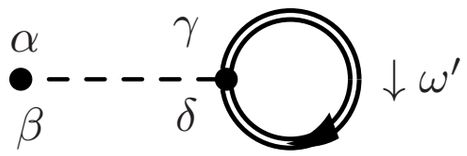
Dressed propagator

$G_{\alpha\beta}(\omega) \equiv$ 

Antisymmetrised interaction

$\bar{v}_{\alpha\beta\gamma\delta} \equiv$ 

⊙ First-order self-energy

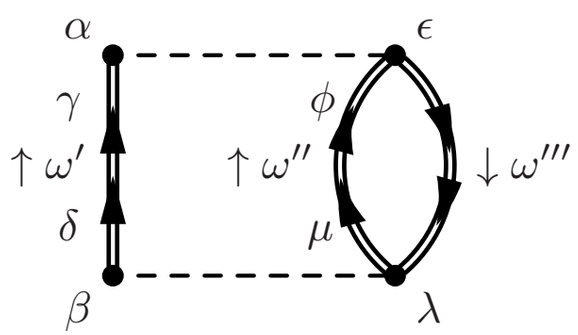
$\Sigma^{(1)}_{\alpha\beta}(\omega) =$ 

$$
\begin{aligned}
\Sigma^{(1)}_{\alpha\beta}(\omega) &= -i \int_{C\uparrow} \frac{d\omega'}{2\pi} \sum_{\gamma\delta} \bar{v}_{\alpha\gamma\beta\delta}\, G_{\delta\gamma}(\omega') \\
&= -i \int_{C\uparrow} \frac{d\omega'}{2\pi} \sum_{\gamma\delta,n} \bar{v}_{\alpha\gamma\beta\delta}\, \frac{U^n_\delta\, U^{n*}_\gamma}{\omega' - E^+_n + i\eta} \\
&\quad - i \int_{C\uparrow} \frac{d\omega'}{2\pi} \sum_{\gamma\delta,k} \bar{v}_{\alpha\gamma\beta\delta}\, \frac{V^{k*}_\delta\, V^k_\gamma}{\omega' - E^-_k - i\eta} \\
&= \sum_{\gamma\delta,k} \bar{v}_{\alpha\gamma\beta\delta}\, V^{k*}_\delta\, V^k_\gamma
\end{aligned}
$$

Second-order self-energy

⊙ **Second-order self-energy**

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



$$\Sigma^{(2)}_{\alpha\beta}(\omega) = \frac{1}{2}\int \frac{d\omega'}{2\pi}\frac{d\omega''}{2\pi}\frac{d\omega'''}{2\pi} \sum_{\gamma\delta\epsilon\phi\mu\lambda} \bar{v}_{\alpha\epsilon\gamma\phi}\,\bar{v}_{\delta\mu\beta\lambda}\,G_{\gamma\delta}(\omega')\,G_{\phi\mu}(\omega'')\,G_{\lambda\epsilon}(\omega''')\,\delta(\omega-\omega'-\omega''+\omega''')$$

$$= \frac{1}{2}\int \frac{d\omega'}{2\pi}\frac{d\omega''}{2\pi} \sum_{\gamma\delta\epsilon\phi\mu\lambda} \bar{v}_{\alpha\epsilon\gamma\phi}\,\bar{v}_{\delta\mu\beta\lambda}\,G_{\gamma\delta}(\omega')\,G_{\phi\mu}(\omega'')\,G_{\lambda\epsilon}(\omega'+\omega''-\omega)$$

$$= -\frac{1}{2}\int \frac{d\omega'}{2\pi i}\frac{d\omega''}{2\pi i} \sum_{\gamma\delta\epsilon\phi\mu\lambda,n_1n_2n_3,k_1k_2k_3} \bar{v}_{\alpha\epsilon\gamma\phi}\,\bar{v}_{\delta\mu\beta\lambda} \left\{\frac{U^{n_1}_{\gamma}\,U^{n_1*}_{\delta}}{\omega'-E^{+}_{n_1}+i\eta}+\frac{V^{k_1*}_{\gamma}\,V^{k_1}_{\delta}}{\omega'-E^{-}_{k_1}-i\eta}\right\}$$

$$\times \left\{\frac{U^{n_2}_{\phi}\,U^{n_2*}_{\mu}}{\omega''-E^{+}_{n_2}+i\eta}+\frac{V^{k_2*}_{\phi}\,V^{k_2}_{\mu}}{\omega''-E^{-}_{k_2}-i\eta}\right\} \left\{\frac{U^{n_3}_{\lambda}\,U^{n_3*}_{\epsilon}}{\omega'+\omega''-\omega-E^{+}_{n_3}+i\eta}+\frac{V^{k_3*}_{\lambda}\,V^{k_3}_{\epsilon}}{\omega'+\omega''-\omega-E^{-}_{k_3}-i\eta}\right\}$$

$$= \frac{1}{2} \sum_{\gamma\delta\epsilon\phi\mu\lambda,n_1n_2n_3,k_1k_2k_3} \bar{v}_{\alpha\epsilon\gamma\phi}\,\bar{v}_{\delta\mu\beta\lambda} \left\{\frac{U^{n_1}_{\gamma}\,U^{n_1*}_{\delta}\,U^{n_2}_{\phi}\,U^{n_2*}_{\mu}\,V^{k_3*}_{\lambda}\,V^{k_3}_{\epsilon}}{\omega-(E^{+}_{n_1}+E^{+}_{n_2}-E^{-}_{k_3})+i\eta}+\frac{V^{k_1*}_{\gamma}\,V^{k_1}_{\delta}\,V^{k_2*}_{\phi}\,V^{k_2}_{\mu}\,U^{n_3}_{\lambda}\,U^{n_3*}_{\epsilon}}{\omega-(E^{+}_{n_3}-E^{-}_{k_1}-E^{-}_{k_2})-i\eta}\right\}$$

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Energy-*independent* eigenvalue problem

- In practise, energy denominators generate (numerical) difficulties
- Eigenvalue problem can be rewritten in an **energy-independent** form

Define new objects

$$M_\alpha^{n_1 n_2 k_3} \equiv \sum_{\beta\gamma\delta} \bar{v}_{\alpha\delta\beta\gamma}\, U_\beta^{n_1} U_\gamma^{n_2} V_\delta^{k_3}$$

2p1h amplitude

$$N_\alpha^{k_1 k_2 n_3} \equiv \sum_{\beta\gamma\delta} \bar{v}_{\alpha\delta\beta\gamma}\, V_\beta^{k_1} V_\gamma^{k_2} U_\delta^{n_3}$$

2h1p amplitude

$$E^+_{n_1 n_2 k_3} \equiv E^+_{n_1} + E^+_{n_2} - E^-_{k_3}$$

2p1h energy

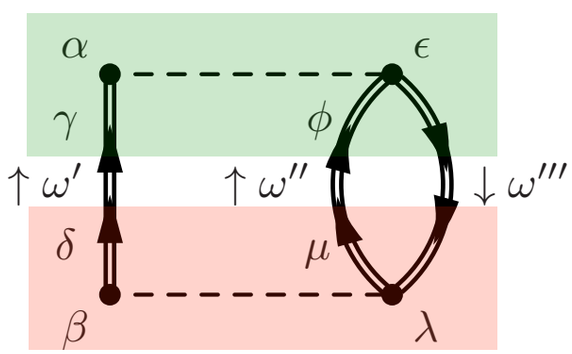
$$E^-_{k_1 k_2 n_3} \equiv E^-_{k_1} + E^-_{k_2} - E^+_{n_3}$$

2h1p energy

Energy-*independent* eigenvalue problem

⊙ **Second-order self-energy**

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



$$\Sigma^{(2)}_{\alpha\beta}(\omega) = \frac{1}{2}\int \frac{d\omega'}{2\pi}\frac{d\omega''}{2\pi}\frac{d\omega'''}{2\pi} \sum_{\gamma\delta\epsilon\phi\mu\lambda} \bar{v}_{\alpha\epsilon\gamma\phi}\,\bar{v}_{\delta\mu\beta\lambda}\,G_{\gamma\delta}(\omega')\,G_{\phi\mu}(\omega'')\,G_{\lambda\epsilon}(\omega''')\,\delta(\omega-\omega'-\omega''+\omega''')$$

$$= \frac{1}{2}\int \frac{d\omega'}{2\pi}\frac{d\omega''}{2\pi} \sum_{\gamma\delta\epsilon\phi\mu\lambda} \bar{v}_{\alpha\epsilon\gamma\phi}\,\bar{v}_{\delta\mu\beta\lambda}\,G_{\gamma\delta}(\omega')\,G_{\phi\mu}(\omega'')\,G_{\lambda\epsilon}(\omega'+\omega''-\omega)$$

$$= -\frac{1}{2}\int \frac{d\omega'}{2\pi i}\frac{d\omega''}{2\pi i} \sum_{\gamma\delta\epsilon\phi\mu\lambda,n_1n_2n_3,k_1k_2k_3} \bar{v}_{\alpha\epsilon\gamma\phi}\,\bar{v}_{\delta\mu\beta\lambda} \left\{\frac{U^{n_1}_{\gamma}\,U^{n_1*}_{\delta}}{\omega'-E^{+}_{n_1}+i\eta}+\frac{V^{k_1*}_{\gamma}\,V^{k_1}_{\delta}}{\omega'-E^{-}_{k_1}-i\eta}\right\}$$

$$\times \left\{\frac{U^{n_2}_{\phi}\,U^{n_2*}_{\mu}}{\omega''-E^{+}_{n_2}+i\eta}+\frac{V^{k_2*}_{\phi}\,V^{k_2}_{\mu}}{\omega''-E^{-}_{k_2}-i\eta}\right\} \left\{\frac{U^{n_3}_{\lambda}\,U^{n_3*}_{\epsilon}}{\omega'+\omega''-\omega-E^{+}_{n_3}+i\eta}+\frac{V^{k_3*}_{\lambda}\,V^{k_3}_{\epsilon}}{\omega'+\omega''-\omega-E^{-}_{k_3}-i\eta}\right\}$$

$$= \frac{1}{2}\sum_{\gamma\delta\epsilon\phi\mu\lambda,n_1n_2n_3,k_1k_2k_3} \bar{v}_{\alpha\epsilon\gamma\phi}\,\bar{v}_{\delta\mu\beta\lambda} \left\{\frac{U^{n_1}_{\gamma}\,U^{n_1*}_{\delta}\,U^{n_2}_{\phi}\,U^{n_2*}_{\mu}\,V^{k_3*}_{\lambda}\,V^{k_3}_{\epsilon}}{\omega-(E^{+}_{n_1}+E^{+}_{n_2}-E^{-}_{k_3})+i\eta}+\frac{V^{k_1*}_{\gamma}\,V^{k_1}_{\delta}\,V^{k_2*}_{\phi}\,V^{k_2}_{\mu}\,U^{n_3}_{\lambda}\,U^{n_3*}_{\epsilon}}{\omega-(E^{+}_{n_3}-E^{-}_{k_1}-E^{-}_{k_2})-i\eta}\right\}$$

Energy-*independent* eigenvalue problem

- In practise, energy denominators generate (numerical) difficulties
- Eigenvalue problem can be rewritten in an **energy-independent** form

Define new objects

$$M_\alpha^{n_1 n_2 k_3} \equiv \sum_{\beta\gamma\delta} \bar{v}_{\alpha\delta\beta\gamma}\, U_\beta^{n_1} U_\gamma^{n_2} V_\delta^{k_3}$$

2p1h amplitude

$$N_\alpha^{k_1 k_2 n_3} \equiv \sum_{\beta\gamma\delta} \bar{v}_{\alpha\delta\beta\gamma}\, V_\beta^{k_1} V_\gamma^{k_2} U_\delta^{n_3}$$

2h1p amplitude

$$E^+_{n_1 n_2 k_3} \equiv E^+_{n_1} + E^+_{n_2} - E^-_{k_3}$$

2p1h energy

$$E^-_{k_1 k_2 n_3} \equiv E^-_{k_1} + E^-_{k_2} - E^+_{n_3}$$

2h1p energy

Compact form of second-order self-energy

$$\Sigma^{(2)}_{\alpha\beta}(\omega) = \frac{1}{2} \sum_{n_1 n_2 n_3, k_1 k_2 k_3} \left\{ \frac{M_\alpha^{n_1 n_2 k_3}\, {M_\beta^{n_1 n_2 k_3}}^*}{\omega - E^+_{n_1 n_2 k_3} + i\eta} + \frac{(N_\alpha^{k_1 k_2 n_3})^*\, N_\beta^{k_1 k_2 n_3}}{\omega - E^-_{k_1 k_2 n_3} - i\eta} \right\}$$

Energy-*independent* eigenvalue problem

Define new objects

$$(E_k - E^+_{n_1 n_2 k_3})\, W_k^{n_1 n_2 k_3} \equiv \sum_\alpha (M_\alpha^{n_1 n_2 k_3})^*\, X_\alpha^k$$

$$(E_k - E^-_{k_1 k_2 n_3})\, Z_k^{k_1 k_2 n_3} \equiv \sum_\alpha N_\alpha^{k_1 k_2 n_3}\, X_\alpha^k$$

Rewrite energy-dependent Dyson equation as

$$\sum_\delta \left[t_{\lambda\delta} + \Sigma^{(1)}_{\lambda\delta} \right] X_\delta^k + \sum_{n_1 n_2 k_3} M_\lambda^{n_1 n_2 k_3}\, W_k^{n_1 n_2 k_3} + \sum_{k_1 k_2 n_3} (N_\lambda^{k_1 k_2 n_3})^*\, Z_k^{k_1 k_2 n_3} = E_k\, X_\lambda^k$$

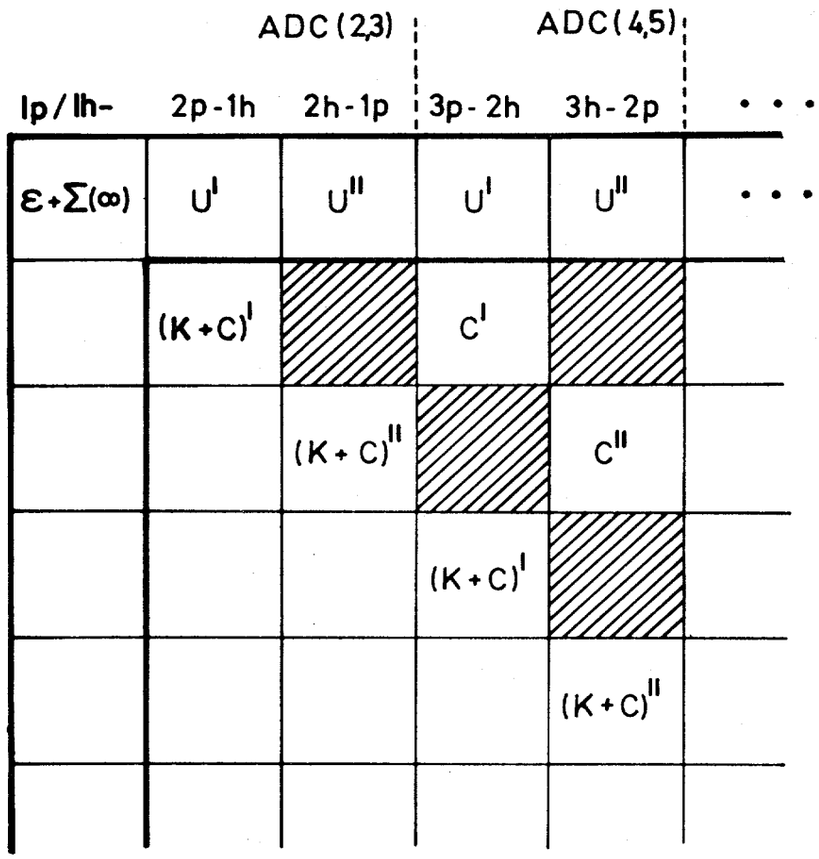
Energy-independent eigenvalue equation

$$E_k \begin{pmatrix} V^* \\ W \\ Z \end{pmatrix}_k = \begin{pmatrix} t + \Sigma^{(1)} & M & N^* \\ M^\dagger & E^+ & 0 \\ N^T & 0 & E^- \end{pmatrix} \begin{pmatrix} X \\ W \\ Z \end{pmatrix}_k \equiv \Xi \begin{pmatrix} X \\ W \\ Z \end{pmatrix}_k$$

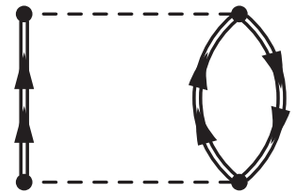
ADC expansion

⊙ **Algebraic Diagrammatic Construction (ADC)** [Schirmer, Cederbaum & Walter 1983]

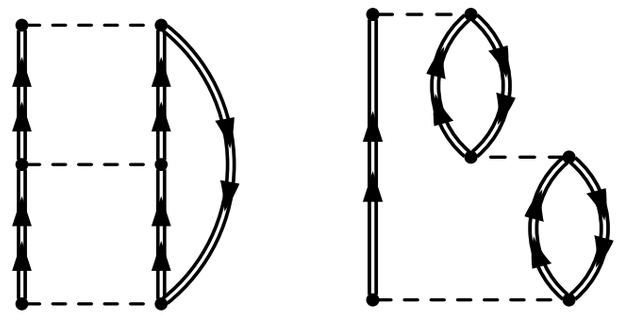
- ○ Exact summation of the self-energy reformulated into a simple algebraic form
- ○ ADC(n) includes complete n-th order (dressed) perturbation theory diagrams for G
- ○ Results in Hermitian eigenvalue problems within limited spaces of $N\pm1$ systems



ADC(2)



ADC(3)



- ○ Pole structure of 2nd order maintained → energy-independent eigenvalue equation to be solved

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   - **Krylov projection**
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Scaling of Dyson matrix

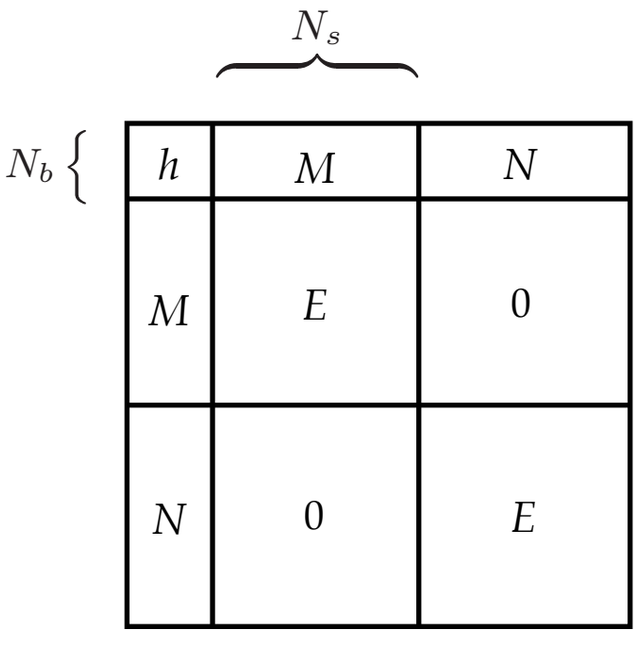
⊙ Dyson (eigenvalue) equation has to be solved iteratively

$$E_k \begin{pmatrix} V^* \\ W \\ Z \end{pmatrix}_k = \begin{pmatrix} t+\Sigma^{(1)} & M & N^* \\ M^\dagger & E^+ & 0 \\ N^T & 0 & E^- \end{pmatrix} \begin{pmatrix} X \\ W \\ Z \end{pmatrix}_k \equiv \Xi \begin{pmatrix} X \\ W \\ Z \end{pmatrix}_k$$

$$E^+_{n_1 n_2 k_3} \equiv E^+_{n_1} + E^+_{n_2} - E^-_{k_3}$$

➟ At each iteration the **number of poles increases** → so does the dimension of Dyson matrix

⊙ Schematically, dimensions grow as follows



○ First iteration

$$N_s \approx \binom{N_b}{3} \approx \frac{N_b^3}{6} \quad \Rightarrow \quad \dim(\Xi) = N_{\text{tot}} \approx N_b^3/3$$

○ Second iteration ⇒ $\dim(\Xi) \approx N_b^9$

○ n^{th} iteration ⇒ $\dim(\Xi) \approx N_b^{3^n}$

➟ **Severe scaling** prevents the exact treatment of all poles

Krylov projection

⊙ Use **Lanczos algorithm** (**Krylov-space** technique) to reduce dimensions of

$$\Xi \equiv \begin{pmatrix} \Xi^{(1)} & \Xi^{(2)} \\ \Xi^{(2)\,\dagger} & \mathcal{E} \end{pmatrix}$$

Project into subspace

⊙ Build set of Lanczos vectors (see next slide) $\mathcal{L}$

$$\mathcal{E} \longrightarrow \mathcal{E}' = \begin{pmatrix} \mathcal{L}^\dagger\, E\, \mathcal{L} & \\ & -\mathcal{L}^\dagger\, E\, \mathcal{L} \end{pmatrix}$$

Projected matrix

and accordingly

$$\Xi^{(2)} \longrightarrow \Xi'^{(2)} = \Xi^{(2)} \begin{pmatrix} \mathcal{L} \\ \mathcal{L} \end{pmatrix}$$

$$\Xi^{(2)\,\dagger} \longrightarrow \Xi'^{(2)\,\dagger} = \begin{pmatrix} \mathcal{L}^\dagger & \mathcal{L}^\dagger \end{pmatrix} \Xi^{(2)\,\dagger}$$

$$\Xi \longrightarrow \Xi' = \begin{pmatrix} \Xi^{(1)} & \Xi'^{(2)} \\ \Xi'^{(2)\,\dagger} & \mathcal{E}' \end{pmatrix}$$

⊙ Krylov subspace can have arbitrary dimensions from 1 to $\dim(E)$

➟ The goal is to choose a small enough $\dim(\mathcal{L}^\dagger\, E\, \mathcal{L}) \ll \dim(E)$ without spoiling the accuracy

Lanczos algorithm

⊙ **Krylov space** defined as

$$\mathcal{K}^{(r)} \equiv \text{span}\left\{\mathbf{p}, E\,\mathbf{p}, E^2\,\mathbf{p}, E^3\,\mathbf{p}, \ldots, E^{r-1}\,\mathbf{p}\right\}$$

⊙ **Lanczos algorithm**: iterative method to build a Krylov space for Hermitian matrices

$$\begin{aligned}
\mathbf{v}_1 &\equiv \mathbf{p} \qquad \text{pivot} \\
E\,\mathbf{v}_1 &\equiv e_{11}\,\mathbf{v}_1 + e_{21}\,\mathbf{v}_2 \\
E\,\mathbf{v}_2 &\equiv e_{12}\,\mathbf{v}_1 + e_{22}\,\mathbf{v}_2 + e_{32}\,\mathbf{v}_3 \\
&\cdots \\
E\,\mathbf{v}_{r-1} &\equiv e_{1(r-1)}\,\mathbf{v}_1 + \cdots + e_{r(r-1)}\,\mathbf{v}_r
\end{aligned}$$

$$e_{ij} = (e_{ji})^* = \mathbf{v}_i^\dagger E\,\mathbf{v}_j \qquad \text{for all } i,j$$

$$e_{ij} = 0 \qquad \text{for } |i-j| \geq 2$$

Projected matrix is Hermitian and tridiagonal

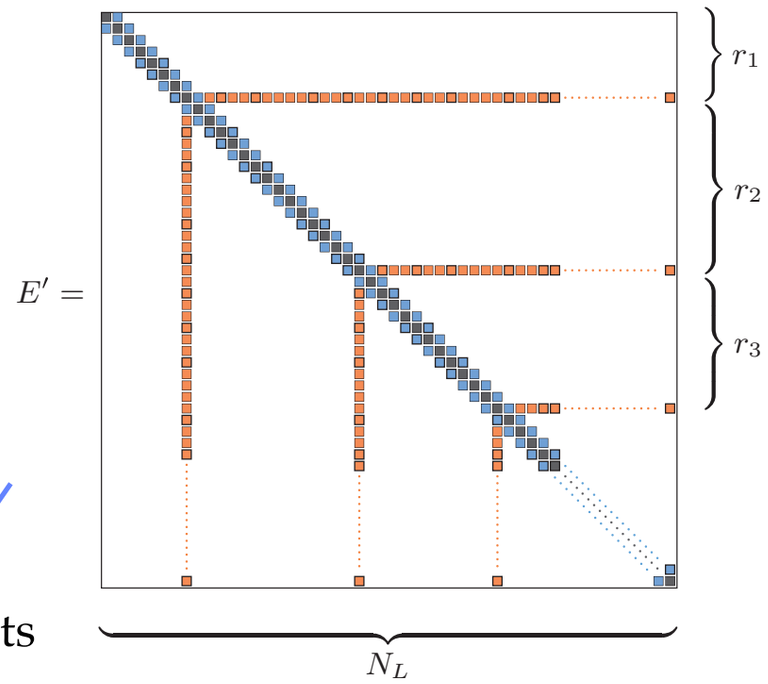
⊙ Possible strategy: use a **multi-pivot** Lanczos algorithm

➠ Consider N_p pivot vectors (typically $N_\text{p} = N_\text{b}$)

$$\{\mathbf{p}^{(i)}; i = 1, \ldots N_p\}$$

➠ Each vector is iterated r_i times

➠ Dimension of projected matrix $\quad N_L = \sum_{i=1}^{N_p} r_i$



Fishbone structure from orthogonalisation of new pivots

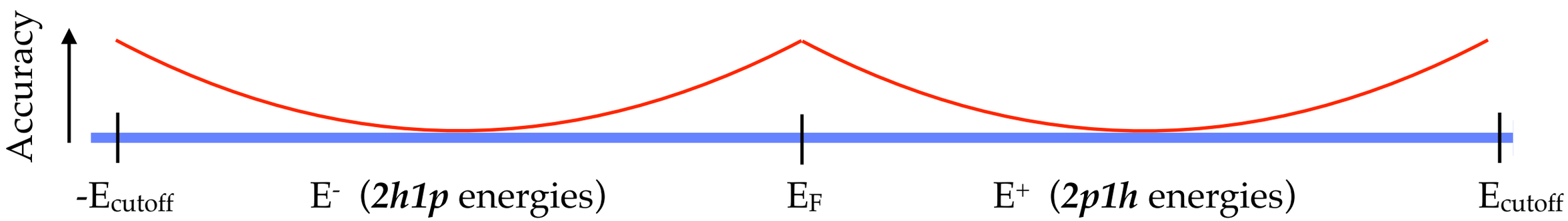
Properties of Krylov projection

- Current implementation different from usual application of Lanczos/Arnoldi
  - ➟ In shell model, CC, … Lanczos algorithm used to extract low-energy eigenvalues
  - ➟ Here we are interested in key/global features of the spectral function

- Krylov projection conserves first moments of the pivots
  - ➟ Choosing components of the spectral function as pivots ensures that its first few moments are approximately conserved

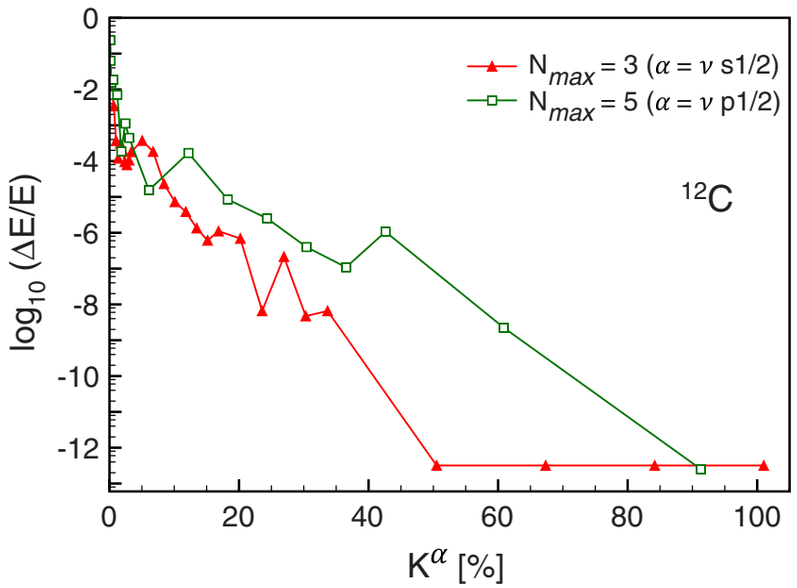
- Lanczos algorithm yields fast convergence at the extremes of the spectrum
  - ➟ Performing separate Lanczos for E^+ and E^- guarantees accuracy around Fermi surface

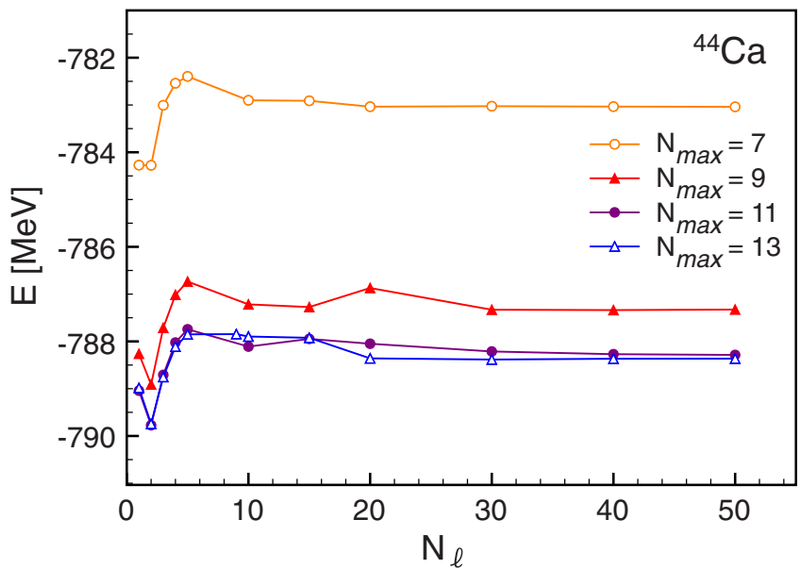
$$\mathcal{E} \longrightarrow \mathcal{E}' = \begin{pmatrix} \mathcal{L}^\dagger E \mathcal{L} & \\ & -\mathcal{L}^\dagger E \mathcal{L} \end{pmatrix}$$



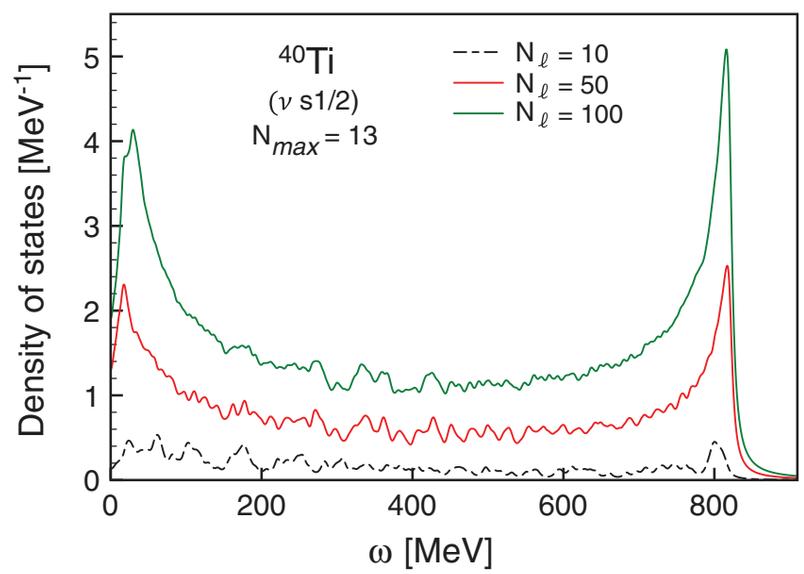
Performance of Krylov projection

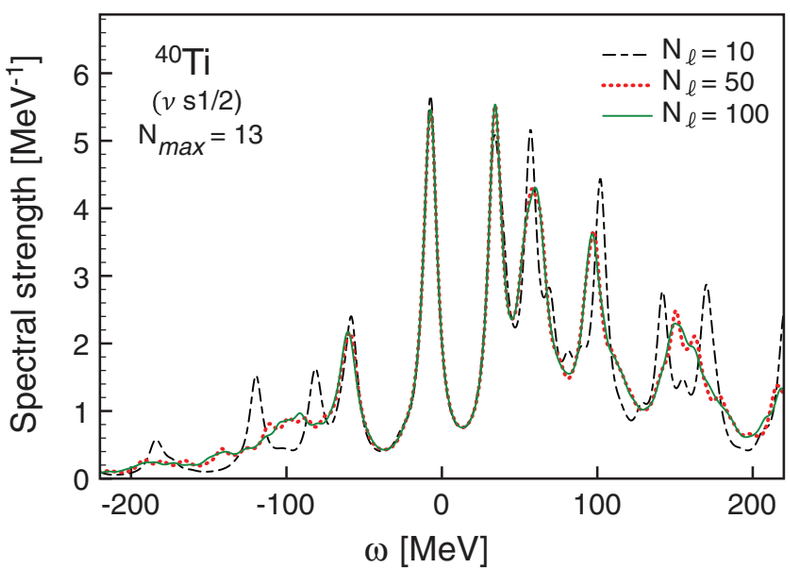
⊙ Krylov-projected energy can be compared with exact result in small model spaces





⊙ Projected **density of states** and **spectral strength distribution**





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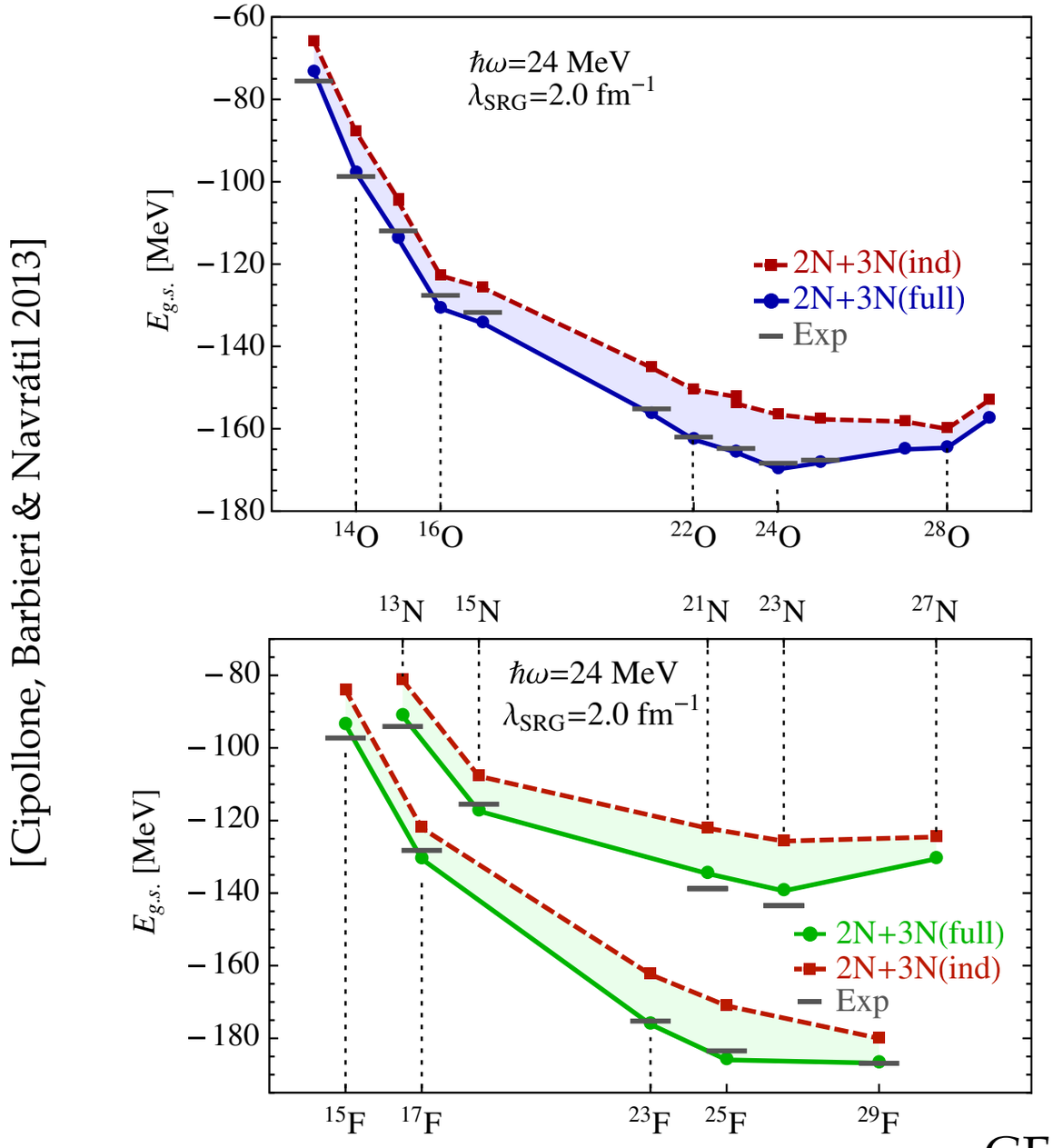
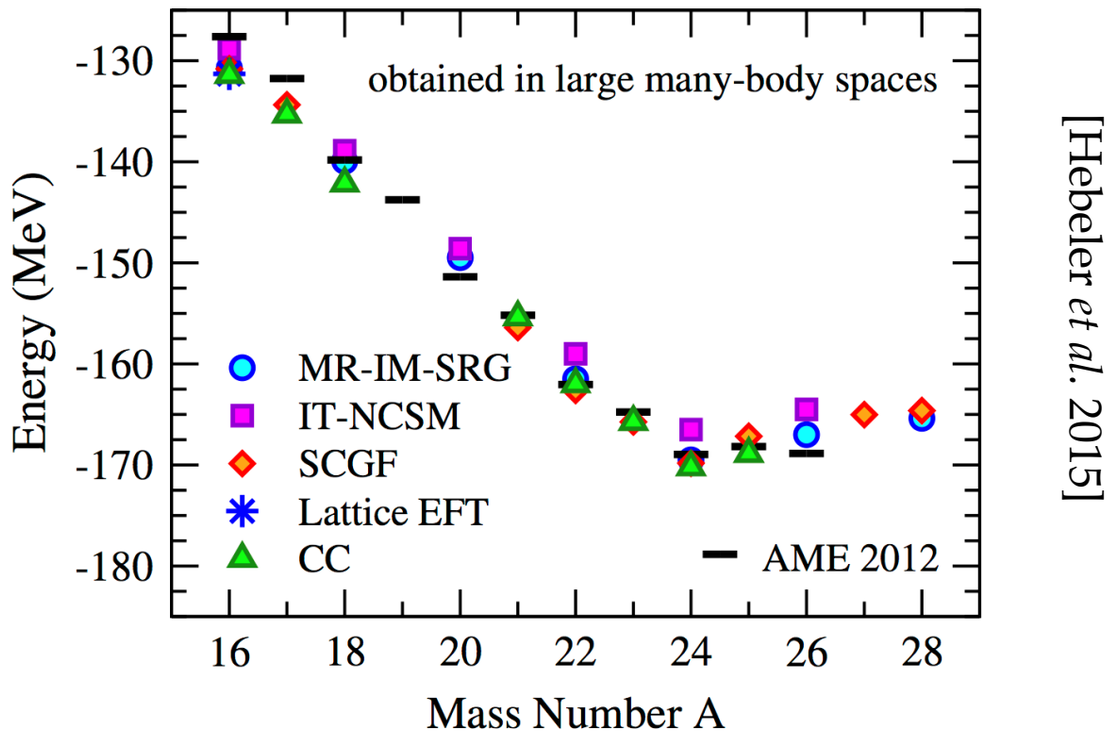
Results: oxygen ground-state energies

- Oxygen chain: importance of **three-body forces** and **benchmark** case for ab initio calculations
  - Hamiltonian: chiral N^3LO 2N (500 MeV) + N^2LO 3N (400 MeV), SRG-evolved to 2.0 fm^{-1}

[Entem & Machleidt 2003; Navrátil 2007; Roth *et al.* 2012]



[Cipollone, Barbieri & Navrátil 2013]



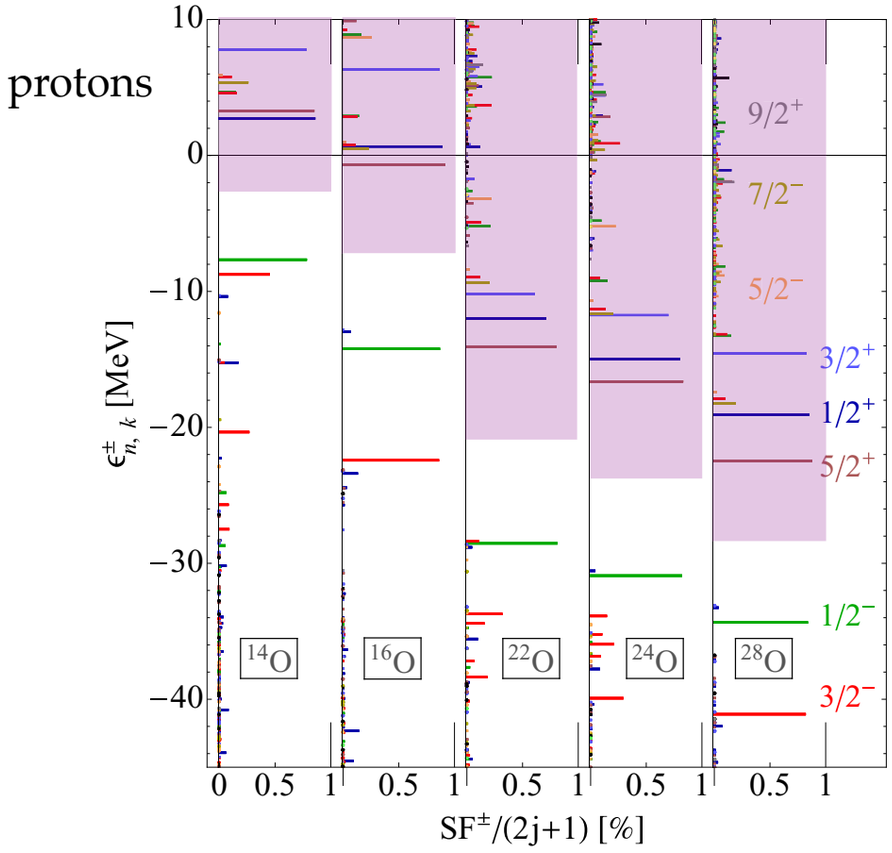
[Hebeler *et al.* 2015]

Different methods yield consistent results

GF access neighbouring F & N chains

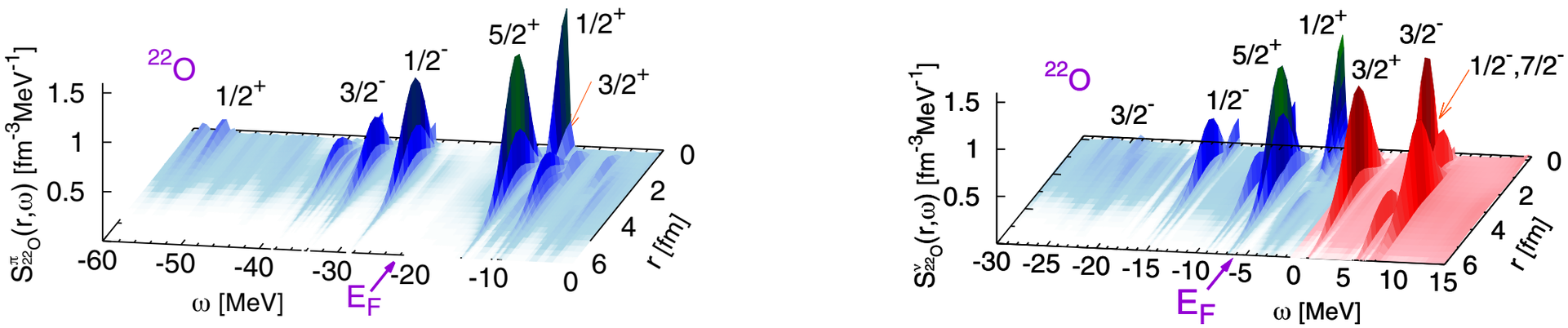
Results: oxygen spectra

⊙ Oxygen chain: spectral strength distribution (**separation energies** and **spectroscopic factors**)



[Cipollone, Barbieri & Navrátil 2015]

⊙ Full spectral function in coordinate space



Plan of the lectures

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5. Three-body forces

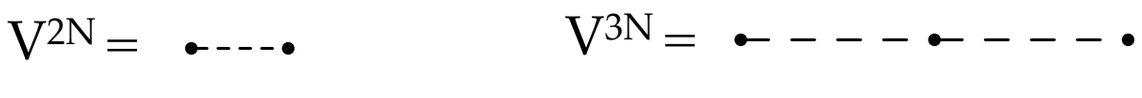
6. Green's functions for open-shell nuclei
   - Degenerate systems and symmetry breaking
   - Gorkov theory
   - Examples of results in open-shell nuclei

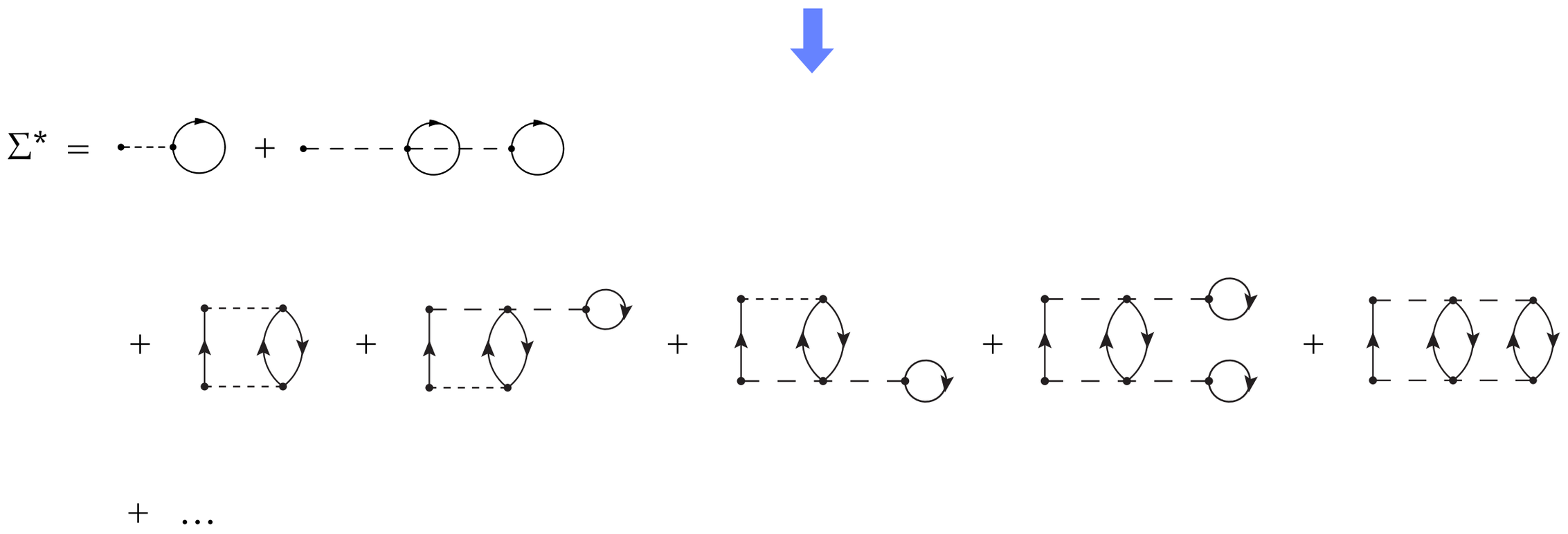
7. Public Green's function code

8. Extras

Three-body forces

- Hamiltonians describing A-nucleon systems contain in principle up to A-body operators
- At least **three-body forces** need to be included in realistic ab initio calculations
- In Green's function theory, one has to re-work out the perturbative expansion of G
- I.e. in the diagrammatic expansion of the self-energy additional terms appear

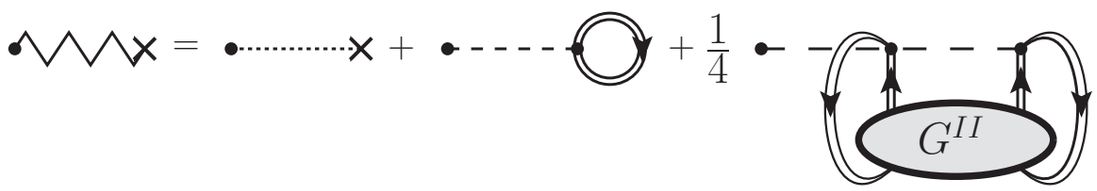




Three-body forces

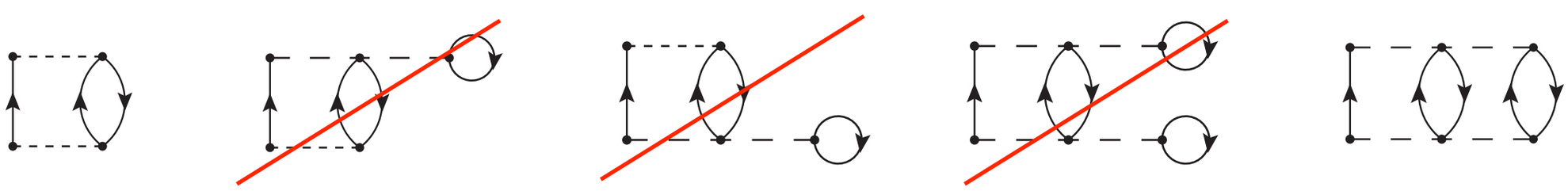
⊙ Diagrammatic expansion can be simplified by exploiting the concept of **effective interactions**

effective 1-body

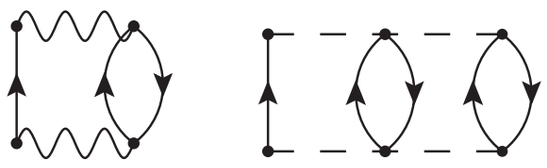


effective 2-body

⊙ One also introduces **interaction-irreducible** diagrams



Combining the two allows to greatly reduce the number of diagrams to be computed

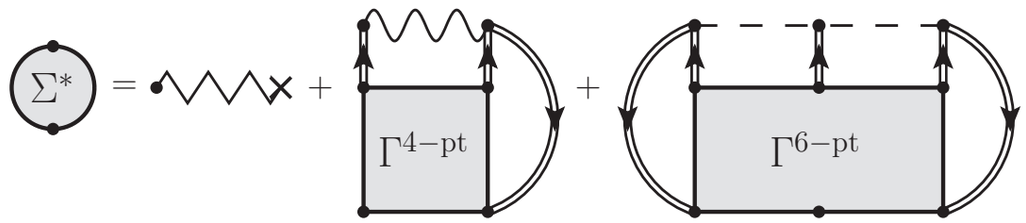


This will generate the first four terms above

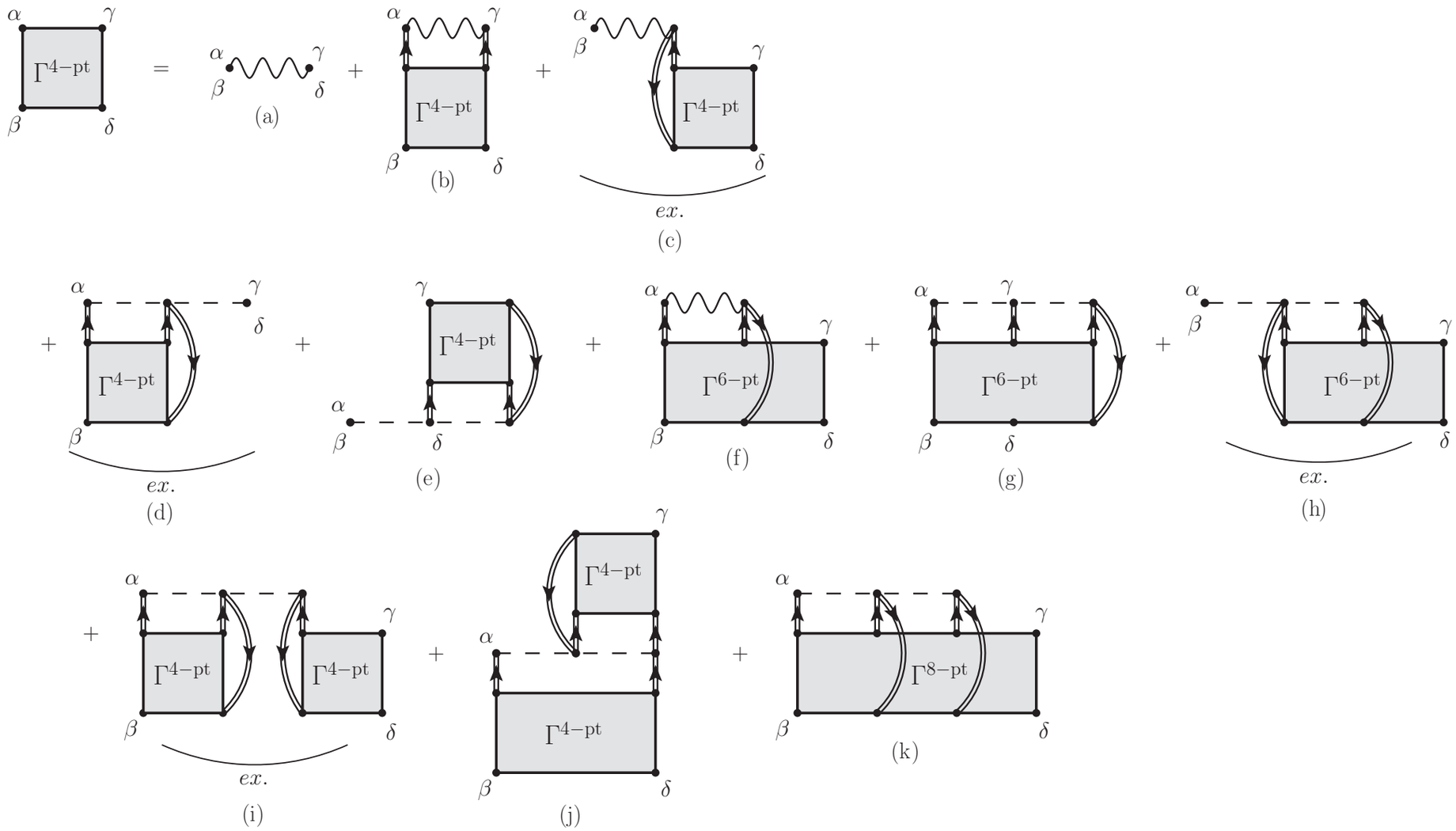
[Carbone, Cipoll
one, Barbieri, Rios, Polls 2013]

Three-body forces

⊙ In general, the irreducible skeleton self-energy is given by



where 4- and 6-point vertices are generated by self-consistent equations



[Carbone, Cipollone, Barbieri, Rios, Polls 2013]

Three-body forces

⊙ Galitskii-Migdal-Koltun sum rule needs to be modified to account for 3N term W

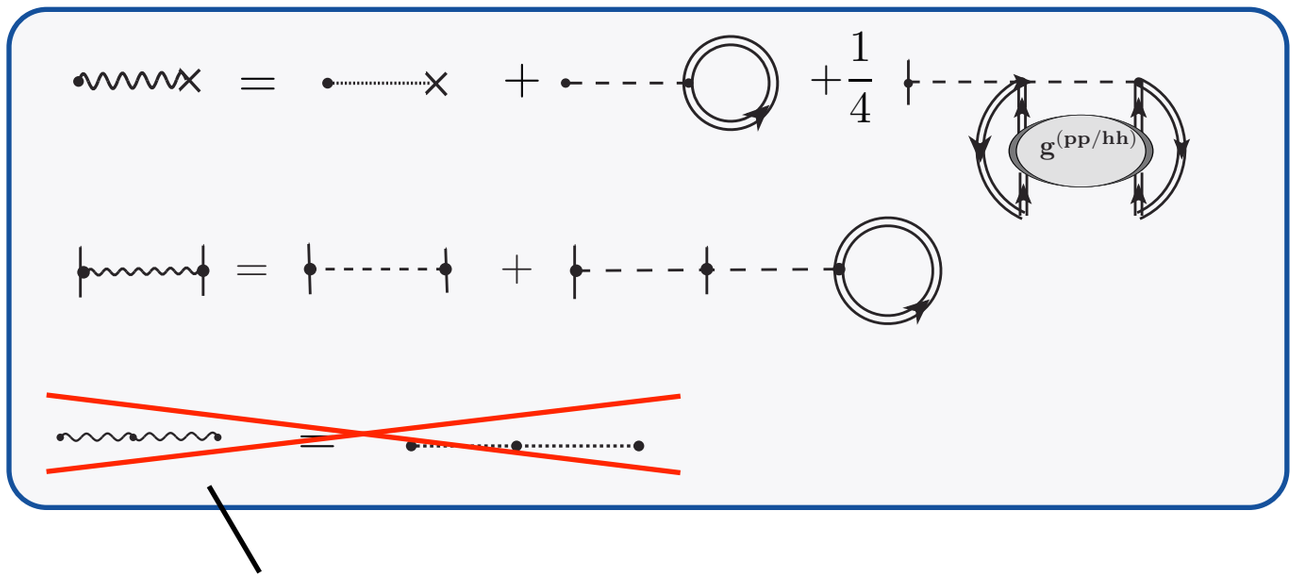
$$E_0^N = \frac{1}{2\pi}\int_{-\infty}^{\bar{\epsilon_F}} d\omega \sum_{\alpha\beta}(T_{\alpha\beta}+\omega\delta_{\alpha\beta})\mathrm{Im}\, G_{\beta\alpha}(\omega) - \frac{1}{2}\left\langle\Psi_0^N\middle|\hat{W}\middle|\Psi_0^N\right\rangle$$

[Carbone, Cipollone, Barbieri, Rios, Polls 2013]

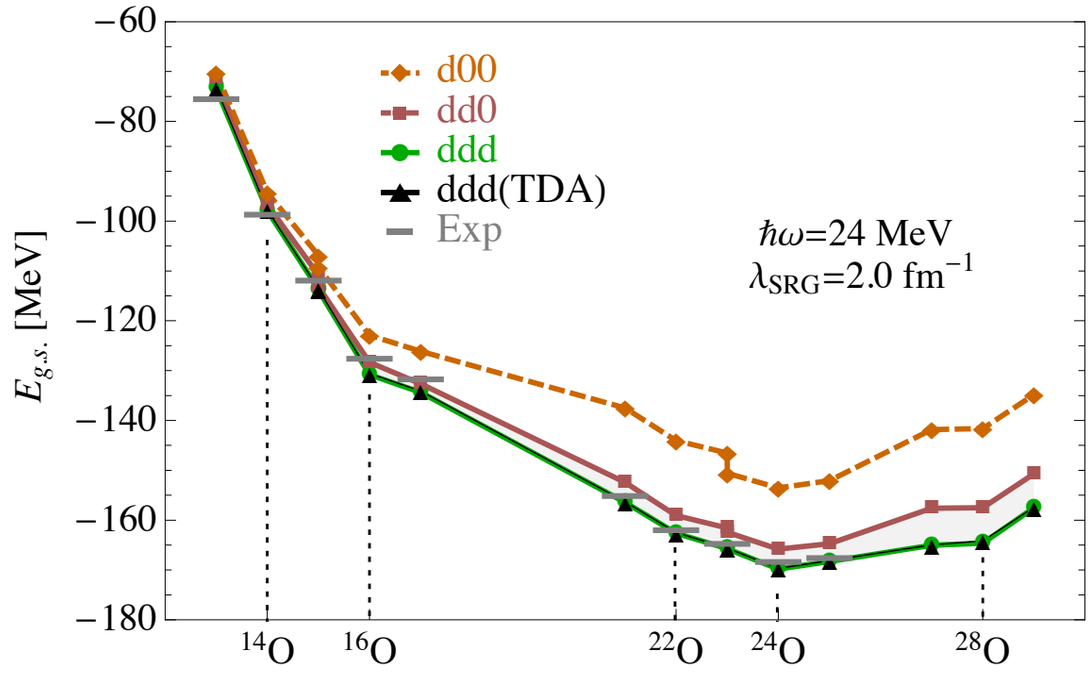
⊙ Effective interactions can be seen as a **generalisation of normal-ordered interactions**

➟ Here contractions are performed with the **fully correlated density matrix**

⊙ Extra correlation provided by the use of dressed propagators can be tested in realistic calculations



Genuine three-body term neglected



[Barbieri *unpublished*]

Plan of the lectures

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6. Green's functions for open-shell nuclei

- **Degenerate systems and symmetry breaking**
- Gorkov theory
- Examples of results in open-shell nuclei

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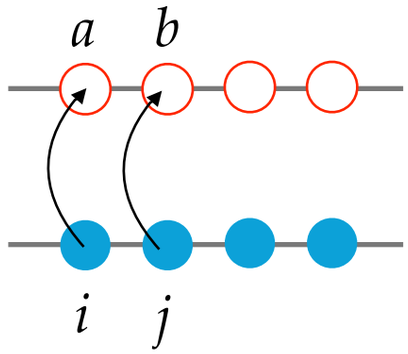
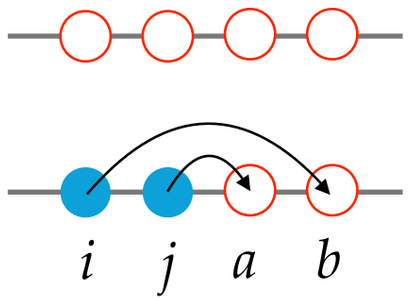
(Near-)degenerate systems

- "Exact" methods grasp all (types of) correlations
  - Hard scaling with A (exponential)
- Approximate/truncated methods grasp some correlations
  - Softer scaling with A (polynomial)
  - Typical way of capturing correlations is via an expansion in **ph excitations**

- Open-shell nuclei are **(near-)degenerate** with respect to ph excitations

closed-shell





open-shell

- E.g. consider MBPT(2) $\Delta E^{(2)} = \frac{1}{4}\sum_{abij}\langle ij|\hat{v}|ab\rangle \frac{\langle ab|\hat{v}|ij\rangle}{\epsilon_i + \epsilon_j - \epsilon_a - \epsilon_b}$

when $\epsilon_i + \epsilon_j = \epsilon_a + \epsilon_b$ the expansion breaks down

Symmetry breaking

- Standard expansion schemes fail when superfluid correlations are essential

- Two possibilities to tackle (near-)degenerate systems:
  - Go to a multi-reference scheme
  - Formulate the expansion around a **symmetry-breaking** reference state
    - ➟ Symmetry-breaking solution allows to **lift the degeneracy**

- Case of open-shell nuclei
  - Singly-open shells (either protons or neutrons)
    - ➟ Breaking of U(1) associated with **particle number** conservation
    - ➟ I.e. work with a Bogoliubov reference state
  - Doubly-open shells (both protons and neutrons)
    - ➟ Breaking of SU(2) associated with **angular momentum** conservation
    - ➟ I.e. work with a deformed Slater determinant

- Symmetries must be eventually restored (see later)

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Gorkov theory

⊙ Idea: expand around an auxiliary many-body state

$$|\Psi_0\rangle \equiv \sum_A^{\text{even}} c_A \, |\psi_0^A\rangle$$

Breaks particle-number symmetry

➟ Introduce a "grand-canonical" potential $\Omega = H - \mu A$

➟ $|\Psi_0\rangle$ minimizes $\Omega_0 = \langle\Psi_0|\Omega|\Psi_0\rangle$ under the constraint $A = \langle\Psi_0|A|\Psi_0\rangle$

➟ Observables of the A-body system $\Omega_0 = \sum_{A'} |c_{A'}|^2 \, \Omega_0^{A'} \approx E_0^A - \mu A$

set of 4 propagators

[Gorkov 1958]

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

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

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

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

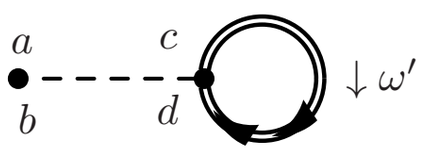
Gorkov equation & self-energy expansion

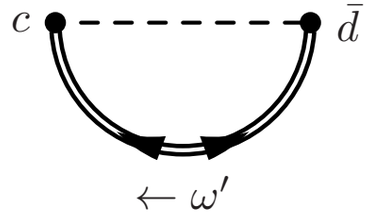
⊙ After perturbation expansion, Wick theorem, definition of self-energy, one gets to

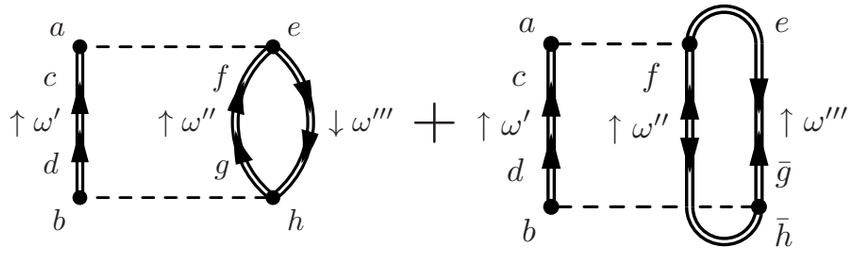
$$\mathbf{G}_{ab}(\omega) = \mathbf{G}^{(0)}_{ab}(\omega) + \sum_{cd} \mathbf{G}^{(0)}_{ac}(\omega)\, \mathbf{\Sigma}^{\star}_{cd}(\omega)\, \mathbf{G}_{db}(\omega) \qquad \text{where} \quad \mathbf{G}(\omega) = \begin{pmatrix} G^{11}(\omega) & G^{12}(\omega) \\ G^{21}(\omega) & G^{22}(\omega) \end{pmatrix}$$

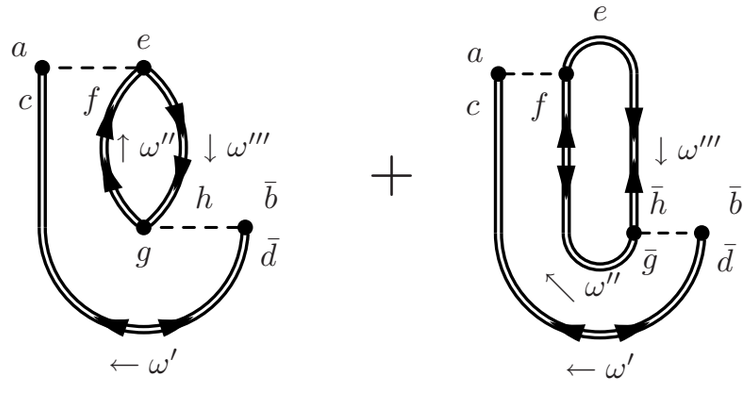
(and similarly for $\mathbf{G^{(0)}}$ and $\mathbf{\Sigma^{*}}$)

⊙ Implemented so far **first**- and **second-order** self-energy diagrams

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

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

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

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

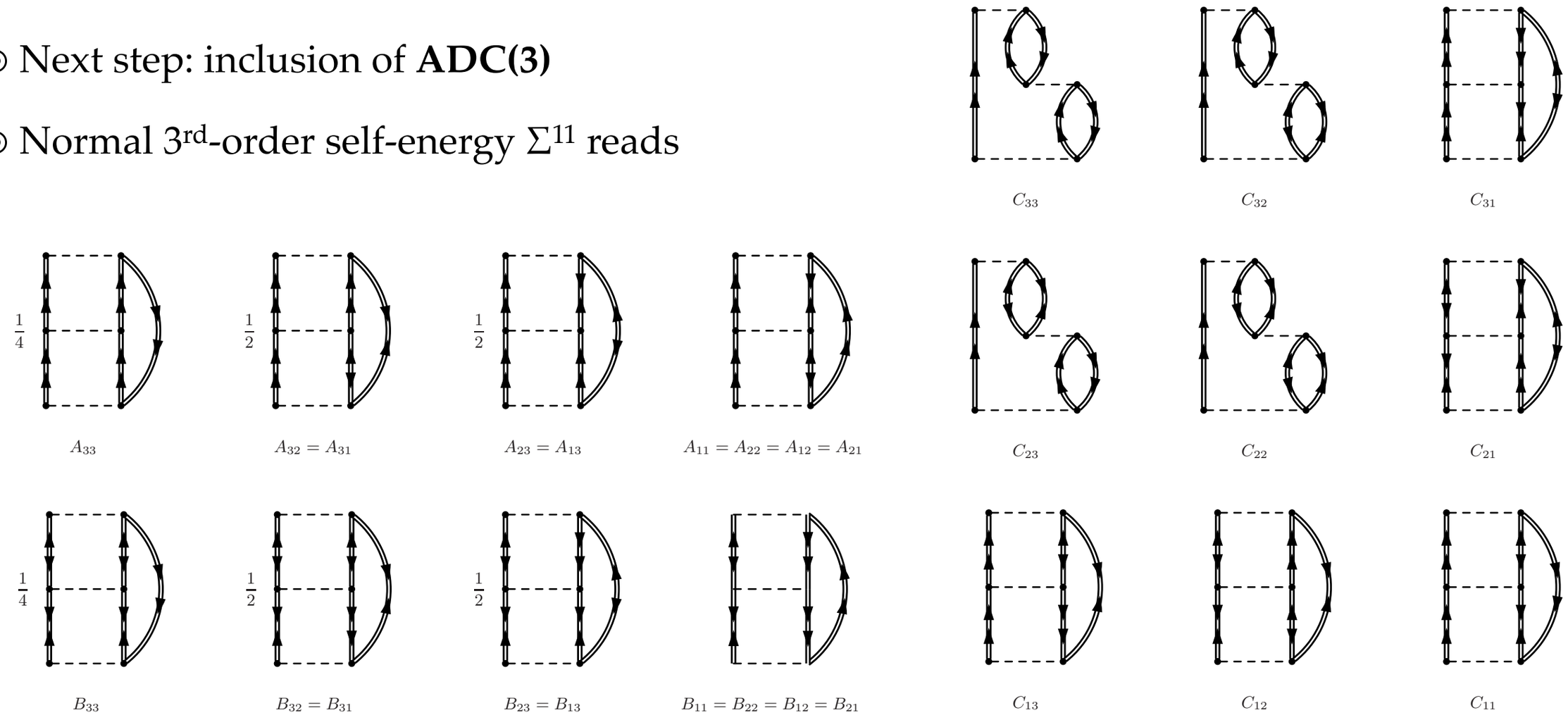
[Somà, Duguet & Barbieri 2011]

➟ Number of **topologically distinct** diagrams increases

➟ Because of symmetry properties, only **2 out of 4** self-energies need to be computed

Gorkov equation & self-energy expansion

- Next step: inclusion of **ADC(3)**
- Normal 3rd-order self-energy Σ^{11} reads



ADC(n)
 # diagrams

n	**1**	**2**	**3**
Dyson	1	1	2
Gorkov	2	4	34

Gorkov equation & self-energy expansion

Gorkov equation

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

where

$$G^{11}_{ab}(\omega) = \sum_k \left\{ \frac{\mathcal{U}^k_a \mathcal{U}^{k*}_b}{\omega - \omega_k + \mathrm{i}\eta} + \frac{\bar{\mathcal{V}}^{k*}_a \bar{\mathcal{V}}^k_b}{\omega + \omega_k - \mathrm{i}\eta} \right\}$$

$$G^{12}_{ab}(\omega) = \sum_k \left\{ \frac{\mathcal{U}^k_a \mathcal{V}^{k*}_b}{\omega - \omega_k + \mathrm{i}\eta} + \frac{\bar{\mathcal{V}}^{k*}_a \bar{\mathcal{U}}^k_b}{\omega + \omega_k - \mathrm{i}\eta} \right\}$$

Energy-*dependent* eigenvalue problem

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

Lehmann representations hold!

using

$$\Sigma^{11\,(2'+2'')}_{ab}(\omega) = \sum_{k_1k_2k_3} \left\{ \frac{\mathcal{C}^{k_1k_2k_3}_a (\mathcal{C}^{k_1k_2k_3}_b)^*}{\omega - E_{k_1k_2k_3} + i\eta} + \frac{(\bar{\mathcal{D}}^{k_1k_2k_3}_a)^* \bar{\mathcal{D}}^{k_1k_2k_3}_b}{\omega + E_{k_1k_2k_3} - i\eta} \right\}$$

$$\Sigma^{12\,(2'+2'')}_{ab}(\omega) = \sum_{k_1k_2k_3} \left\{ \frac{\mathcal{C}^{k_1k_2k_3}_a (\mathcal{D}^{k_1k_2k_3}_b)^*}{\omega - E_{k_1k_2k_3} + i\eta} + \frac{(\bar{\mathcal{D}}^{k_1k_2k_3}_a)^* \bar{\mathcal{C}}^{k_1k_2k_3}_b}{\omega + E_{k_1k_2k_3} - i\eta} \right\}$$

Energy-*independent* eigenvalue problem

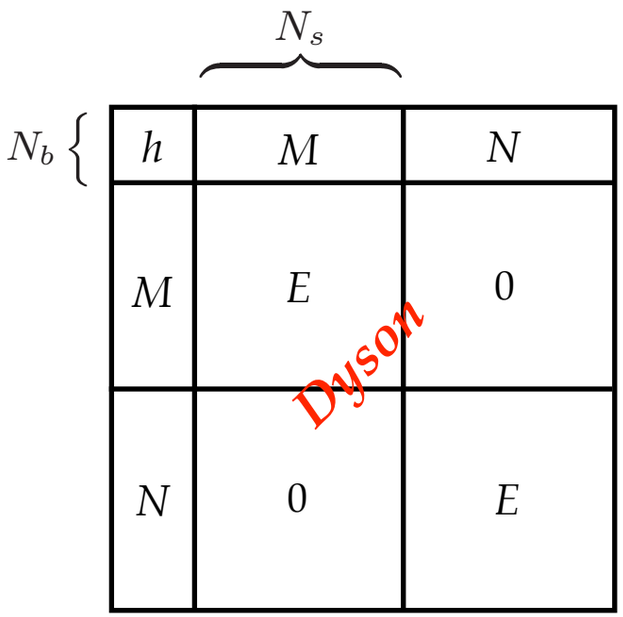
$$\begin{pmatrix} T - \mu + \Lambda & \tilde{h} & \mathcal{C} & -\mathcal{D}^\dagger \\ \tilde{h}^\dagger & -T + \mu - \Lambda & -\mathcal{D}^\dagger & \mathcal{C} \\ \mathcal{C}^\dagger & -\mathcal{D} & E & 0 \\ -\mathcal{D} & \mathcal{C}^\dagger & 0 & -E \end{pmatrix} \begin{pmatrix} \mathcal{U}^k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

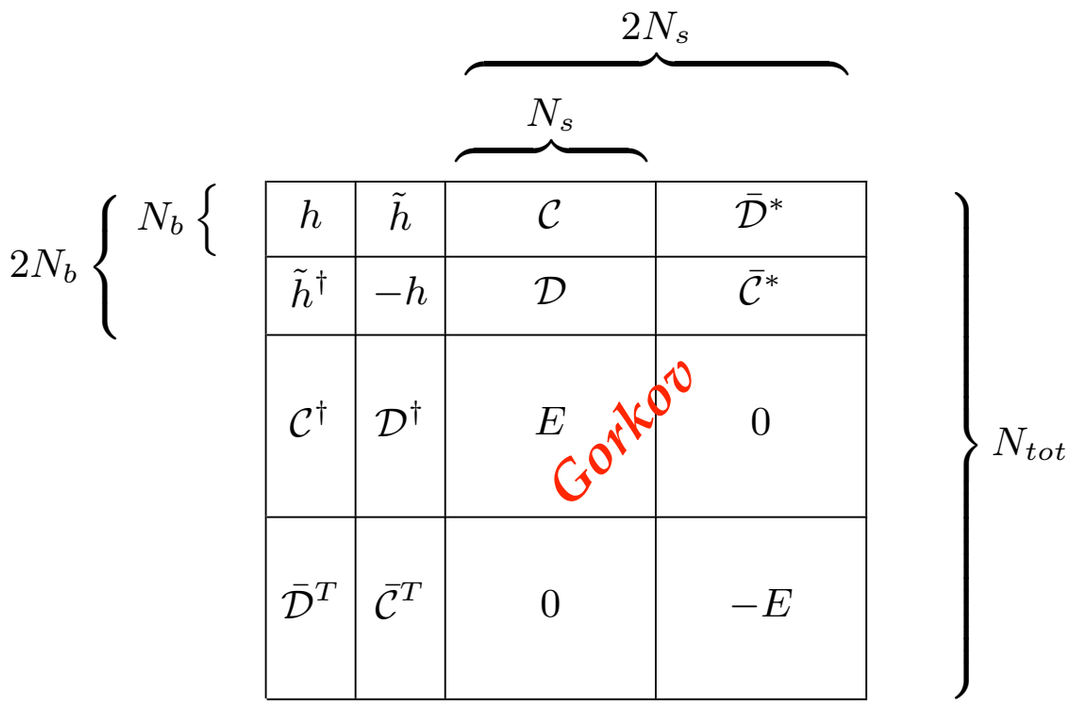
From **2p-1h** & **2h-1p** to **3qp**

➟ Many more possibilities

Dyson vs Gorkov dimensions

- In Gorkov theory, no distinction between "particles" and "holes"
  - ➟ Dimension of Gorkov matrix larger than in Dyson case





$$N_b = N_h + N_p$$

$$N_s^N = N_h^2\, N_p$$
$$N_s^M = N_p^2\, N_h$$
$$\Rightarrow \quad N_s^{\text{tot}} = N_h^2\, N_p + N_p^2\, N_h$$

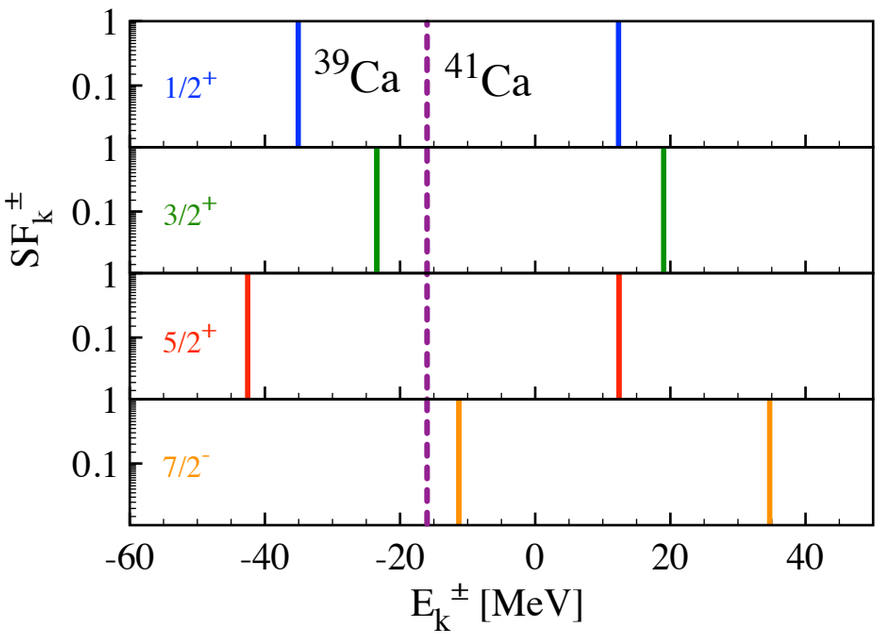
$$2N_b = 2(N_h + N_p)$$

$$N_s^{\text{tot}} = 2(N_h + N_p)^3$$

- Both computation of the matrix itself and Krylov projection numerically more costly
  - ➟ Generalised Lanczos algorithm can be developed → small Krylov spaces work fine

Spectral strength distribution: Dyson vs Gorkov

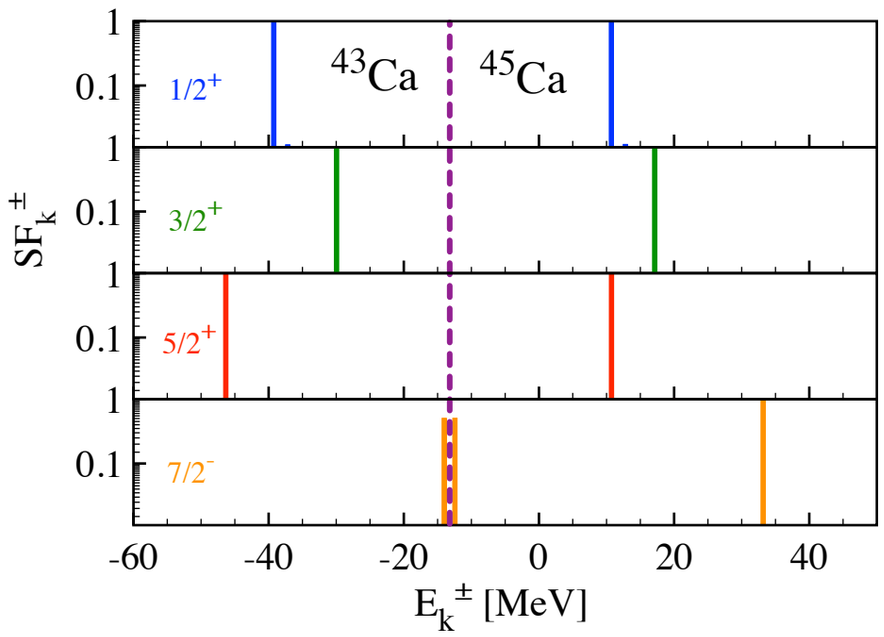
Dyson 1st order (HF)



Fragmentation

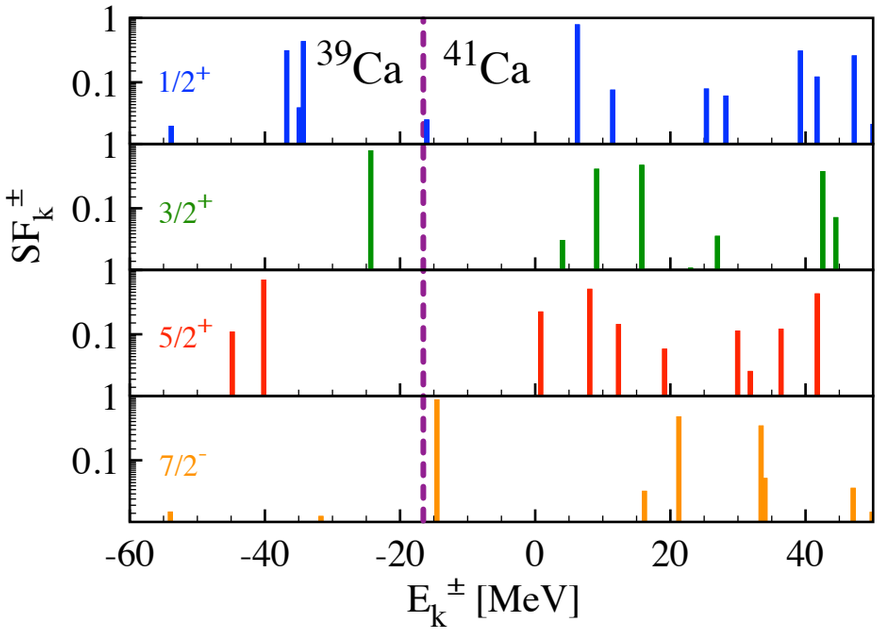
Static pairing

Gorkov 1st order (HFB)

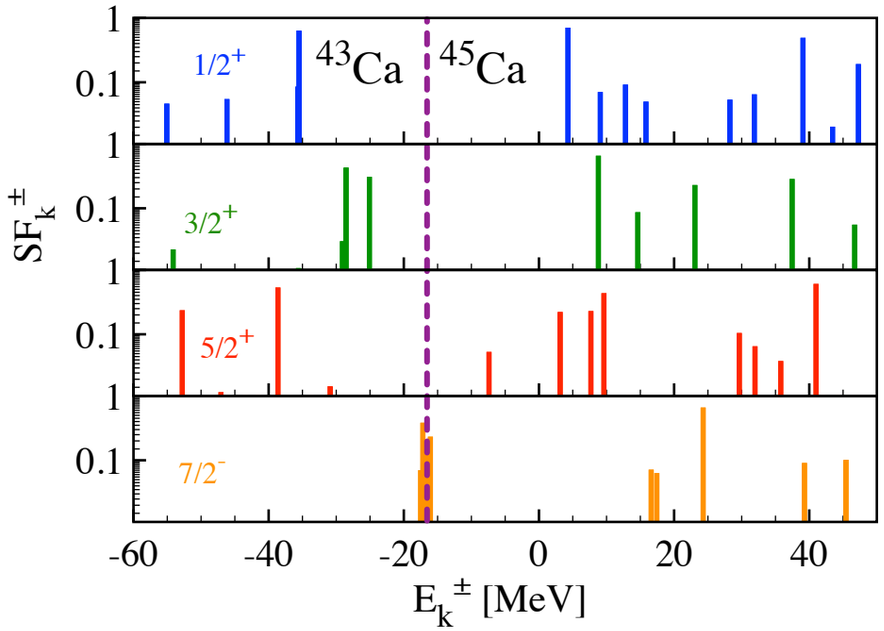


Dynamical fluctuations

Dyson 2nd order



Gorkov 2nd order



Plan of the lectures

5. Three-body forces

6. Green's functions for open-shell nuclei

- Degenerate systems and symmetry breaking
- Gorkov theory
- **Examples of results in open-shell nuclei**

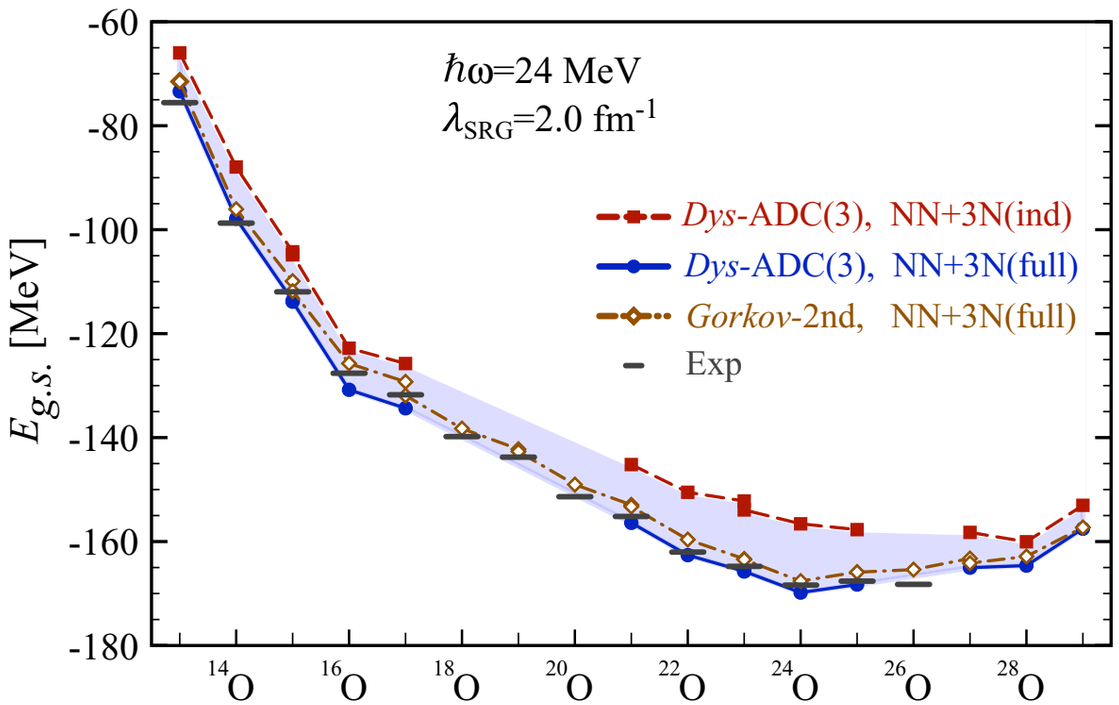
7. Public Green's function code

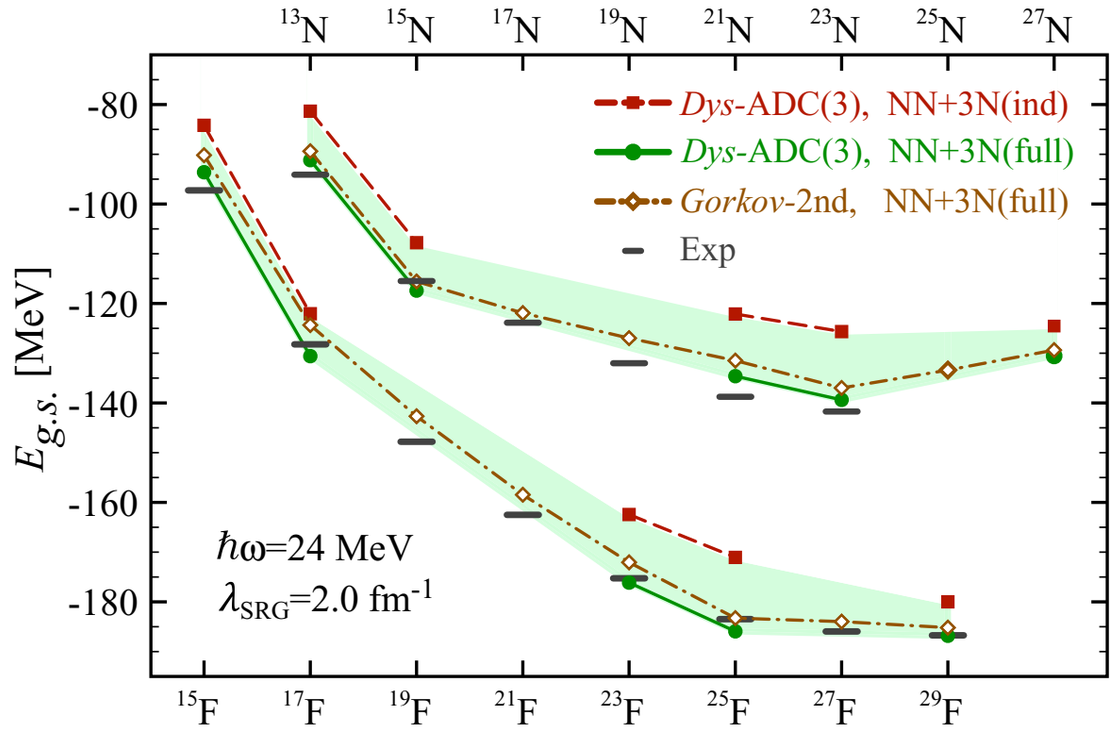
8. Extras

Oxygen g.s. energies

- Calculation of **full isotopic chains** becomes possible
- Example of oxygen: **Dyson-ADC(3) vs Gorkov-ADC(2)**
  - Hamiltonian: chiral N^{3}LO 2N (500 MeV) + N^{2}LO 3N (400 MeV), SRG-evolved to 2.0 fm^{-1}

[Entem & Machleidt 2003; Navrátil 2007; Roth *et al*. 2012]





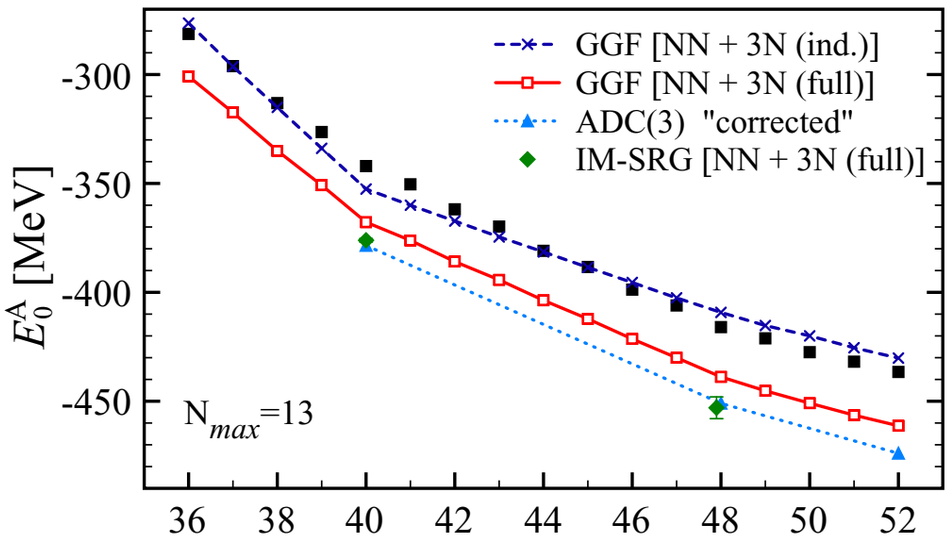
[Cipollone, Barbieri & Navrátil 2015]

➠ Correlation energy from 3rd order amount to a few percent (for soft interactions)

➠ Trend (i.e. energy differences) well captured at second order

Up to the calcium region

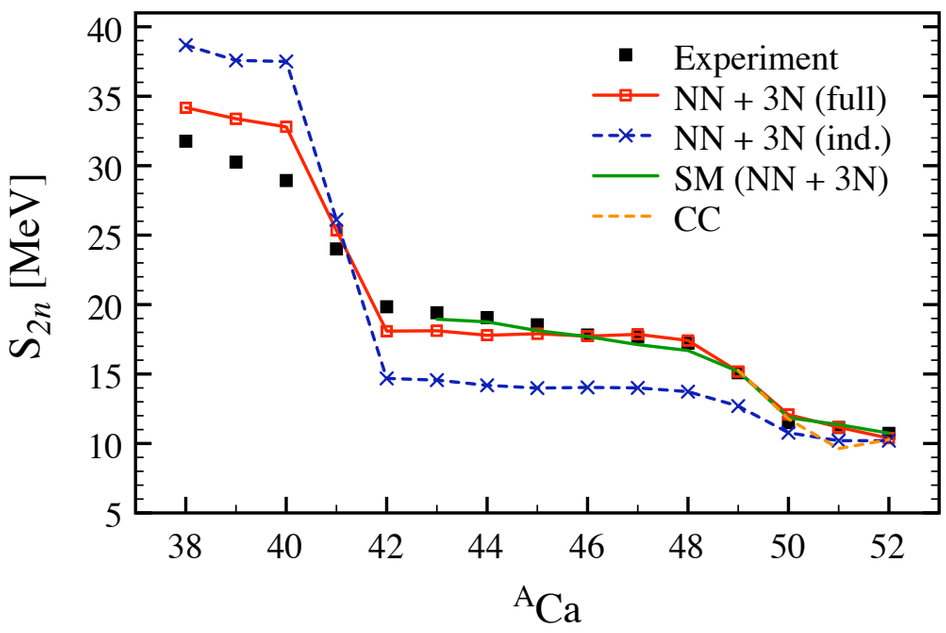
⊙ Gorkov GF led to the first ab initio calculations of **isotopic chains around Z=20**

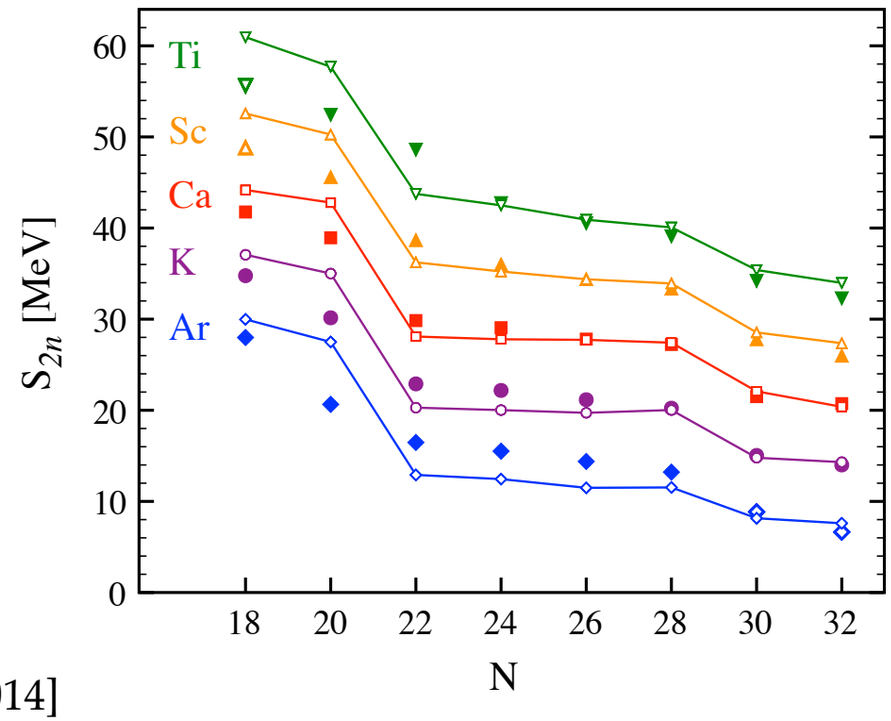


- 3NF overbind but correct overall trend
- Two-neutron separation energies reproduced

$$S_{2n} \equiv E_0^{Z,N} - E_0^{Z,N-2}$$

- **3NF necessary for magic gaps**
- Consistent picture across 5 chains



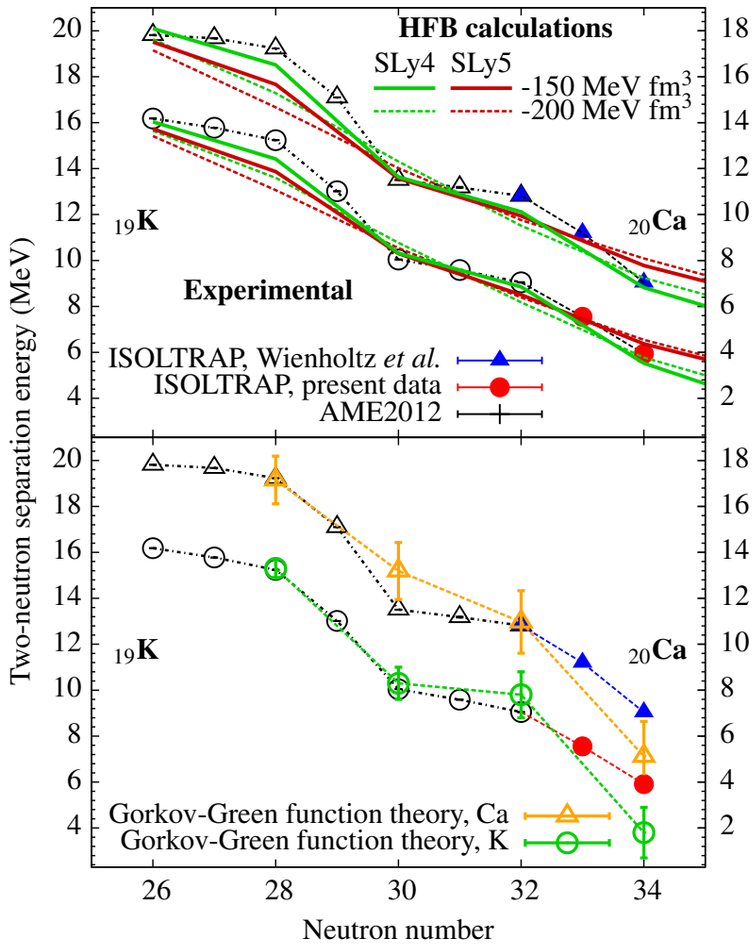


[Somà *et al.* 2014]

Potassium masses and g.s. (re)inversion

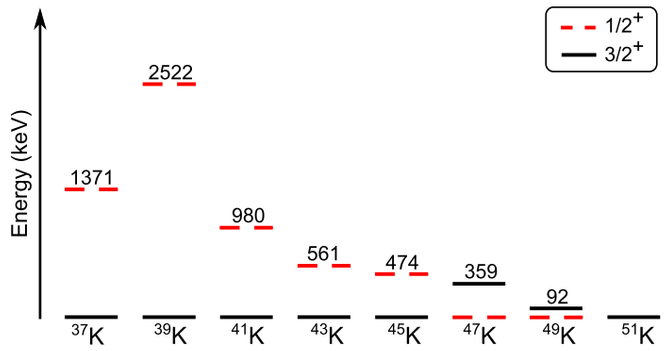
⊙ Gorkov-Green's functions can tackle **odd Z** chains

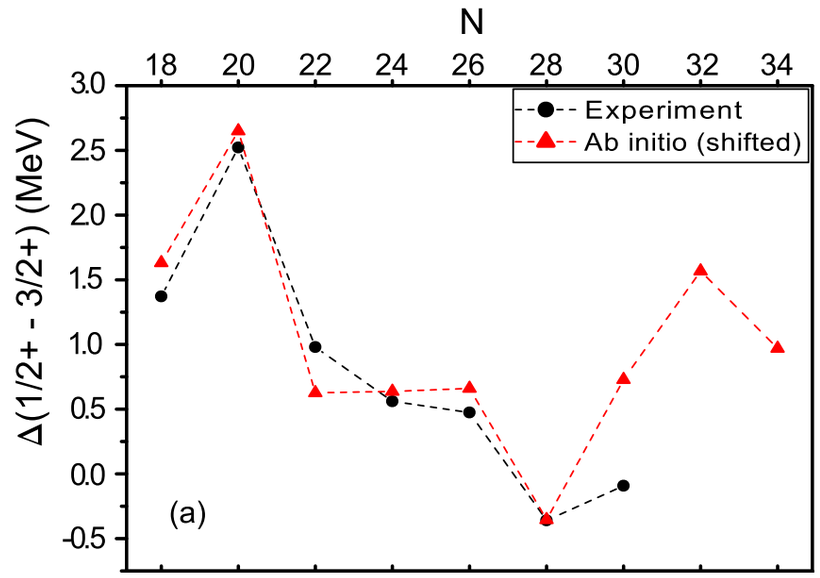
ISOLTRAP



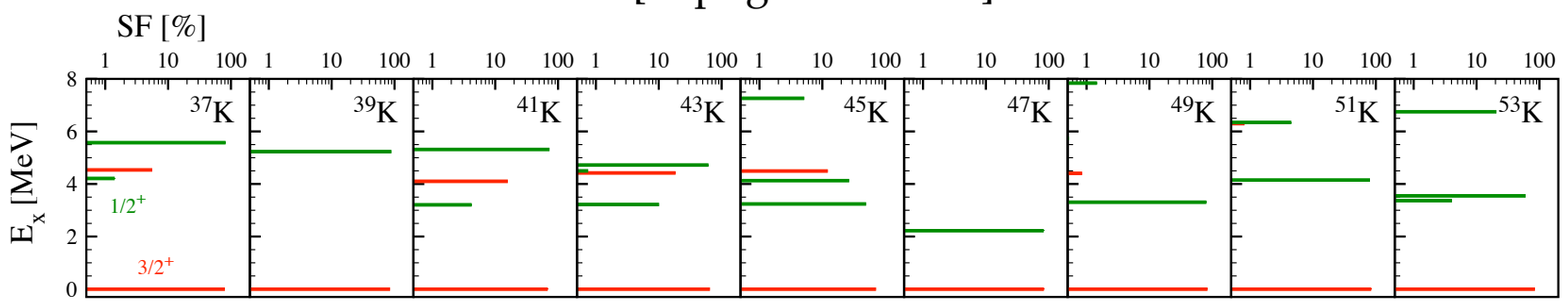
[Rosenbusch *et al.* 2015]

COLLAPS





[Papuga *et al.* 2014]



➟ Relative trend well reproduced

➟ New mass measurements challenge theory

➟ General fair agreement, but N=32 gap overestimated

Oxygen & calcium radii

⊙ Ab initio calculations over mid-mass chains as test tools to develop new Hamiltonians

⊙ Example: two sets of 2N+3N chiral interactions

➟ Conventional* N^3LO 2N (500 MeV) + N^2LO 3N (400 MeV) [**EM**]

[Entem & Machleidt 2003; Navrátil 2007; Roth *et al*. 2012]

➟ Unconventional* N^2LO 2N+3N (450 MeV) [**$NNLO_{sat}$**]

[Ekström *et al*. 2015]

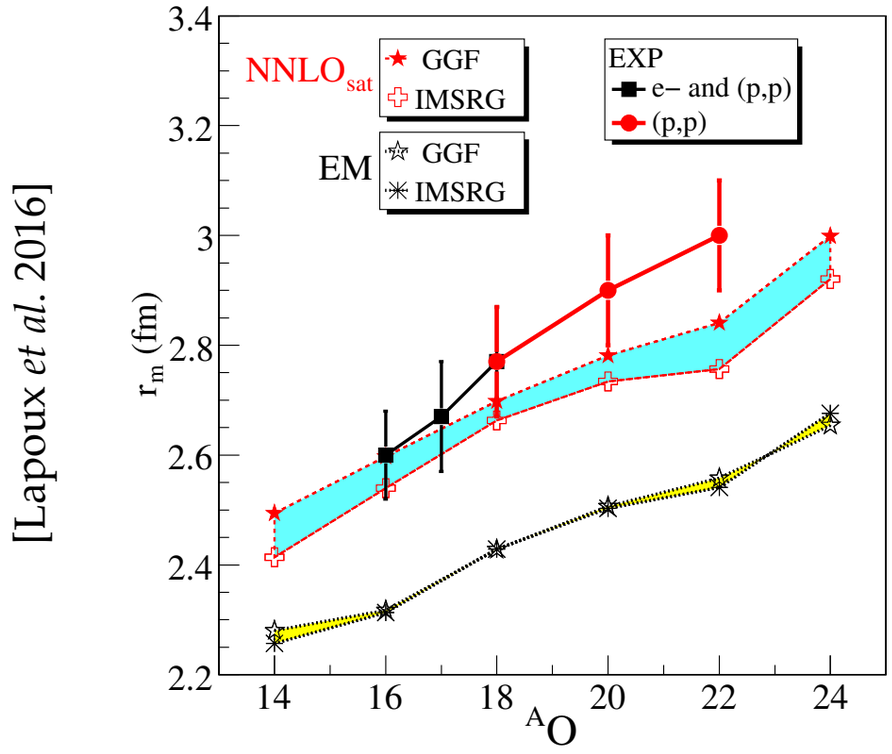
○ LECs fitted on $A \leq 25$

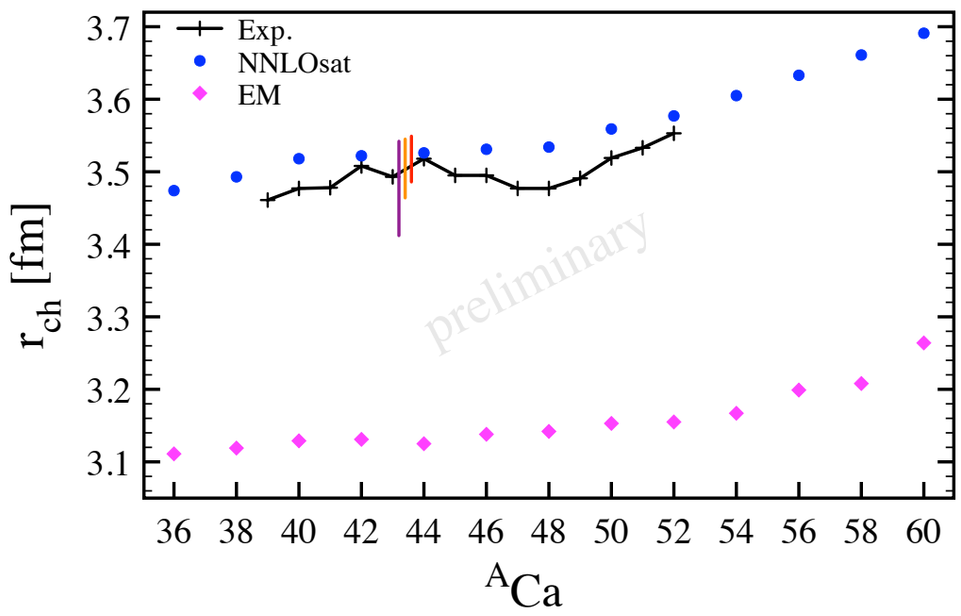
○ **Simultaneous** optimisation

○ **Non-local** 3NF regulator

** With respect to the usual reductionist strategy of ab initio calculations*

⊙ $NNLO_{sat}$ considerably improves on the description of nuclear radii

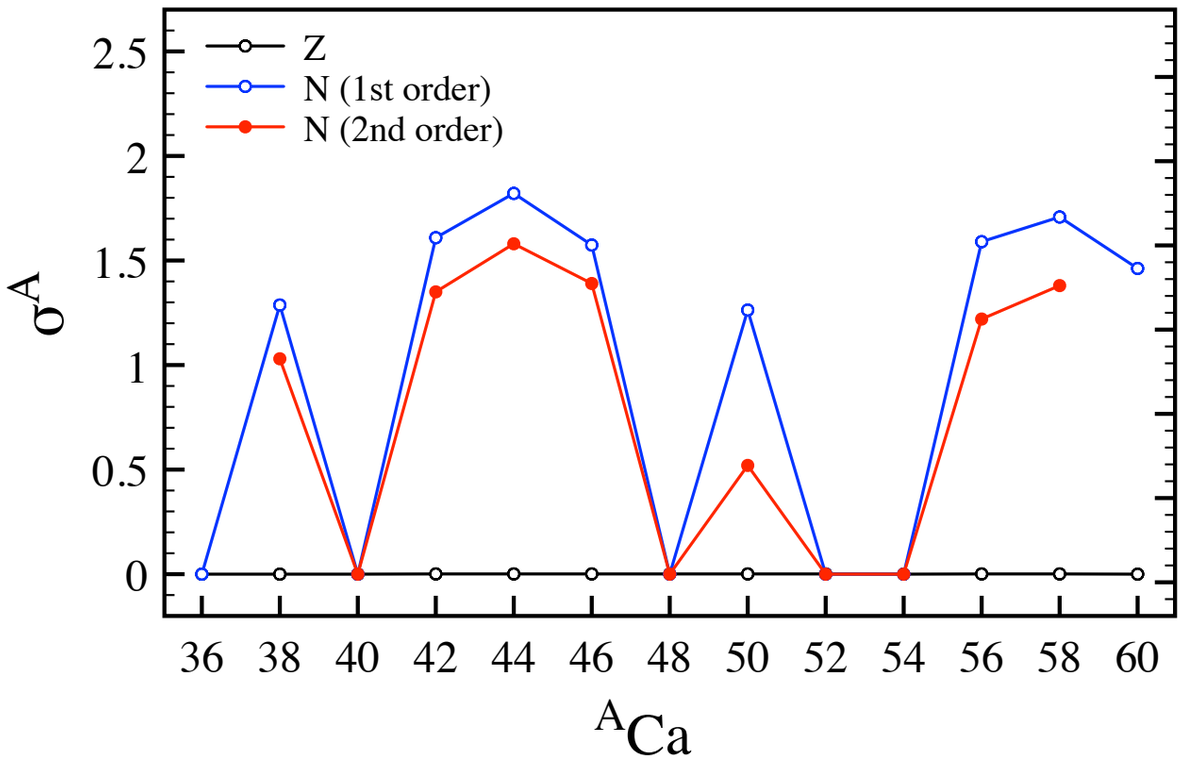




[Somà *et al*. in preparation]

Symmetry breaking and restoration

⊙ Variance in particle number as an indicator of symmetry breaking



$$\sigma_A = \sqrt{\langle \hat{A}^2 \rangle - \langle \hat{A} \rangle^2}$$

➟ Only concerns neutron number

➟ Decreases as many-body order increases

⊙ Eventually, symmetries need to be restored

⊙ Only recently the formalism was developed for MBPT and CC

- ○ Case of **SU(2)** [Duguet 2014]
- ○ Case of **U(1)** [Duguet & Signoracci 2016]

⊙ Symmetry-restored Gorkov GF formalism still to be developed

Plan of the lectures

5. Three-body forces

6. Green's functions for open-shell nuclei
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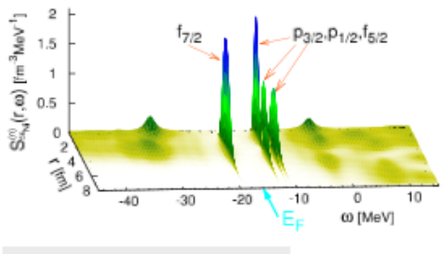
8. Extras

BoccaDorata code

- A public version of a GF code implemented for finite nuclei is **publicly available** at

  http://personal.ph.surrey.ac.uk/~cb0023/bcdor/bcdor/Comp_Many-Body_Phys.html

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 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 the coupled cluster CCD (doubles only!) equations for the correlation energy.

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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Last updated: Monday 27nd July, 2015

BoccaDorata code

✓ The name **Bocca Dorata** comes from a Brazilian priestess in the comic series *Corto Maltese* by Hugo Pratt

- Self-consistent Green's function code for finite systems
- Public version of the code includes **up to 2nd-order** self-energy and handles **two-body interactions**
- **Bonus** (also in the public version):
  - MBPT(2)
  - Coupled-cluster doubles
- **Extensions** (non-public):
  - ADC(3) (and more, in fact) self-energy
  - Treatment of three-body interactions
  - Gorkov scheme (for open-shells)

✓ Main developer: C. Barbieri (Surrey)

✓ Other developers:

A. Cipollone (Surrey/Bologna)
V. Somà (Saclay)

Data types

- BoccaDorata builds on 4 main data types (C++ classes)

1. **Model space**
   - Defines the set of (HO) basis states that enter the calculation
   - Serves as reference for other data types
   - Can be generated within the code or read from file

2. **One-body propagator**
   - Central object on which most operation are performed
   - Can be generated within the code or read from file

3. **Self-energy**
   - Mainly used to build Dyson matrix (final eigenvalue problem)
   - Can be generated within the code or read from file

4. **(Two-body) interaction**
   - Needs to be generated externally (but can be manipulated in BoccaDorata)

General structure

- Needed objects are loaded/initialised
- (If it's a 2nd-order calculation) dimensions of self-energy/propagator arrays are estimated
- Iterations start
  - ➟ Loop over partial waves starts
    - ➟ HF self-energy is computed
    - ➟ Kinetic energy is added
    - ➟ (If it's a 2nd-order calculation) dynamic self-energy is computed/read from file
    - ➟ (If it's a 2nd-order calculation) Lanczos algorithm is run
    - ➟ Dyson matrix is built and diagonalised
    - ➟ Partial wave contributions to N, Z and E are computed
  - ➟ Loop over partial waves ends
  - ➟ Old G is erased, new G will be input for the next iteration
- Iterations end
- Final results are written to screen/file

Single-particle propagator

- This is how a one-body propagator looks like

$$G_{ab}(z) = \sum_{\mu} \frac{U_a^{\mu}(U_b^{\mu})^*}{z - E_{\mu}^{+} + i\eta} + \sum_{\nu} \frac{(V_a^{\nu})^* V_b^{\nu}}{z - E_{\nu}^{-} - i\eta}$$

E_{μ}^{+} U_a^{μ} E_{ν}^{-} V_a^{ν}

```
#  Quasi- particle and hole fragments of the sp propagator
#-------------------------------------------------------

# number of (ilj\pi) subshells, max n. of radial orbitals:
#      30       4       0

# Total numbers of qp and qh stored here:
#      66       6

# Subshell:
# v_s1/2
#       3  # -> tot n. of quasiparticles
       45.300293       100.000      -3.779214e-03      -1.081792e-01       4.159454e-01       9.029243e-01
       16.812094       100.000       1.102827e-01      -2.187659e-01      -8.901109e-01       3.842940e-01
        0.324998       100.000      -2.221997e-01       9.395954e-01      -1.753774e-01       1.924329e-01
#       1  # -> tot n. of quasiholes
      -55.090909       100.000      -9.687367e-01      -2.399983e-01      -6.272807e-02      -3.912206e-03

# Subshell:
# v_p1/2
#       3  # -> tot n. of quasiparticles
       60.401165       100.000      -7.885525e-02      -1.627880e-02       5.268234e-01       8.461524e-01
       27.506481       100.000      -1.638212e-01       5.133379e-01       7.126959e-01      -4.491230e-01
        7.710524       100.000       1.200694e-01      -8.372168e-01       4.506958e-01      -2.855253e-01
#       1  # -> tot n. of quasiholes
      -16.294481       100.000       9.759753e-01       1.878491e-01       1.067473e-01       2.810576e-02

# Subshell:
# v_p3/2
#       3  # -> tot n. of quasiparticles
       56.750438       100.000      -6.220491e-02      -5.608834e-02       4.954804e-01       8.645714e-01
       25.320437       100.000      -1.987774e-01       4.398073e-01       7.659408e-01      -4.247255e-01
        6.715028       100.000       2.021342e-01      -8.552241e-01       3.952311e-01      -2.674431e-01
#       1  # -> tot n. of quasiholes
      -26.046202       100.000       9.569534e-01       2.683567e-01       1.078248e-01       2.446737e-02

# Subshell:
# v_d3/2
#       3  # -> tot n. of quasiparticles
       50.931715       100.000      -3.039998e-02       4.831755e-01       8.749956e-01
       21.326080       100.000       3.975944e-01       8.090090e-01      -4.329239e-01
        7.058846       100.000       9.170576e-01      -3.347324e-01       2.167017e-01
#       0  # -> tot n. of quasiholes
```

Plan of the lectures

5. Three-body forces

6. Green's functions for open-shell nuclei
   - Degenerate systems and symmetry breaking
   - Gorkov theory
   - Examples of results in open-shell nuclei

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8. Extras

Literature

- **Books**
  - Dickhoff & Van Neck, ***Many-body theory exposed!*** (World Scientific, Singapore, 2007)
  - Fetter & Walecka, ***Quantum theory for many-particle physics*** (McGraw-Hill, New York, 1971)
  - Abrikosov, Gorkov & Dzyaloshinski, ***Methods of quantum field theory in statistical physics*** (Dover, New York, 1975)
  - Mattuck, ***A guide to Feynman diagrams in the many-body problem*** (Dover, New York, 1992)
  - Economou, ***Green's functions in quantum physics*** (Springer, Berlin, 2006)
  - Blaizot & Ripka, ***Quantum theory of finite systems*** (MIT press, Cambridge MA, 1986)
  - Negele & Orland, ***Quantum many-particle systems*** (Benjamin, Redwood City, 1988)

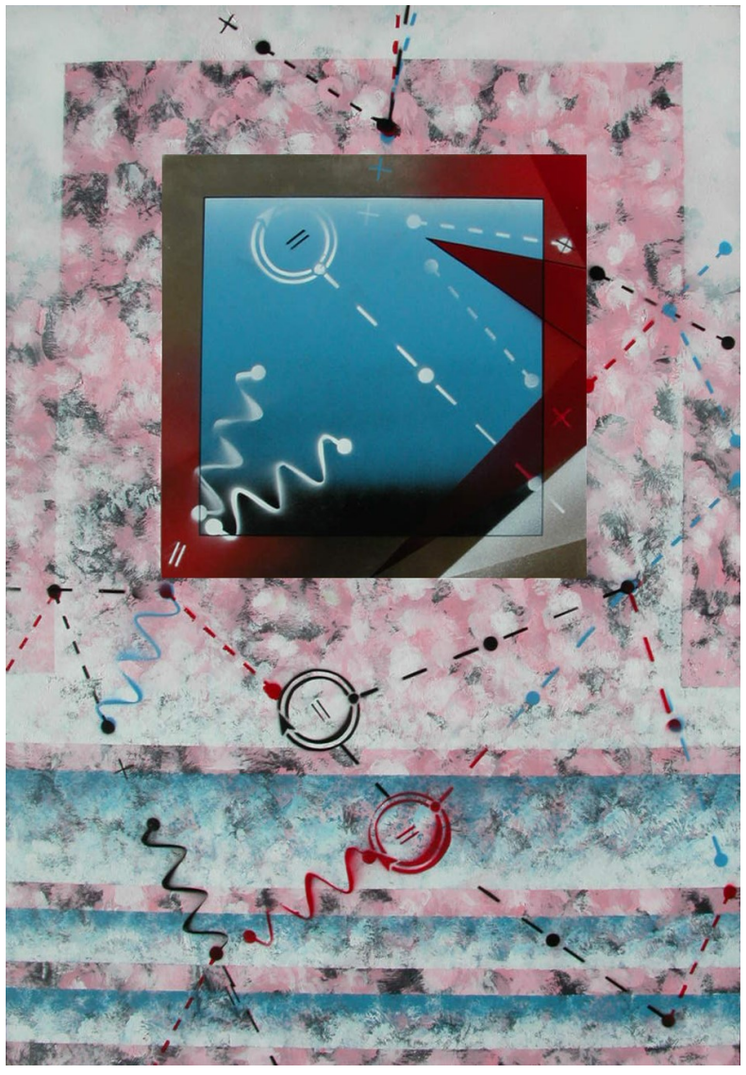
Literature

- **Recent review articles**
  - Onida, Reining & Rubio, *Rev. Mod. Phys.* **74**, 601 (2002)
  - Dickhoff & Barbieri, *Prog. Part. Nucl. Phys.* **52**, 377 (2004)

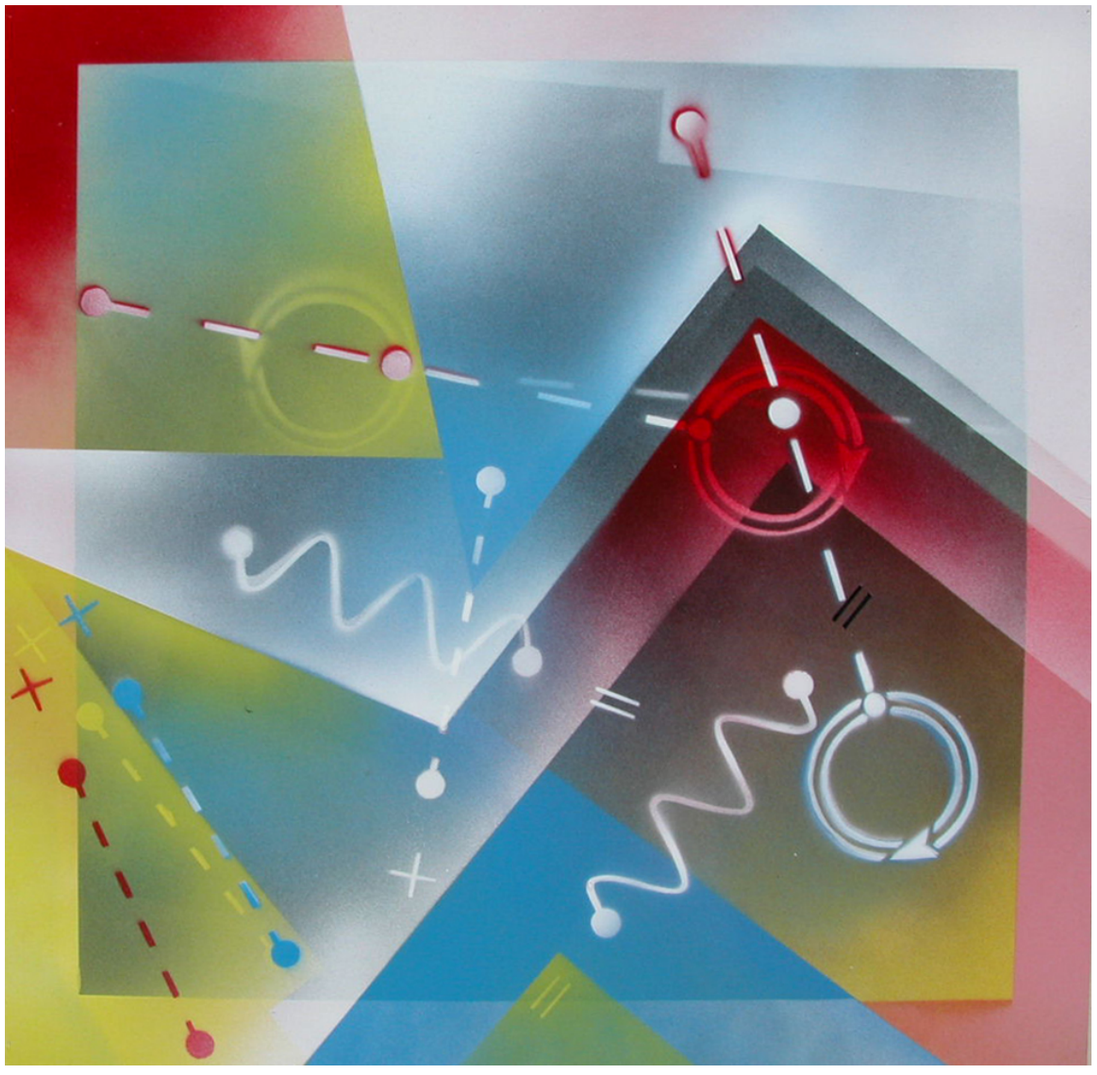
- **Recent papers** (theory)
  - Somà, Barbieri & Duguet, *Phys. Rev. C* **84**, 064317 (2011)
  - Lani, Romaniello & Reining, *New J. Phys.* **17**, 093045 (2012)
  - Carbone, Cipollone, Barbieri, Polls & Rios, *Phys. Rev. C* **88**, 054326 (2013)

- **Recent papers** (applications)
  - Rios & Somà, *Phys. Rev. Lett.* **108**, 012501 (2012)
  - Cipollone, Barbieri & Navrátil, *Phys. Rev. Lett.* **111**, 062501 (2013)
  - Somà, Cipollone, Barbieri, Navrátil & Duguet, *Phys. Rev. C* **89**, 061301 (2014)
  - Carbone, Polls & Rios, *Phys. Rev. C* **90**, 054322 (2014)
  - Lapoux et al., *Phys. Rev. Lett.* **117**, 052501 (2016)

Green's functions in art



Forze nello spazio I



Forze nello spazio II

Meo Carbone (2014)