Recent progress in nuclear Green's function theory

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A journey into nuclear structure and reaction theory
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Ab initio nuclear many-body problem

➪ Nuclei described as a collection of interacting protons and neutrons

Goals

- ○ Understand how nucleons organise themselves into nuclei starting from basic interactions (← QCD)
- ○ Provide reliable predictions for nuclear observables (→ applications)

Solve ***A*-body Schrödinger equation** (for any A=Z+N)

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

- H: many-nucleon Hamiltonian
- $|\Psi_k^A\rangle$: A-body wave function
- E_k^A: A-body energies of ground and excited states

1. Model interactions between nucleons — input → / ← feedback — **2. Solve many-body Schrödinger eq.**

➪ Each of them constitutes a **formal & computational** complex task

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many-nucleon Hamiltonian

A-body wave function

A-body energies of ground and excited states

This lecture:
one particular many-body technique

⇧

1. Model interactions between nucleons

input

feedback

2. Solve many-body Schrödinger eq.

➪ **van Kolck**

➪ **Duguet**

Nuclear Hamiltonian

⦿ Model inter-nucleon forces via **effective field theories**

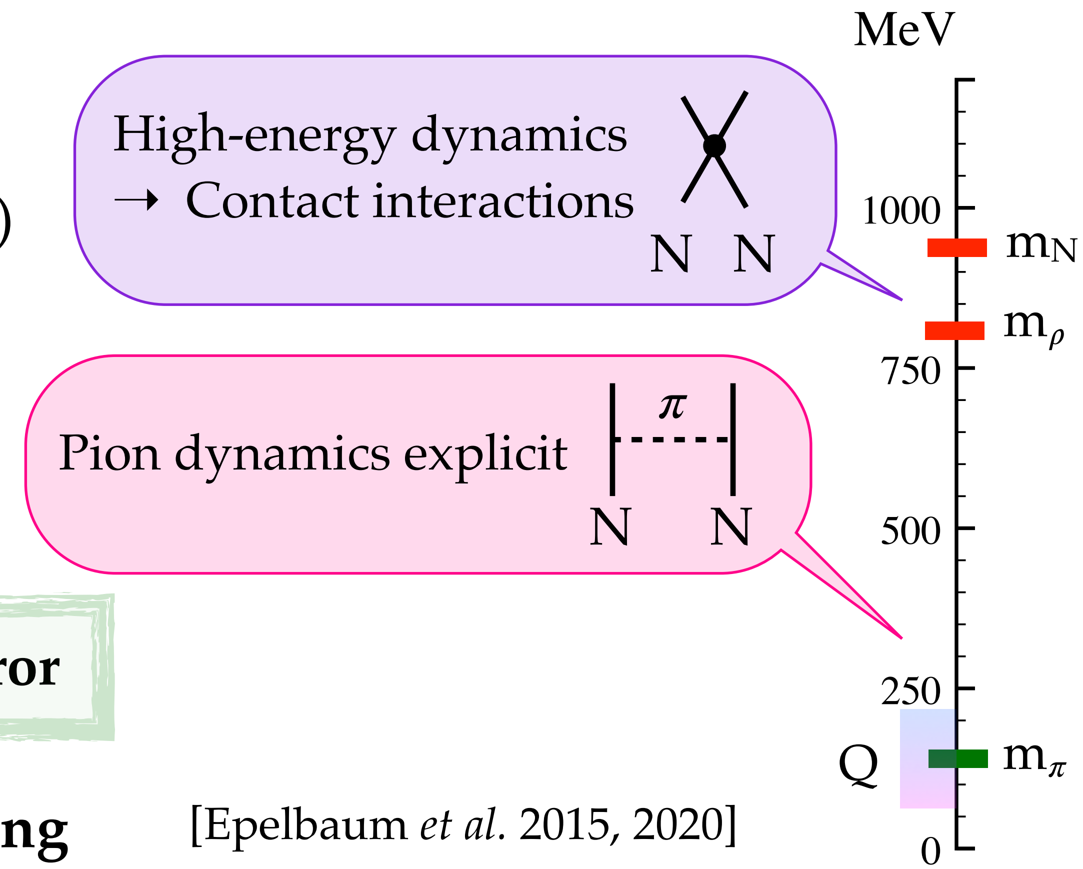
○ Systematic framework to build *A*N interactions (*A*=2, 3, …)

○ Chiral EFT → Nucleons and pions as explicit d.o.f.

[Weinberg 1990-91, Ordóñez & van Kolck 1992, ….]

○ Truncate expansion → **Error** assigned to each order

➪ **Apply to many-nucleon systems + propagate theoretical error**

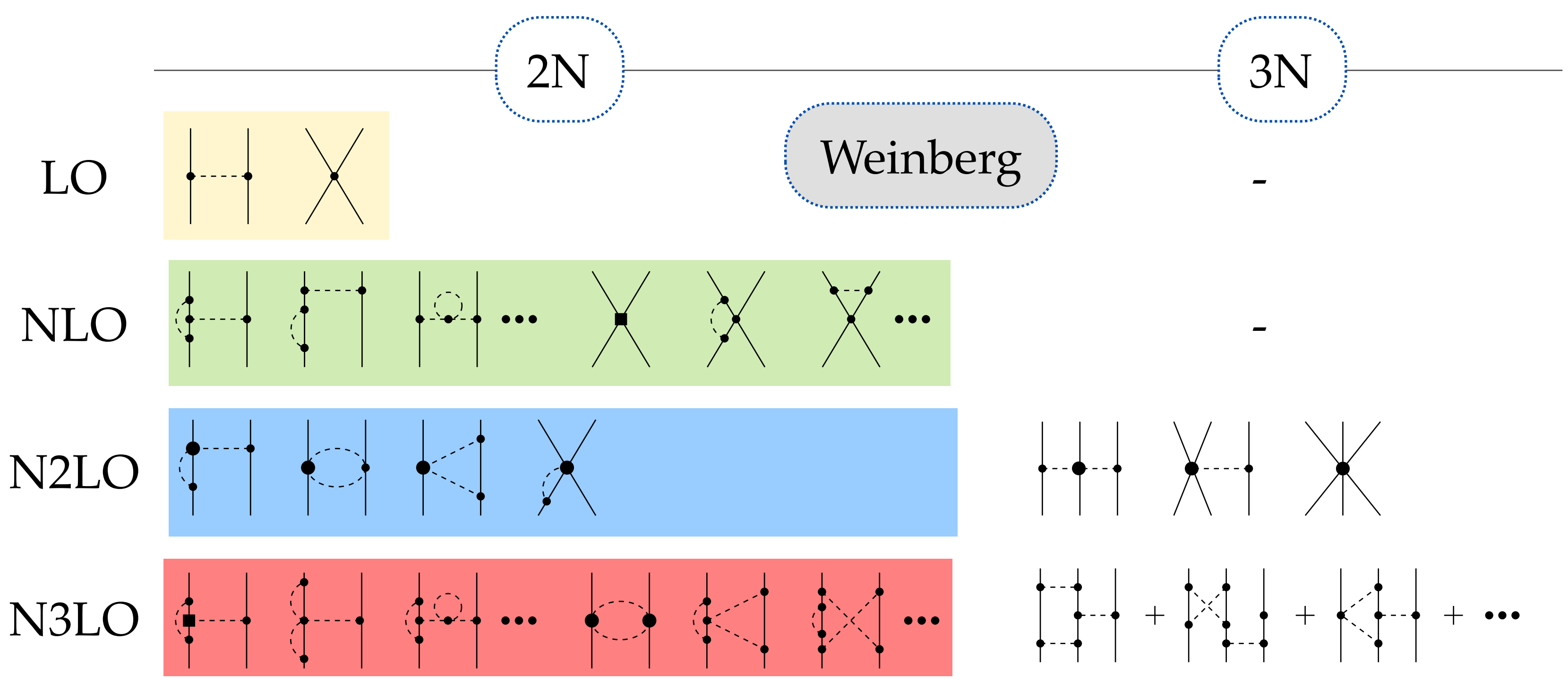


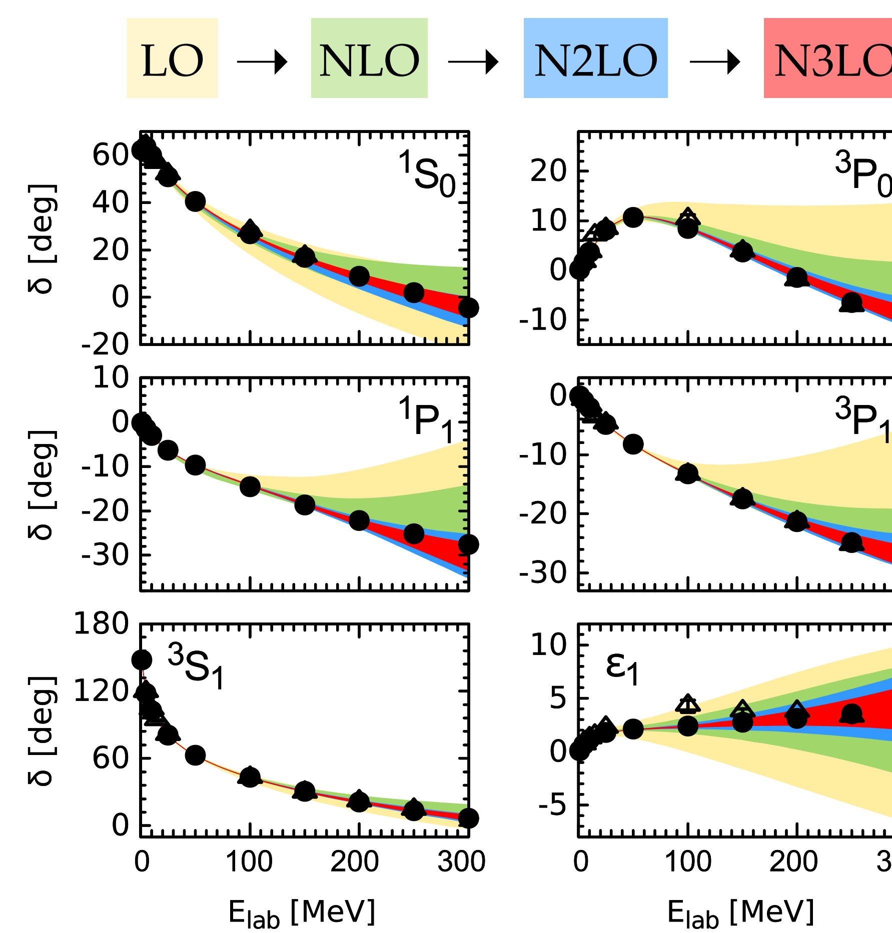
○ Current implementation follows **Weinberg's power counting**

→ Known issues with renormalisability

→ Alternative power counting being investigated

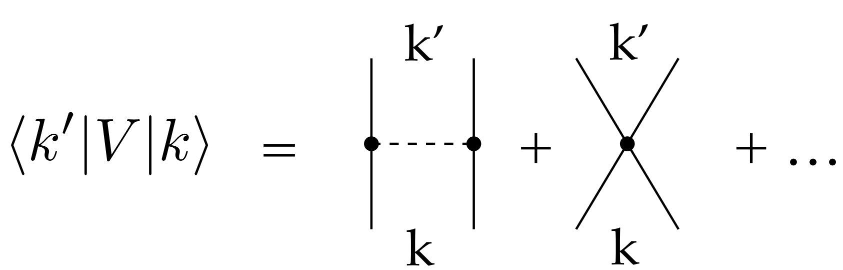
[Epelbaum *et al.* 2015, 2020]

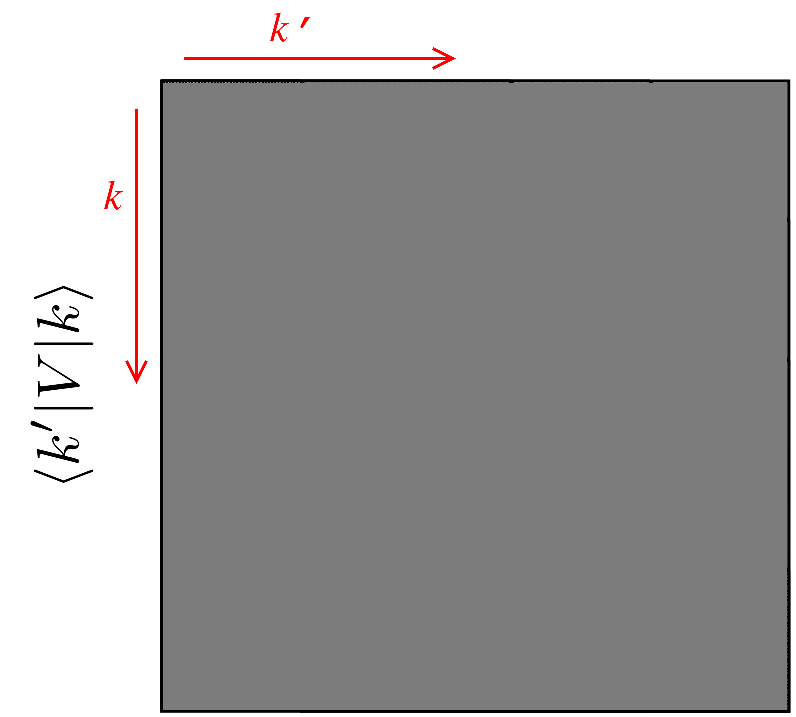




Pre-processing of the nuclear Hamiltonian

- Interactions usually represented in the space of relative nucleon momenta

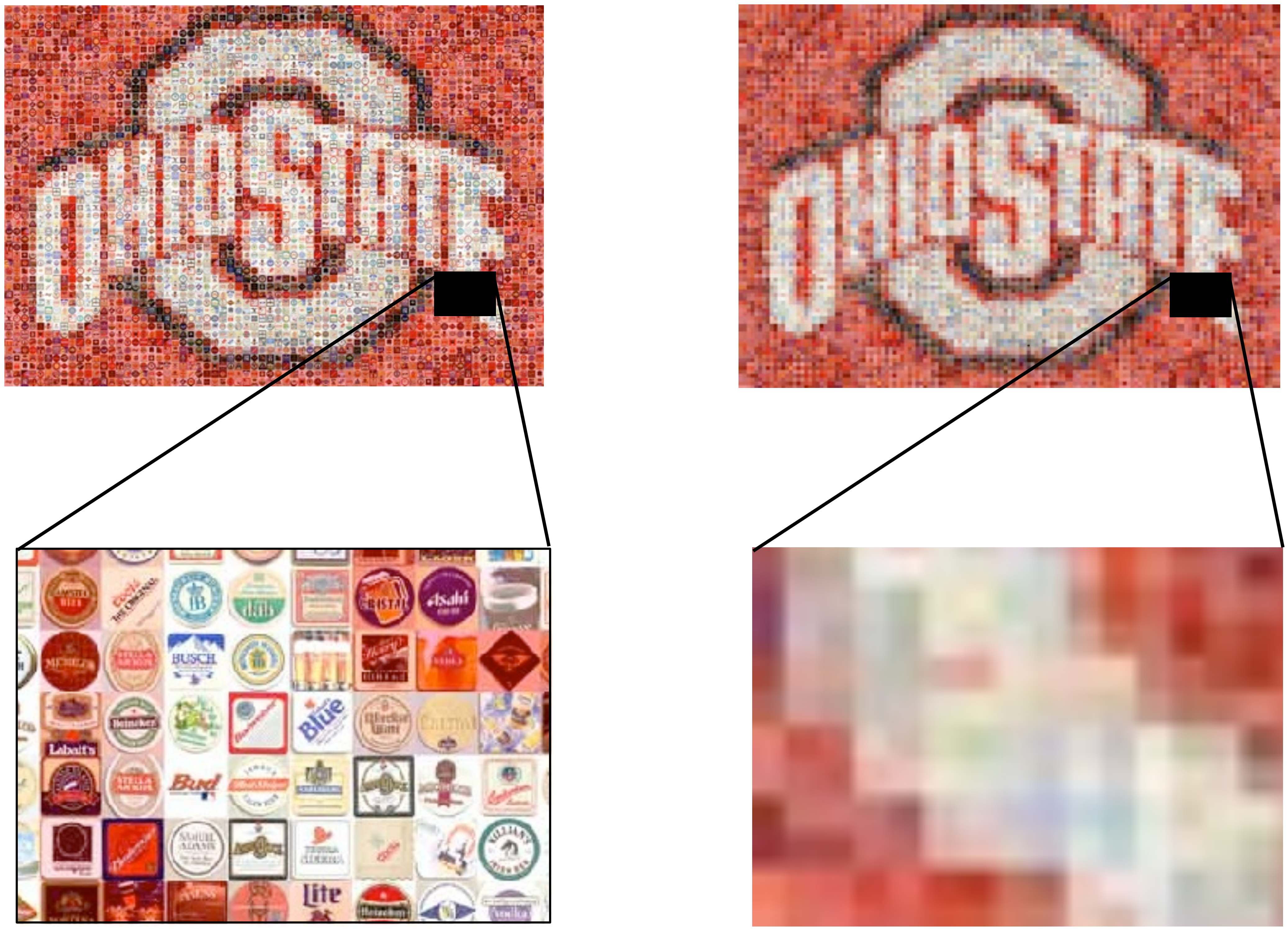




- Large off-diagonal matrix elements generate **strong correlations between low & high momenta**
  - Usually referred to as **short-range correlations** in the many-body wave function
    - → Traditionally linked to "**hard core**" of one-boson exchange potentials
    - → **Weaker but present** in modern chiral interactions
  - Short distance / high momenta / high energy → **large Hilbert space needed**

➪ **Are these large momenta necessary to compute low-energy observables?**

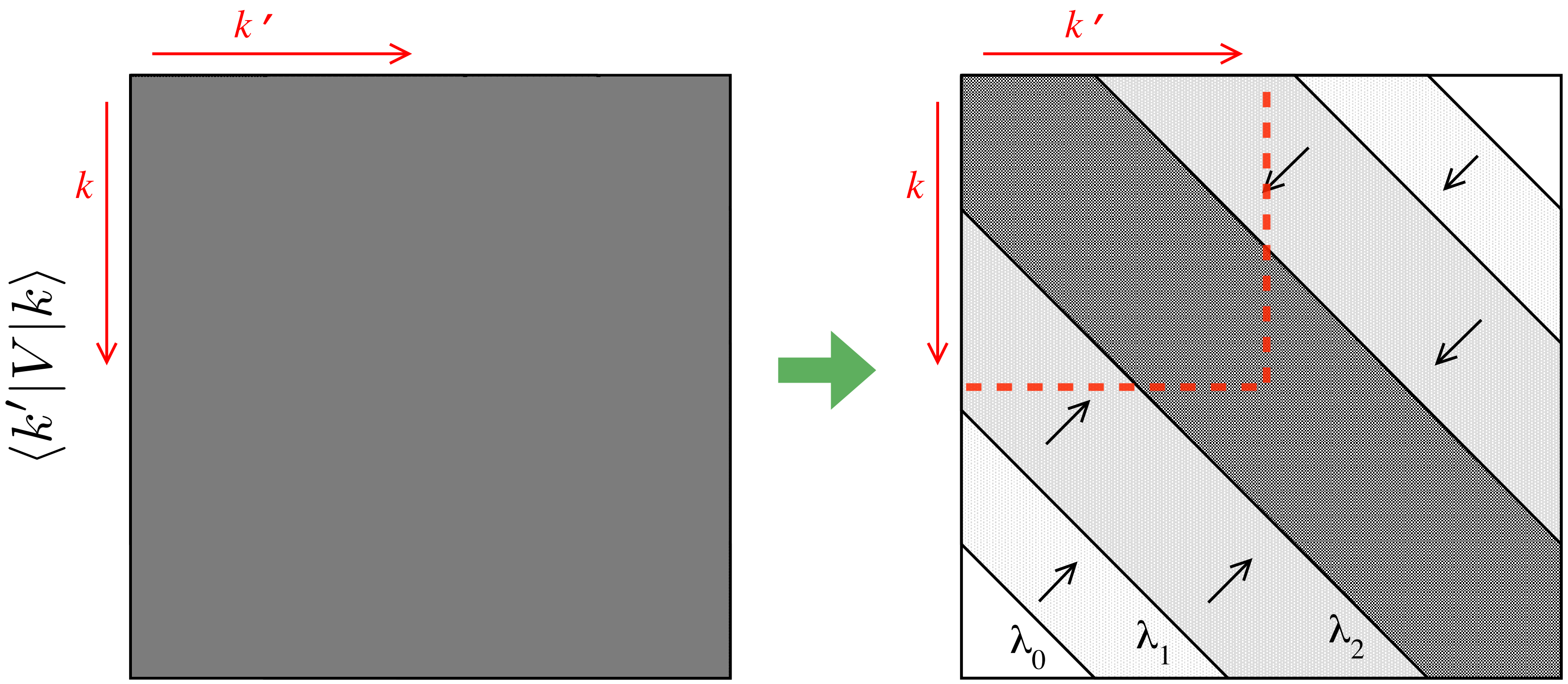
A matter of resolution



[figures from K. Hebeler]

Pre-processing of the nuclear Hamiltonian

⦿ Idea: use **unitary transformations** on H to suppress these correlations



✓ Decouple low- & high-momenta

✓ Can work in small Hilbert space

✓ Observables unchanged!

$$U^\dagger H U U^\dagger |\Psi\rangle = E U^\dagger |\Psi\rangle$$

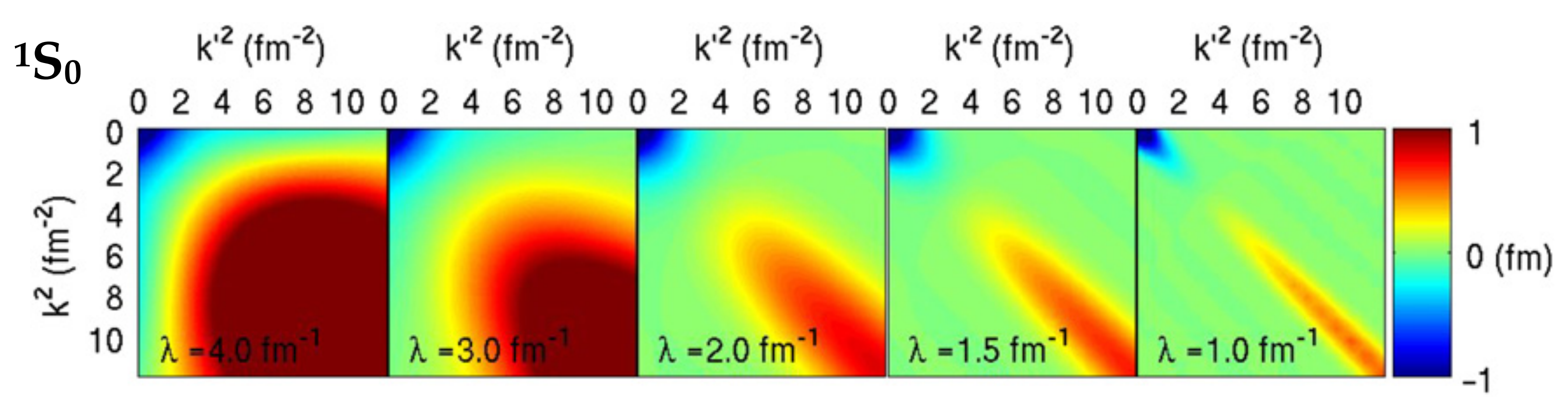
$$\tilde{H}|\tilde{\Psi}\rangle = E|\tilde{\Psi}\rangle$$

✗ Many-body forces generated

⦿ In practice: use **similarity renormalisation group** (SRG) to transform H

○ Transformation governed by one continuous parameter (denoted λ or α)

○ Unitarity of the transformation depends on neglected many-body forces



[Bogner *et al*. 2010]

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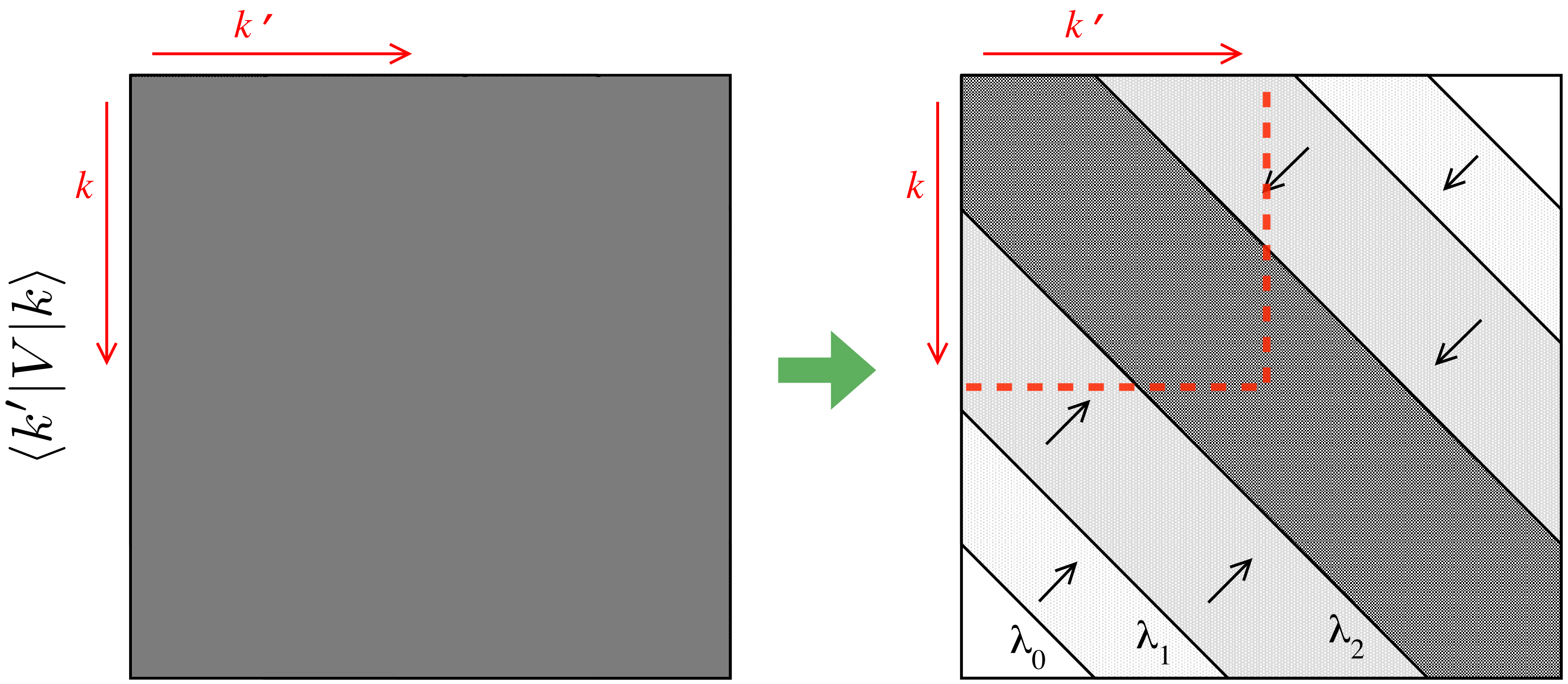

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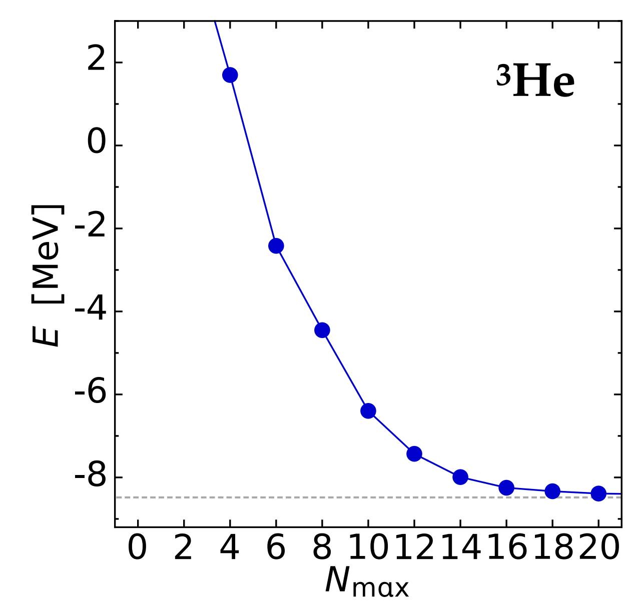
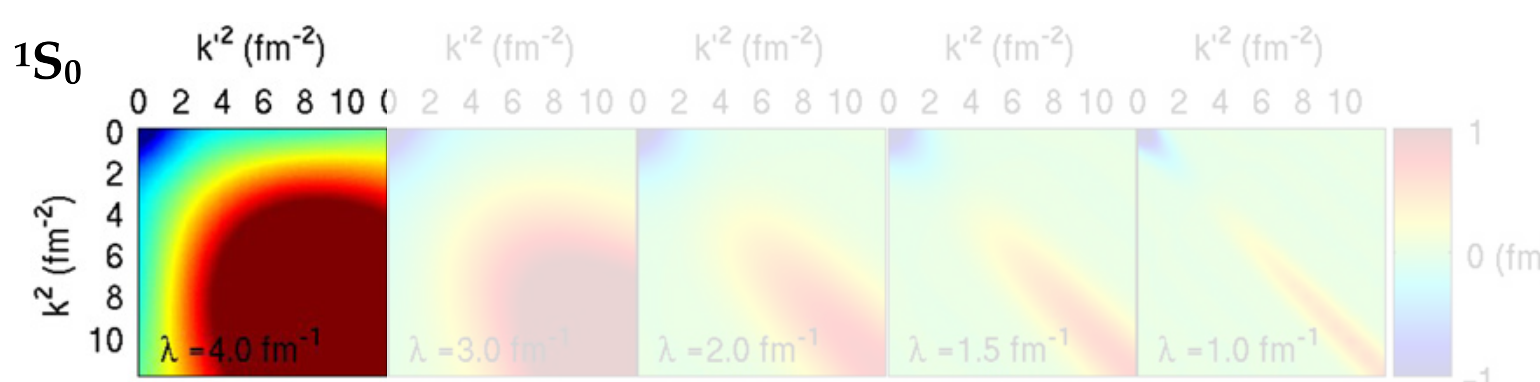


[Roth]



[Bogner *et al.* 2010]

Pre-processing of the nuclear Hamiltonian

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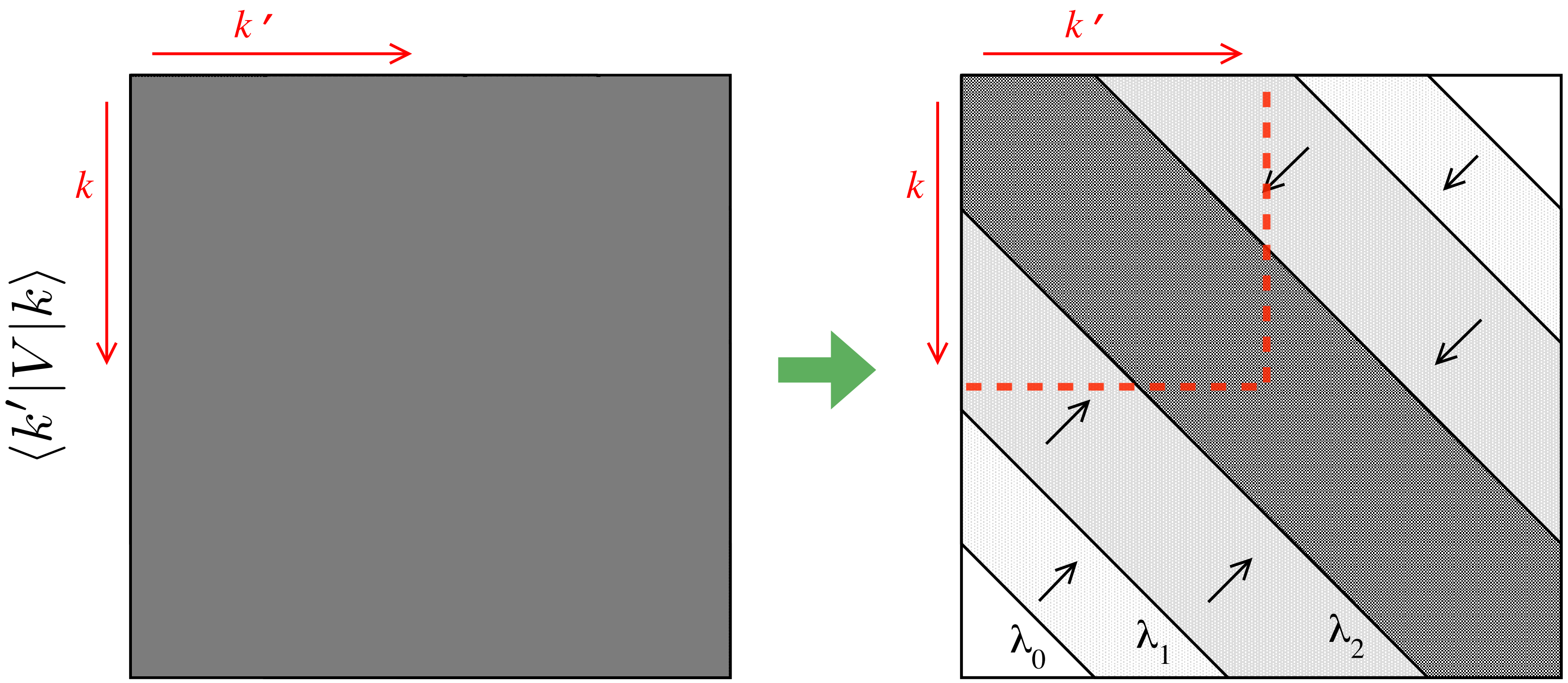

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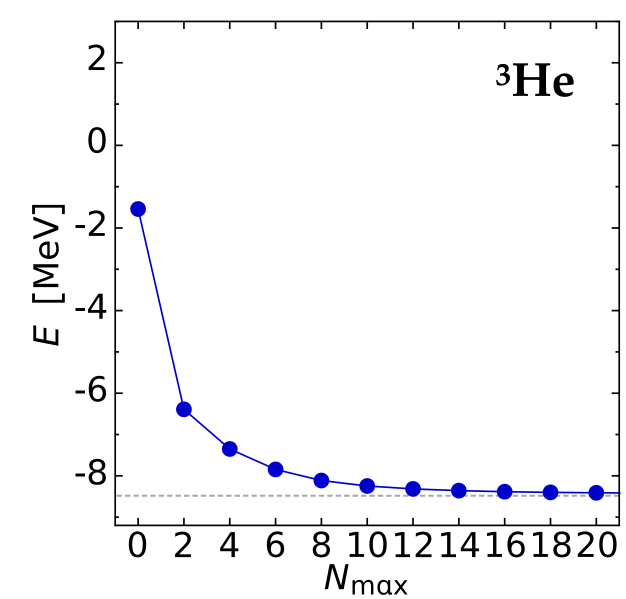

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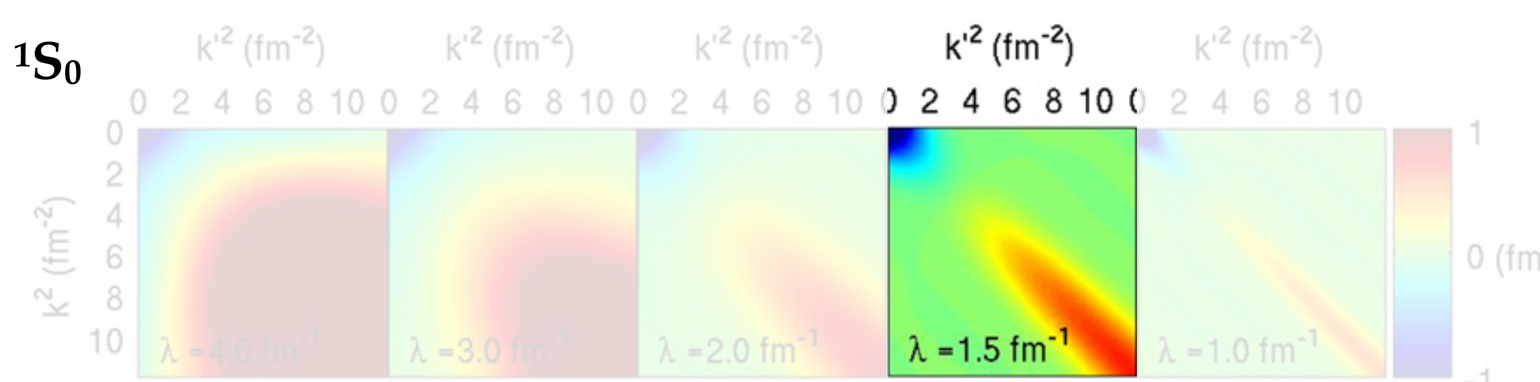


[Bogner *et al.* 2010]

Many-body approaches

Exponential scaling

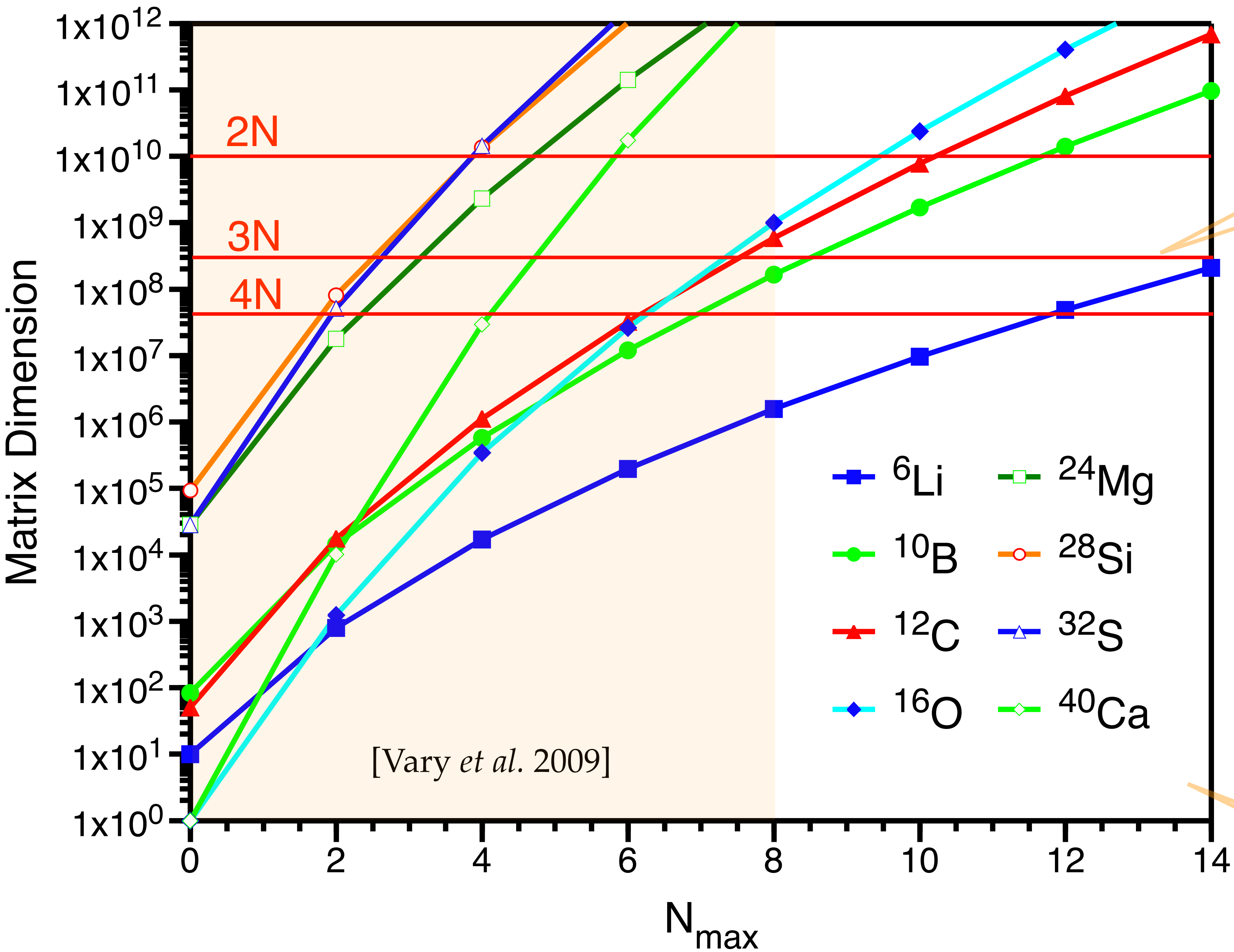
- **Exact methods**
  - Aim to solve the A-body Schrödinger eq. virtually exactly
    - ➪ Coordinate space → Quantum Monte Carlo, nuclear lattice EFT, …
    - ➪ Configuration space → FCI, No-core shell model, …

Exact methods

⦿ Example: **full diagonalisation** of the Hamiltonian matrix in configuration space (NCSM)

$$|\Psi_k(D)\rangle = \sum_{i=1}^{D} C_i^{(k)} |\Phi_i\rangle \quad ➪ \quad \sum_{i=1}^{D} \underbrace{\langle \Phi_j | H | \Phi_i \rangle}_{\equiv H_{ji}} C_i^{(k)} = E_k \sum_{i=1}^{D} C_i^{(k)} \underbrace{\langle \Phi_j \,|\, \Phi_i \rangle}_{= \delta_{ij}}$$

D = D(N_{max}) configurations



800 TB aggregate memory

➪ **Computational limits** are quickly reached

$N_{max} \geq 8$ needed to converge

Many-body approaches

Exact methods

Exponential scaling

- Aim to solve the A-body Schrödinger eq. virtually exactly
  - ➪ Coordinate space → Quantum Monte Carlo, nuclear lattice EFT, …
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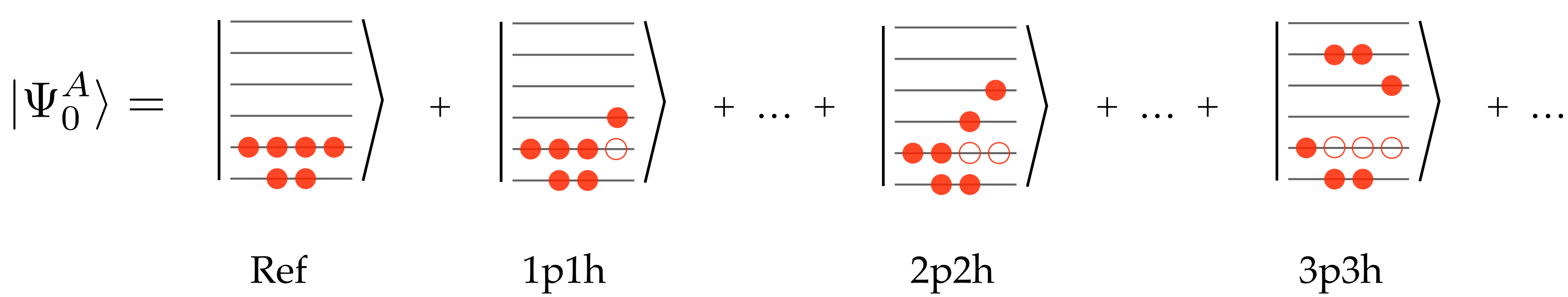
Correlation-expansion methods

Polynomial scaling

- Splitting $H = H_0 + H_1$ → Reference state $|\phi_0\rangle$
- Expand $|\Psi_0^A\rangle = \Omega_0 |\phi_0\rangle \approx |\phi_0\rangle + |\phi_1\rangle + |\phi_2\rangle + \dots$

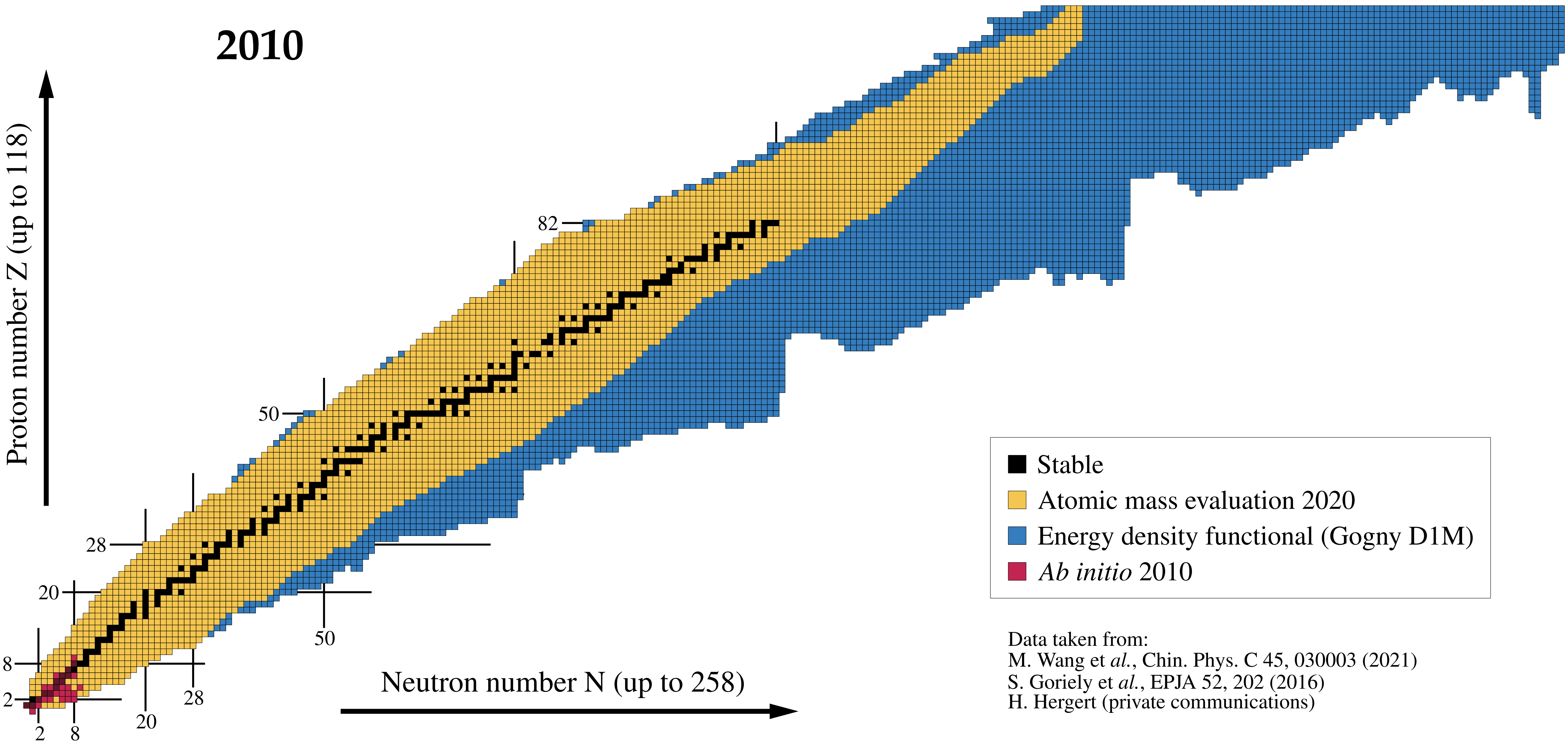
Cost reduced from e^N to N^α with $\alpha \geq 4$

Expansion in terms of **particle-hole excitations**



- However: **no small expansion parameter**
  - ➪ Convergence assessed via benchmarks and/or computing higher orders
  - ➪ Variety of methods essential (benchmarks, observables, interpretation, …)

Ab initio nuclear chart



Data taken from:
M. Wang et *al.*, Chin. Phys. C 45, 030003 (2021)
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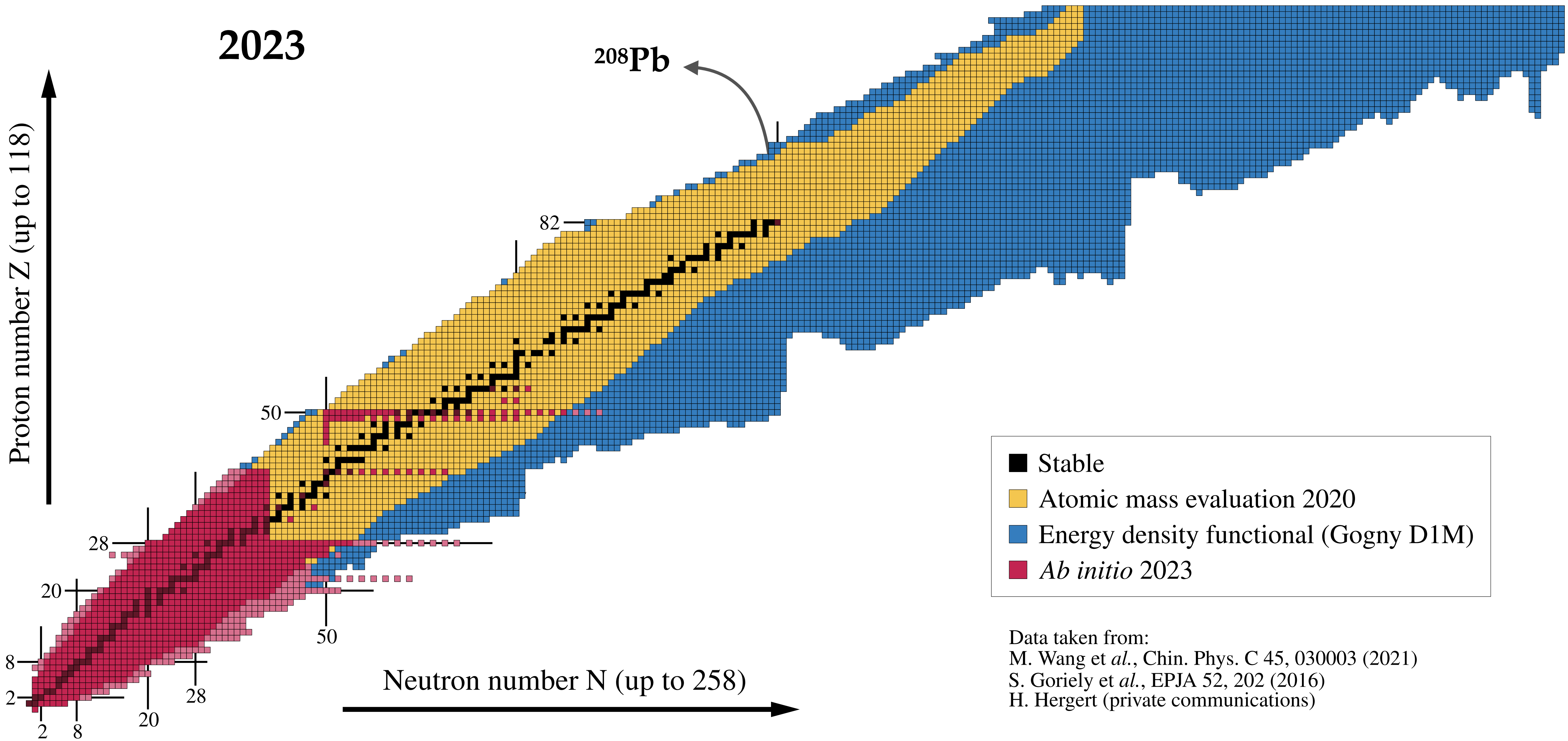
H. Hergert (private communications)

[*Figure*: B. Bally]

Ab initio nuclear chart



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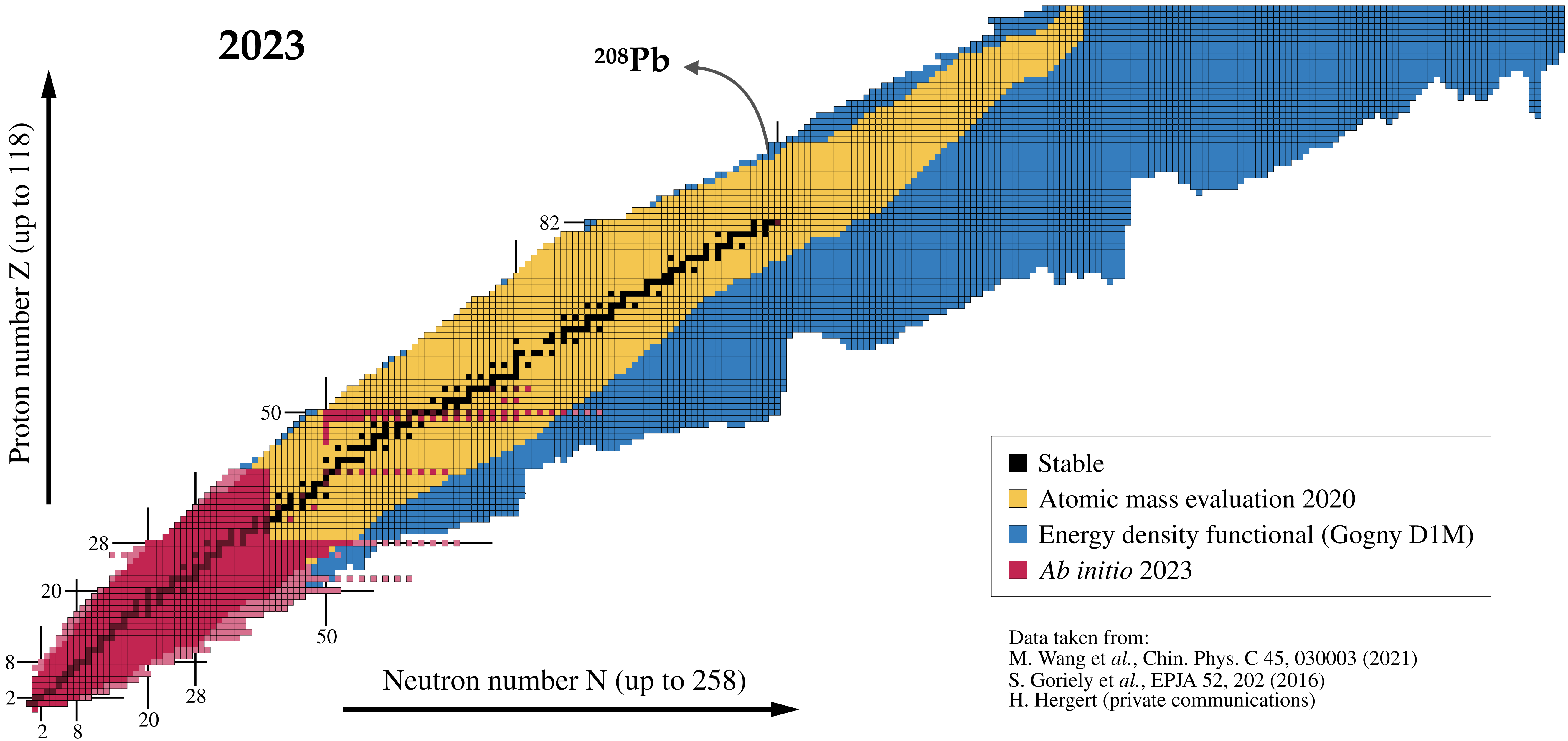
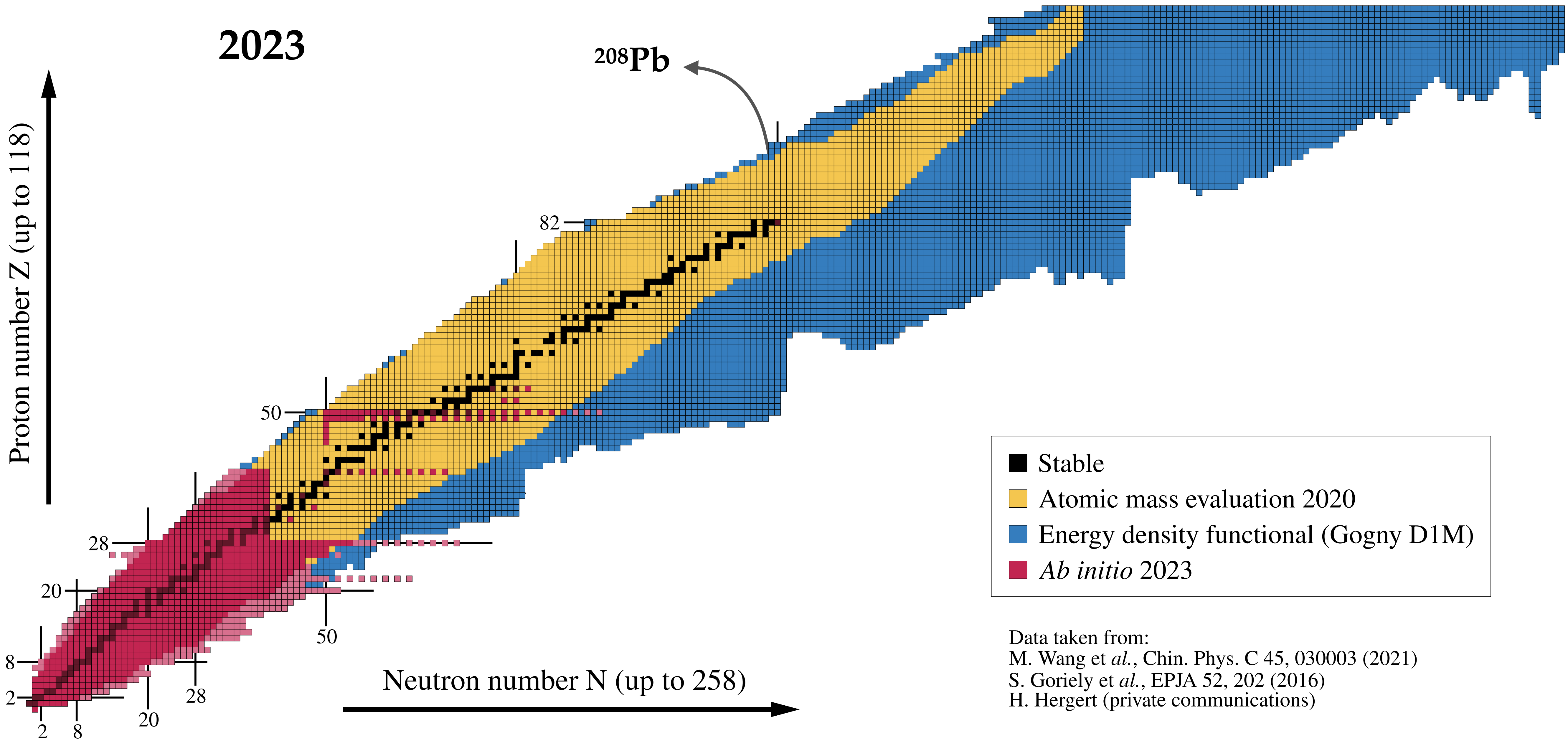


[*Figure*: B. Bally]

○ **Progress** thanks to

- Development of many-body techniques
- Chiral EFT interactions
- SRG pre-processing
- Increase of computational resources

Ab initio nuclear chart



[*Figure*: B. Bally]

○ **Limitations** because of

- Handling of 3N forces
- Applicability of many-body techniques
- Need for optimisation, adaptation to new architectures, …

Semantics & history

- **Many-body Green's function** theory
  - → Set of techniques originated in QFT and then imported to the many-body problem
- Few names for the same thing
  - *Green's function*
  - *Propagator*
  - *Correlation function*
  - → Defined for one-, two-, … up to A-body
- Applicable to different many-body systems: crystals, molecules, atoms, atomic nuclei, …
- **Self-consistent** Green's functions: many-body GF with dressed propagators (see later)
- *Many-body Green's functions* are **not** *Green's function Monte Carlo*
- Some ideas are old, but ab initio implementations are recent
  - Late 1950s, 1960s: import of concepts from QFT & development of many-body formalism
  - 1970s → today: technical developments & applications in several fields of physics
  - 2000s → today: implementation as an *ab initio* method in nuclear physics

Many-body Green's functions in one slide

A-body wave function → **Green's functions**

$$|\Psi_k^A\rangle$$

$$\mathrm{i}\, g_{\alpha\beta}(t_\alpha, t_\beta) \equiv \langle \Psi_0^A | \mathcal{T}[a_\alpha(t_\alpha) a_\beta^\dagger(t_\beta)] | \Psi_0^A \rangle$$

$$\mathrm{i}\, g^{4-\mathrm{pt}}_{\alpha\gamma\beta\delta}(t_\alpha, t_\gamma, t_\beta, t_\delta) \equiv \langle \Psi_0^A | \mathcal{T}[a_\gamma(t_\gamma) a_\alpha(t_\alpha) a_\beta^\dagger(t_\beta) a_\delta^\dagger(t_\delta)] | \Psi_0^A \rangle$$

$$\dots$$

A-body Schrödinger equation ⇢ **Martin-Schwinger equations**

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

$$g_{\alpha\beta}(\omega) = g_{0\,\alpha\beta}(\omega) - \sum_{\gamma\delta} g_{0\,\alpha\gamma}(\omega)\, u_{\gamma\delta}\, g_{\delta\beta}(\omega) - \frac{1}{2} \sum_{\substack{\gamma\epsilon \\ \delta\mu}} g_{0\,\alpha\gamma}(\omega)\, v_{\gamma\epsilon,\delta\mu} \int \frac{d\omega_1}{2\pi} \int \frac{d\omega_2}{2\pi} g^{4-\mathrm{pt}}_{\delta\mu,\beta\epsilon}(\omega_1, \omega_2; \omega, \omega_1 + \omega_2 - \omega)$$

Decouple

$$\dots$$

Observables: exp. values

$$\mathrm{O} = \langle \Psi_0^A | O | \Psi_0^A \rangle$$

Many-body Green's functions in one slide

A-body wave function → **Green's functions**

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$$\mathrm{i}\, g^{4-\mathrm{pt}}_{\alpha\gamma\beta\delta}(t_\alpha, t_\gamma, t_\beta, t_\delta) \equiv \langle\Psi_0^A|\mathcal{T}[a_\gamma(t_\gamma) a_\alpha(t_\alpha) a_\beta^\dagger(t_\beta) a_\delta^\dagger(t_\delta)]|\Psi_0^A\rangle$$

$$\dots$$

A-body Schrödinger equation → **Dyson equation**

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

$$g_{\alpha\beta}(\omega) = g_{0\,\alpha\beta}(\omega) + \sum_{\gamma\delta} g_{0\,\alpha\gamma}(\omega)\, \Sigma^\star_{\gamma\delta}(\omega)\, g_{\delta\beta}(\omega)$$

Self-energy expansion → Many-body approximations

Observables: exp. values → **Observables: convolutions with GFs**

$$\mathrm{O} = \langle\Psi_0^A|O|\Psi_0^A\rangle$$

$$\langle\Psi_0^A\,|\,O^{1\mathrm{B}}\,|\,\Psi_0^A\rangle = \sum_{\alpha\beta}\int \frac{d\omega}{2\pi i}\, g_{\beta\alpha}(\omega)\, o_{\alpha\beta}$$

Koltun sum rule $E_0 = \langle\Psi_0^A\,|\,H\,|\,\Psi_0^A\rangle = \frac{1}{2}\sum_{\alpha\beta}\int \frac{d\omega}{2\pi i}\, g_{\beta\alpha}(\omega)\, [t_{\alpha\beta} + \omega\,\delta_{\alpha\beta}]$

Many facets of Green's functions

Mathematical object

$$\mathrm{i}\, g_{\alpha\beta}(t_\alpha, t_\beta) \equiv \langle \Psi_0^A | \mathcal{T}[a_\alpha(t_\alpha) a_\beta^\dagger(t_\beta)] | \Psi_0^A \rangle$$

Green's functions in maths

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

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

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

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

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

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

one-body

$$G(\boldsymbol{r},\boldsymbol{r}';z) = \sum_\mu \frac{\langle \Psi_0^N | a_{\boldsymbol{r}} \,|\, \Psi_\mu^{N+1} \rangle \langle \Psi_\mu^{N+1} \,|\, a^\dagger_{\boldsymbol{r}'} | \Psi_0^N \rangle}{z - E^+_\mu} + \sum_\nu \frac{\langle \Psi_0^N | a^\dagger_{\boldsymbol{r}'} \,|\, \Psi_\nu^{N-1} \rangle \langle \Psi_\nu^{N-1} \,|\, a_{\boldsymbol{r}} | \Psi_0^N \rangle}{z - E^-_\nu}$$

many-body

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

with

$\lvert \Psi_0^N \rangle$	→	(Exact) ground state of N-body system
$\lvert \Psi_\kappa^{N\pm 1} \rangle$	→	κ-excited state of (N±1)-body system
$E^+_\mu \equiv E_\mu^{N+1} - E_0^N$	→	one-particle (addition) separation energy
$E^-_\nu \equiv E_0^N - E_\nu^{N-1}$	→	one-particle (removal) separation energy

Many facets of Green's functions

Mathematical object

Spectral representation

$$\mathrm{i}\, g_{\alpha\beta}(t_\alpha, t_\beta) \equiv \langle \Psi_0^A | \mathcal{T}[a_\alpha(t_\alpha) a_\beta^\dagger(t_\beta)] | \Psi_0^A \rangle$$

Källén-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

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

Use integral representation of Heaviside function

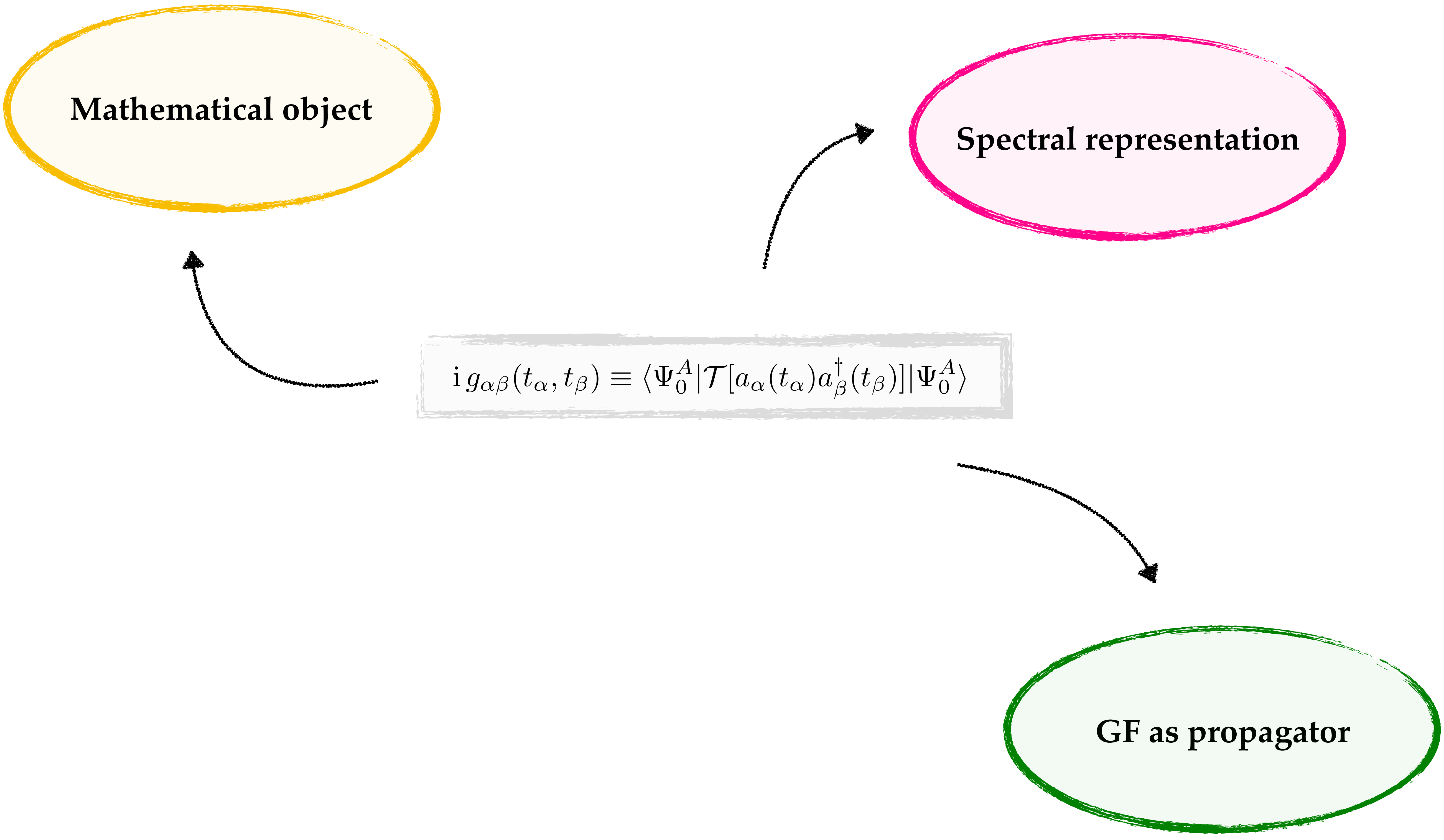
$$\Theta(t) = \lim_{\eta\to 0^+}\frac{1}{2\pi i}\int_{-\infty}^{+\infty} dz\,\frac{e^{itz}}{z-i\eta}$$

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

Källén-Lehmann representation

[Källén 1952, Lehmann 1954]

Many facets of Green's functions



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Propagator

⦿ General definition

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

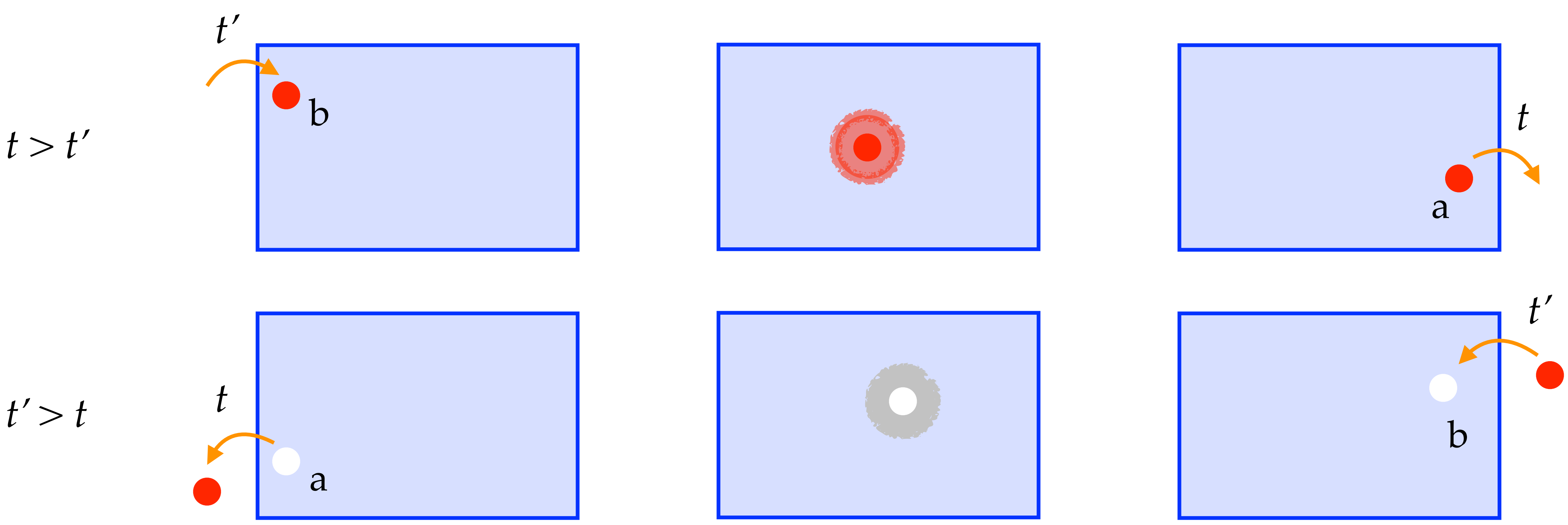
single-particle labels

time-ordering operator

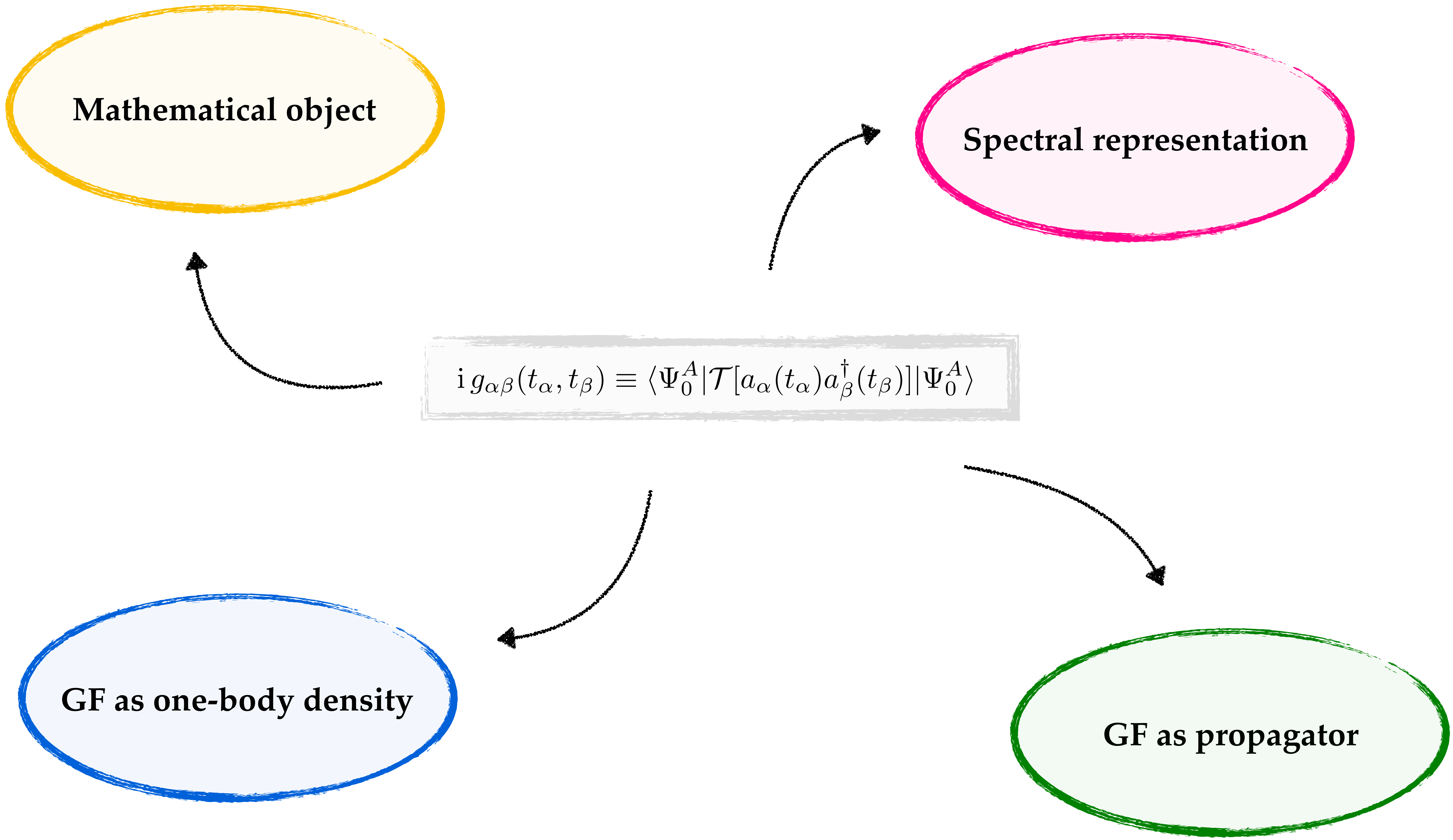
(Exact) ground state of N-body system

➟ 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**



Many facets of Green's functions



$$\mathrm{i}\, g_{\alpha\beta}(t_\alpha, t_\beta) \equiv \langle \Psi_0^A | \mathcal{T}[a_\alpha(t_\alpha) a_\beta^\dagger(t_\beta)] | \Psi_0^A \rangle$$

Green's functions as density matrices

- Many-body GFs can be easily related to **many-body density matrices**

$$\rho_{\delta\gamma} \equiv \langle \Psi_0^A | \, a_\gamma^\dagger a_\delta \, | \Psi_0^A \rangle = -\mathrm{i}\, g_{\delta\gamma}^{2-\mathrm{pt}}(t, t^+) \; ,$$

$$\rho_{\delta\eta\gamma\epsilon} \equiv \langle \Psi_0^A | \, a_\gamma^\dagger a_\epsilon^\dagger a_\eta a_\delta \, | \Psi_0^A \rangle = \mathrm{i}\, g_{\delta\eta\gamma\epsilon}^{4-\mathrm{pt}}(t, t, t^+, t^+) \; ,$$

$$\rho_{\delta\eta\xi\gamma\epsilon\zeta} \equiv \langle \Psi_0^A | \, a_\gamma^\dagger a_\epsilon^\dagger a_\zeta^\dagger a_\xi a_\eta a_\delta \, | \Psi_0^A \rangle = -\mathrm{i}\, g_{\delta\eta\xi\gamma\epsilon\zeta}^{6-\mathrm{pt}}(t, t, t, t^+, t^+, t^+)$$

$$\dots$$

- Correspondingly, observables can be computed as

$$\langle \Psi_0^A | O^{1B} \, | \Psi_0^A \rangle = \sum_{\delta\gamma} o_{\delta\gamma} \; \rho_{\gamma\delta} \; ,$$

$$\langle \Psi_0^A | O^{2B} \, | \Psi_0^A \rangle = \sum_{\substack{\delta\eta \\ \gamma\epsilon}} o_{\delta\eta\gamma\epsilon} \; \rho_{\gamma\epsilon\delta\eta} \; ,$$

$$\langle \Psi_0^A | O^{3B} \, | \Psi_0^A \rangle = \sum_{\substack{\delta\eta\xi \\ \gamma\epsilon\zeta}} o_{\delta\eta\xi\gamma\epsilon\zeta} \; \rho_{\gamma\epsilon\zeta\delta\eta\xi}$$

$$\dots$$

- One exception is constituted by the **Galitski-Migdal-Koltun sum rule** for the total g.s. energy

$$E_0^A = \frac{1}{3\pi} \int_{-\infty}^{\epsilon_F^-} \mathrm{d}\omega \; \sum_{\alpha\beta} (2 t_{\alpha\beta} + \omega \, \delta_{\alpha\beta}) \, \mathrm{Im} \, g_{\beta\alpha}(\omega) + \frac{1}{3} \sum_{\substack{\alpha\gamma \\ \beta\delta}} v_{\alpha\gamma\beta\delta} \, \rho_{\beta\delta\alpha\gamma}$$

[Galitskii, Migdal 1958; Koltun 1972]

with 3NF → [Carbone *et al*. 2013]

Dyson equation: basic idea

- **Schrödinger** equation for many-body ψ → **Dyson** equation for one-body GF
  - Equation of motion technique
  - **Perturbative expansion**

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:

$$G(z) = (z - \mathcal{H}_0 - \mathcal{H}_1)^{-1} = \left\{(z - \mathcal{H}_0)\left[1 - (z - \mathcal{H}_0)^{-1}\mathcal{H}_1\right]\right\}^{-1}$$

$$= \left[1 - (z - \mathcal{H}_0)^{-1}\mathcal{H}_1\right]^{-1}(z - \mathcal{H}_0)^{-1}$$

$$= [1 - G_0(z)\mathcal{H}_1]^{-1} G_0(z) \ .$$

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

- **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

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

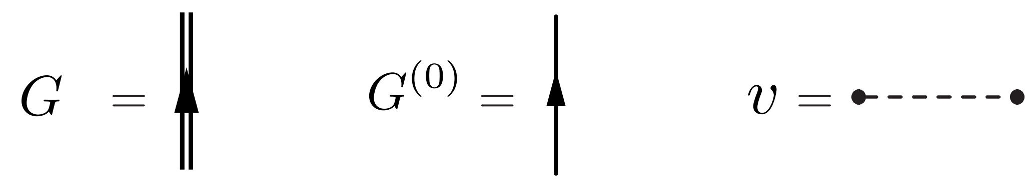
  - ➟ Several terms cancel out (all disconnected combinations of variables), at the end:

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

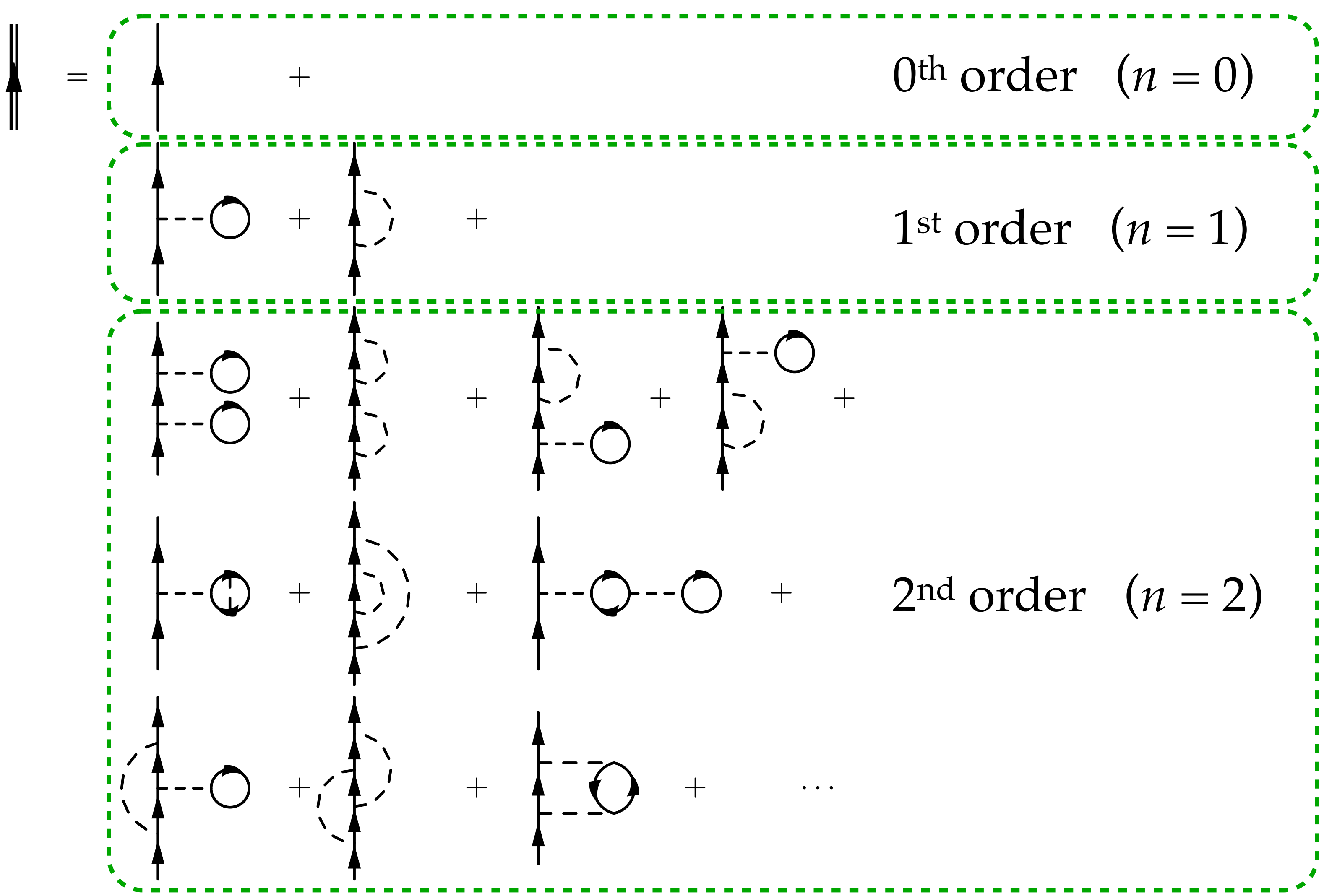
- In practice it is convenient to introduce **Feynman diagrams**
  - ➟ Expansion worked out diagrammatically

Dyson equation: diagrammatic expansion

⊙ Feynman diagrams: **exact & unperturbed propagators** and **interaction lines** depicted as

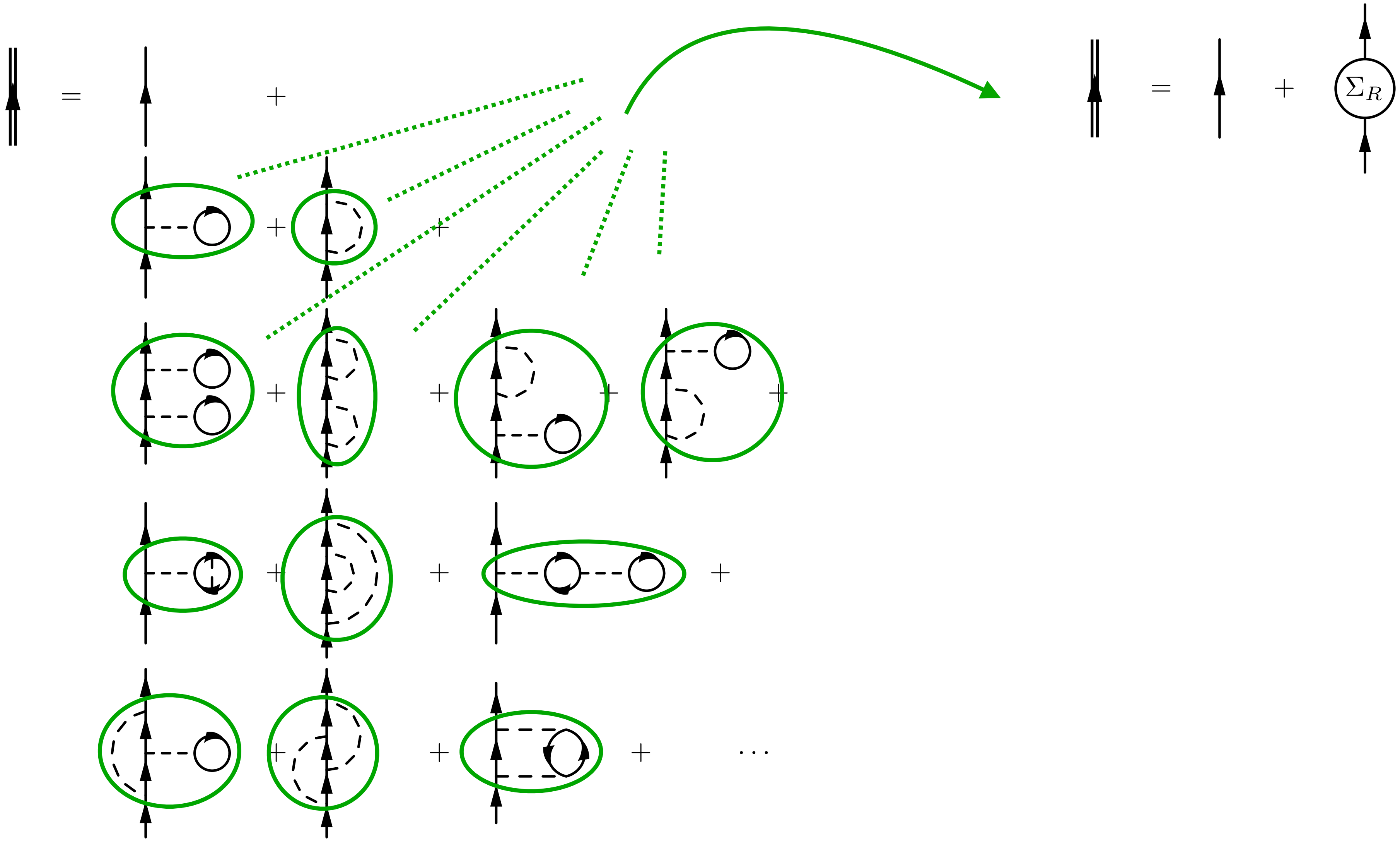


⊙ Expansion for $G = \sum_{n} \sum_{\text{connected}} \underbrace{G^{(0)} \cdots G^{(0)} \cdots}_{2n+1 \text{ propagators}} \underbrace{v \cdots v \cdots}_{n \text{ interactions}}$ reads as



Dyson equation: diagrammatic expansion

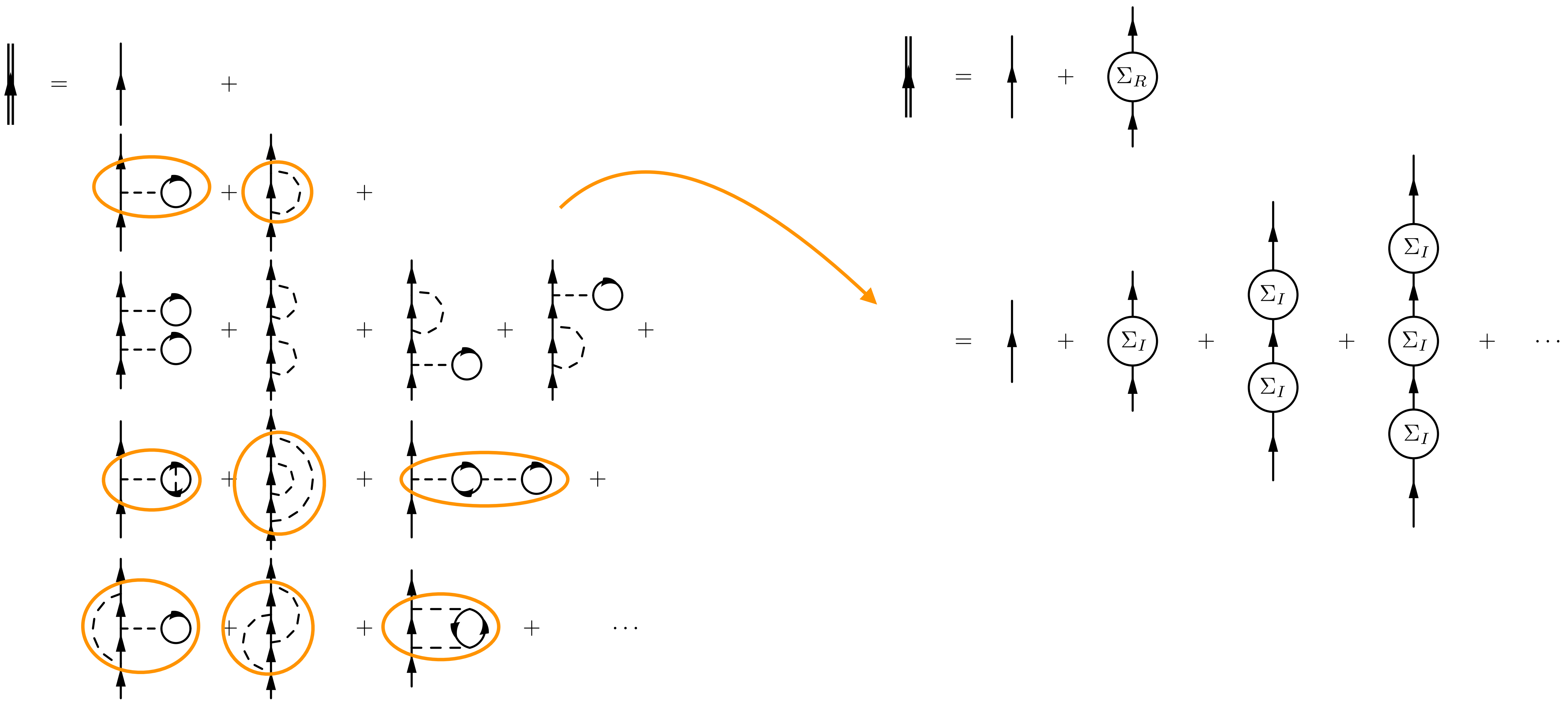
- Introduce *reducible* **self-energy**
  - ➟ Includes all diagrams after external legs are cut off



Dyson equation: diagrammatic expansion

⊙ Select **one-particle irreducible** self-energy diagrams → ***Irreducible* self-energy**

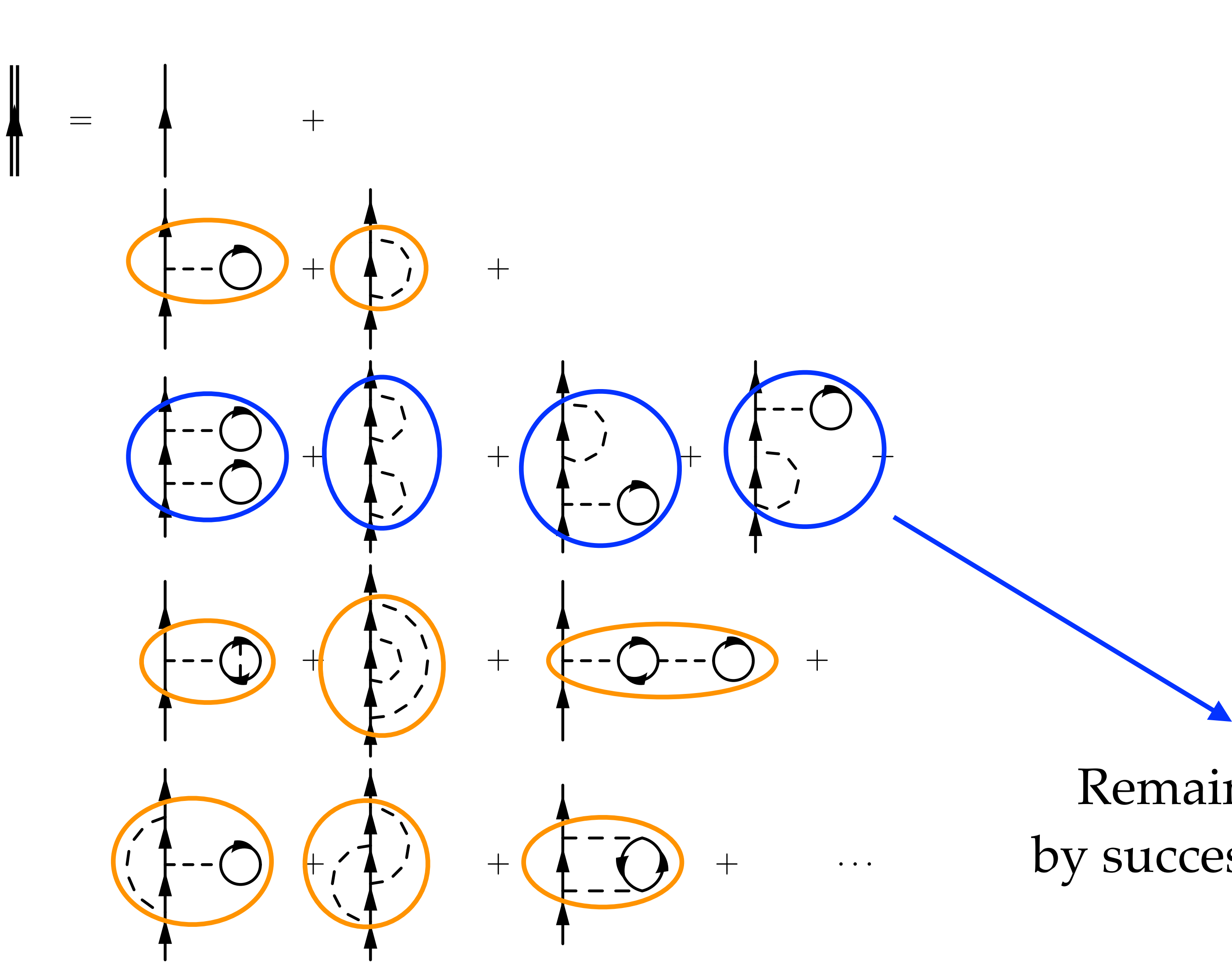
➟ All contributions that cannot be separated in two parts by cutting a propagation line

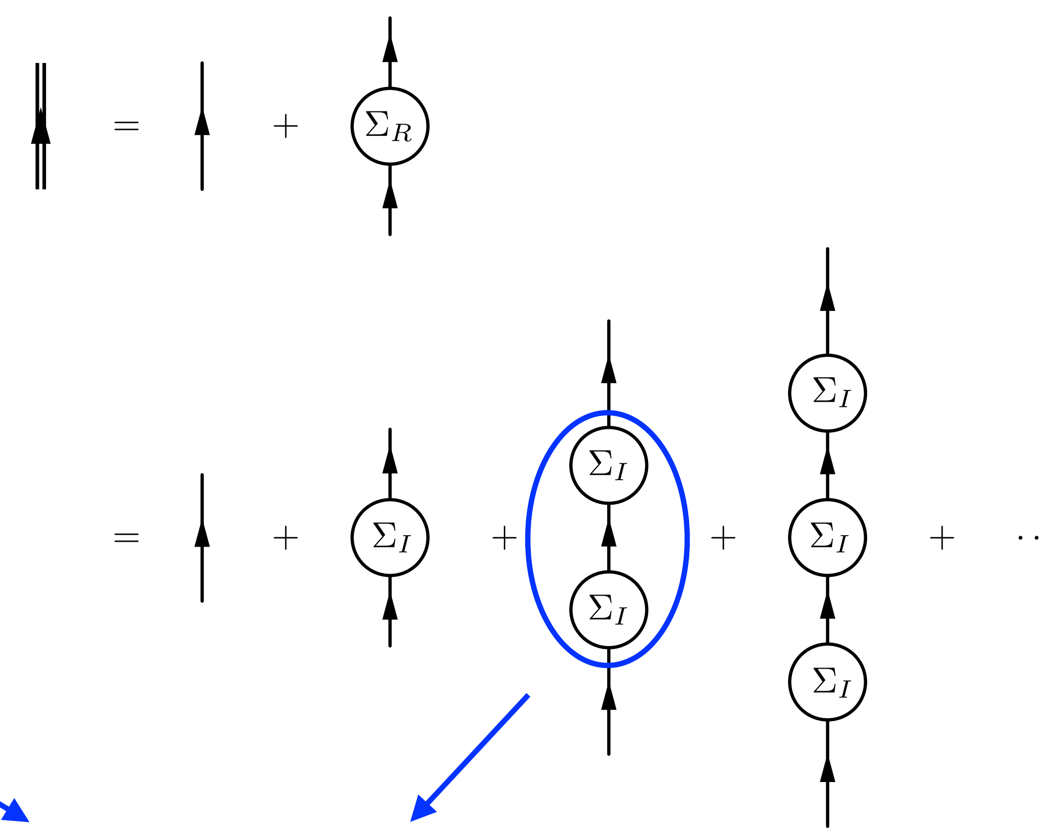


Dyson equation: diagrammatic expansion

⦿ Select **one-particle irreducible** self-energy diagrams → ***Irreducible* self-energy**

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

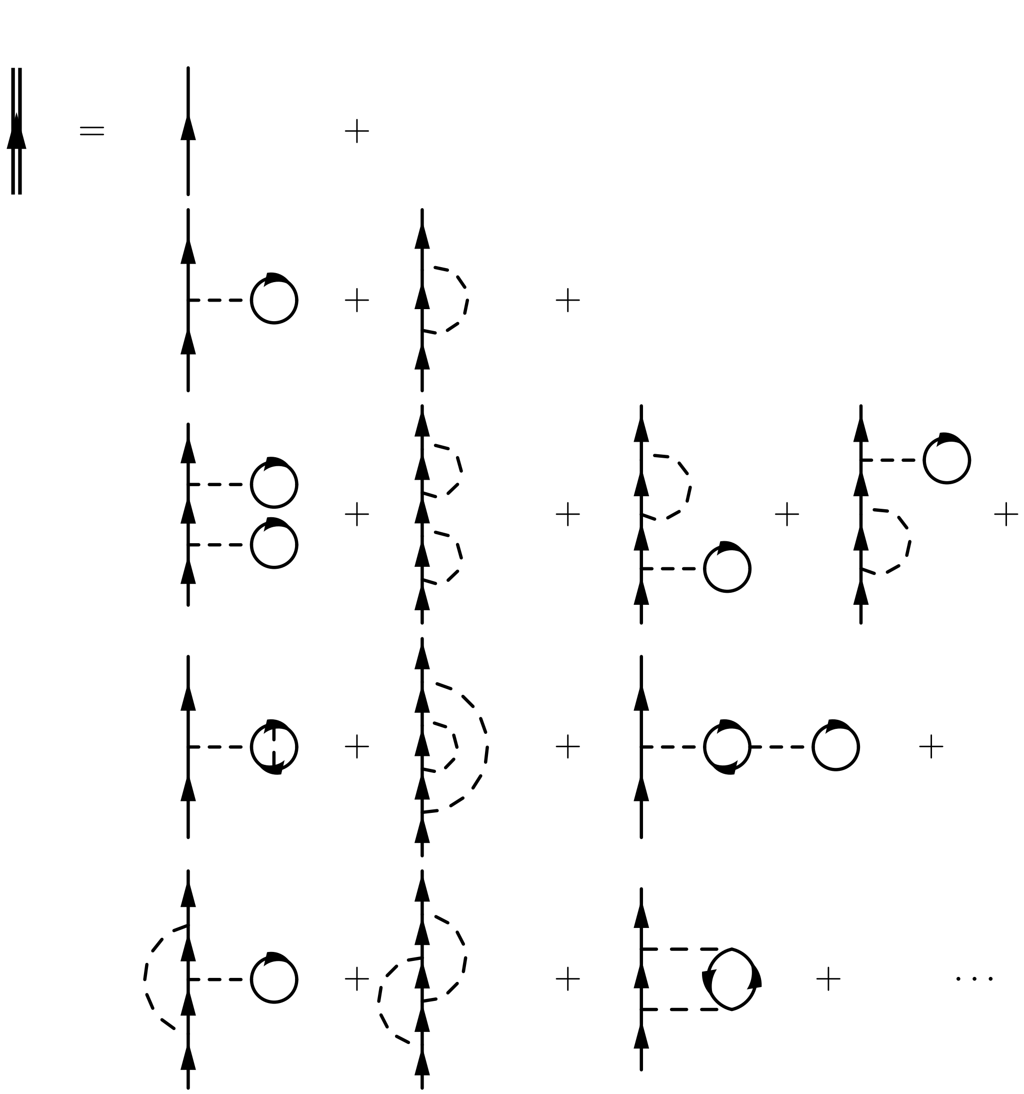


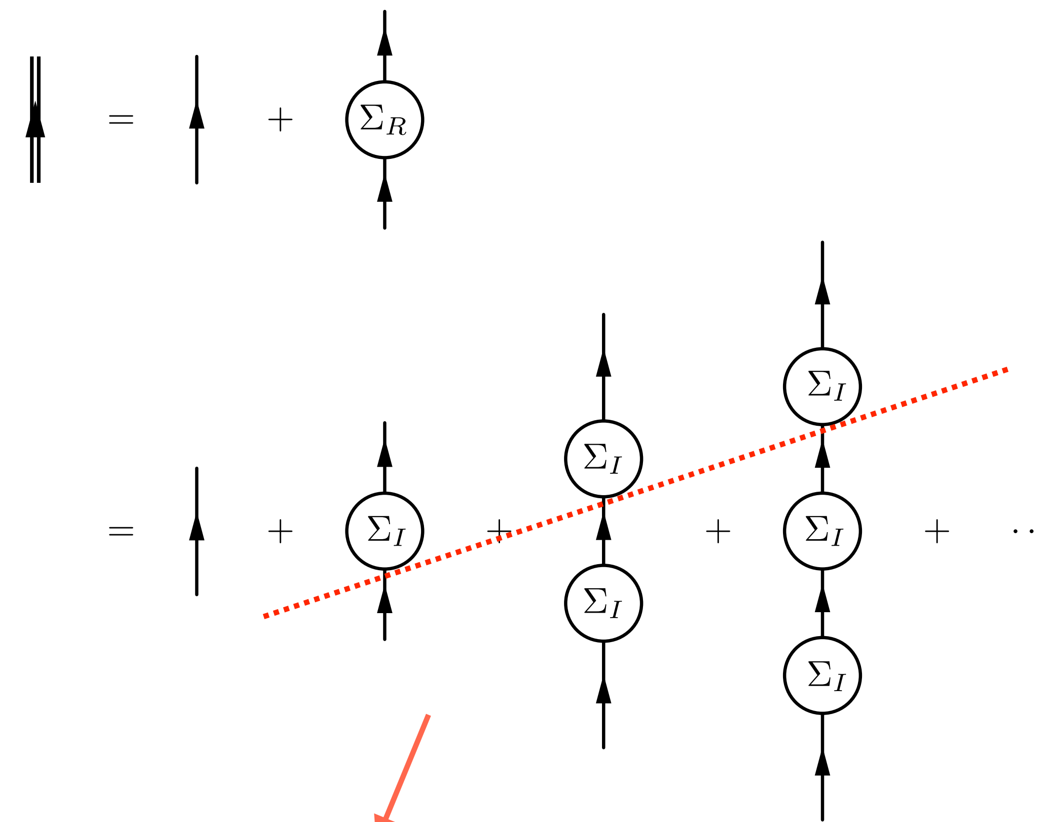


Remaining diagrams generated
by successive self-energy insertions

Dyson equation: diagrammatic expansion

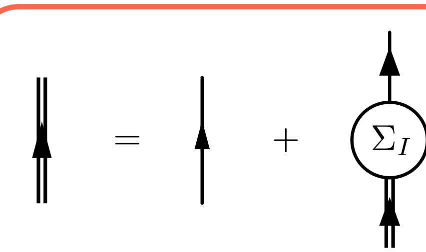
- Rewrite the expansion in the form of an **iterative** equation
  - ➟ Implicit equation that generates all orders





This is itself the expansion for the dressed propagator

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

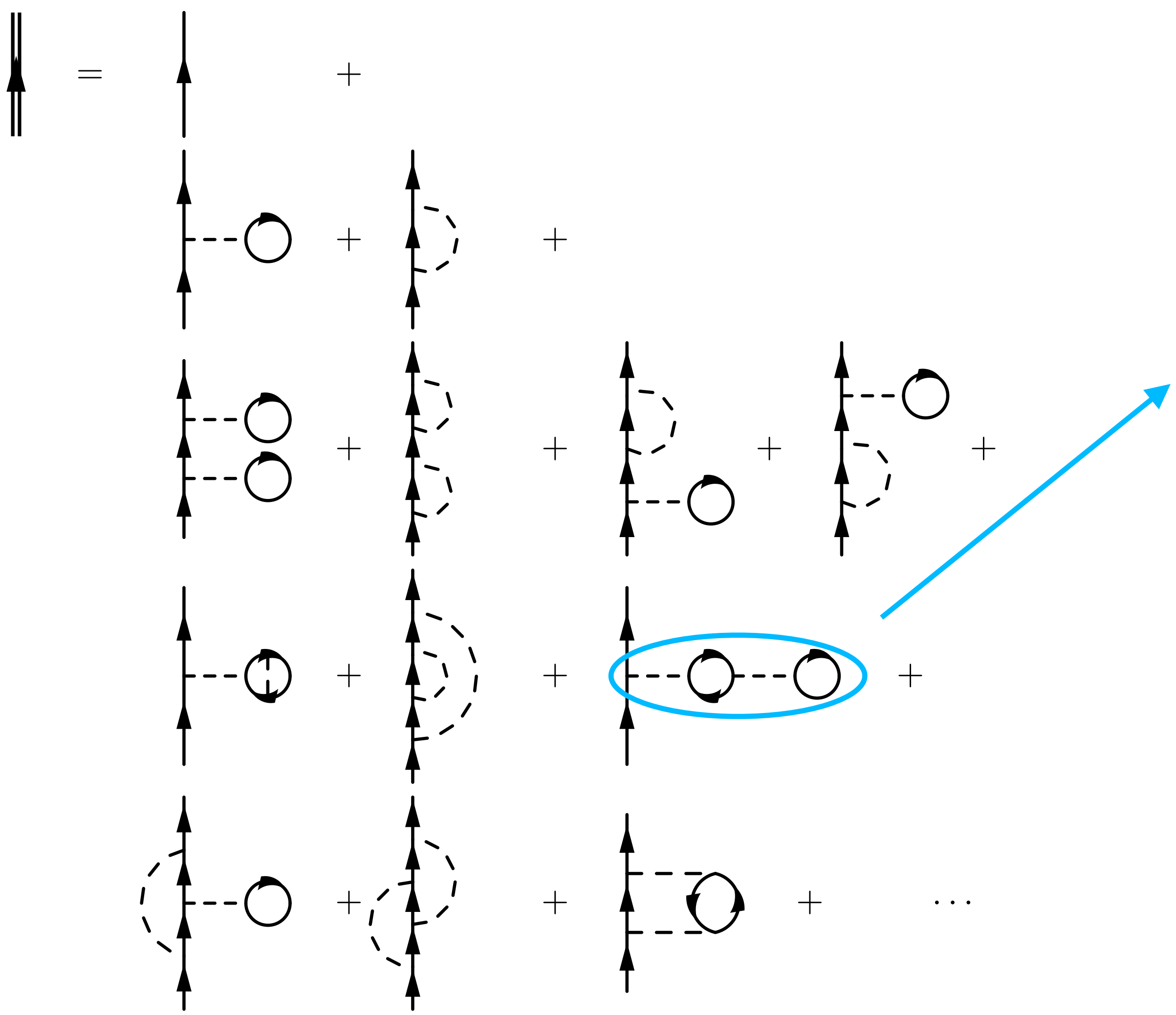


Dyson equation

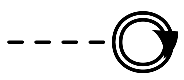
Dyson equation: diagrammatic expansion

⦿ Further select **two-particle irreducible** self-energy diagrams → ***Skeleton* self-energy**

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



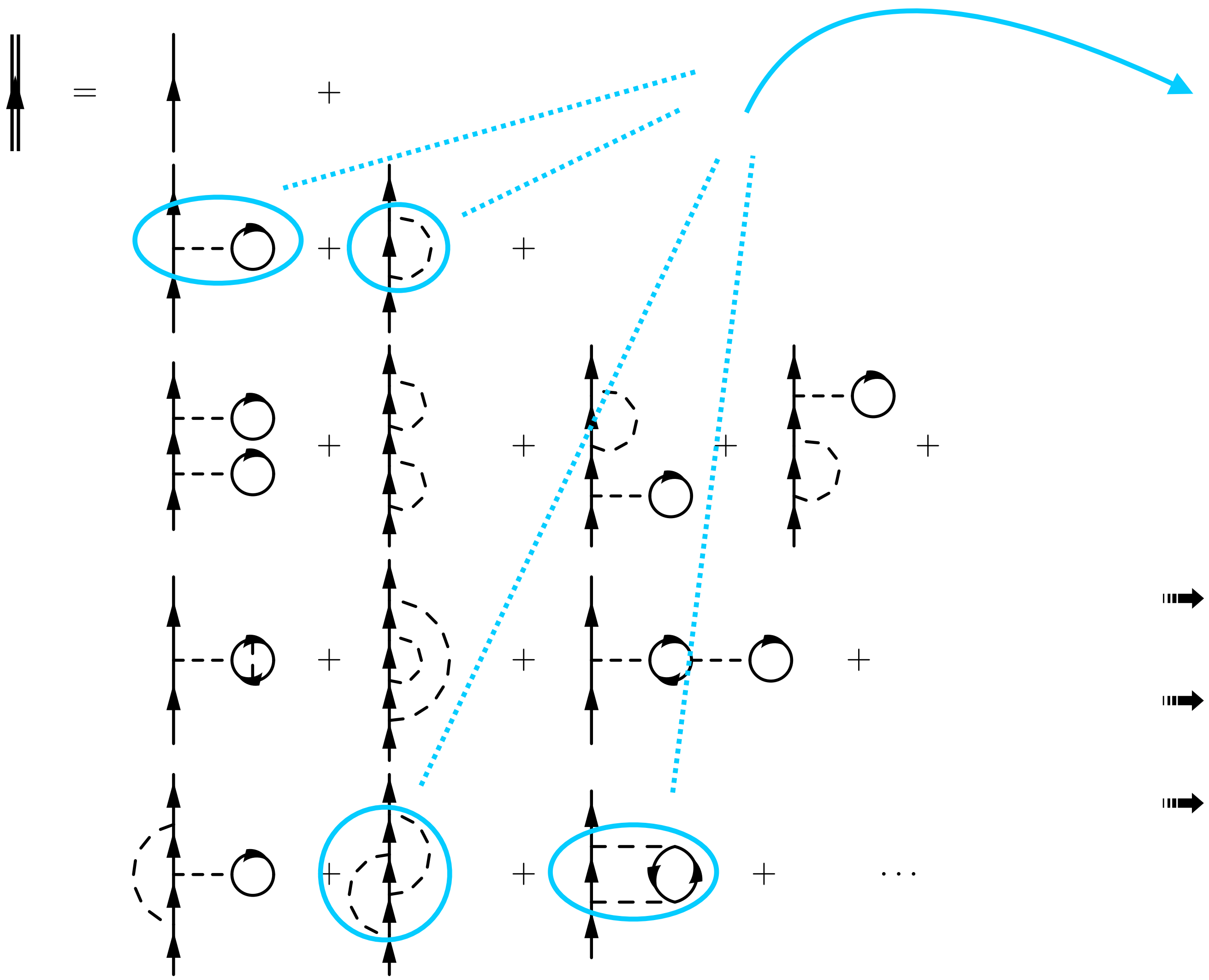
E.g. this can be generated by the self-energy term



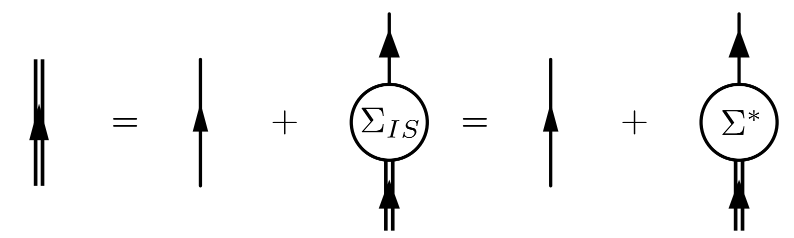
Dyson equation: diagrammatic expansion

⦿ Further select **two-particle irreducible** self-energy diagrams → ***Skeleton* self-energy**

➟ 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

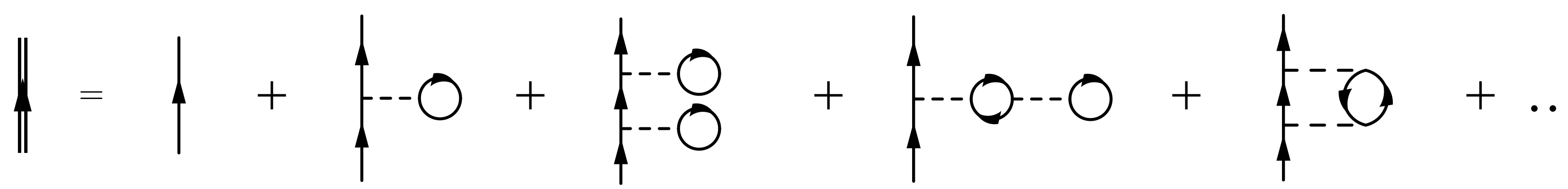
Approximations to the full Dyson equation

⦿ Full solution as expensive as (exact) configuration interaction

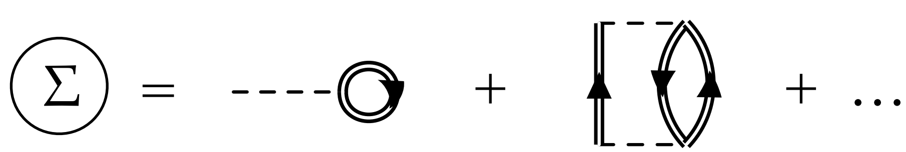
➟ Approximated solutions achieved via **truncated** diagrammatic expansions

⦿ Several possibilities

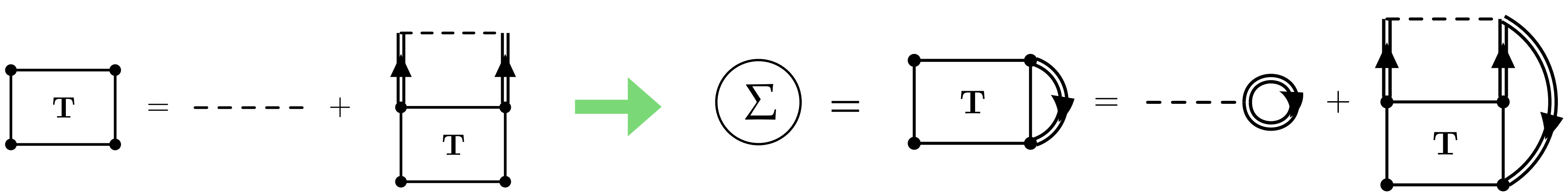
○ Truncate perturbative expansion of one-body propagator (no Dyson eq.)



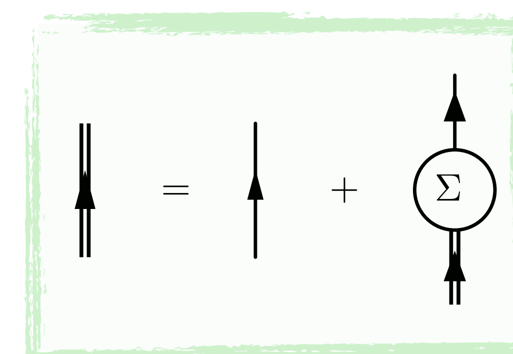
○ Truncate perturbative/skeleton expansion of self-energy



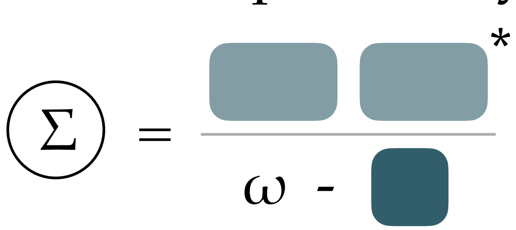
○ Resum (to infinite order) certain types of diagrams



Dyson eq.



○ Truncate & impose analytic form of exact self-energy



complete at perturbative order n

➟ Algebraic diagrammatic construction (ADC)

Spectral representation

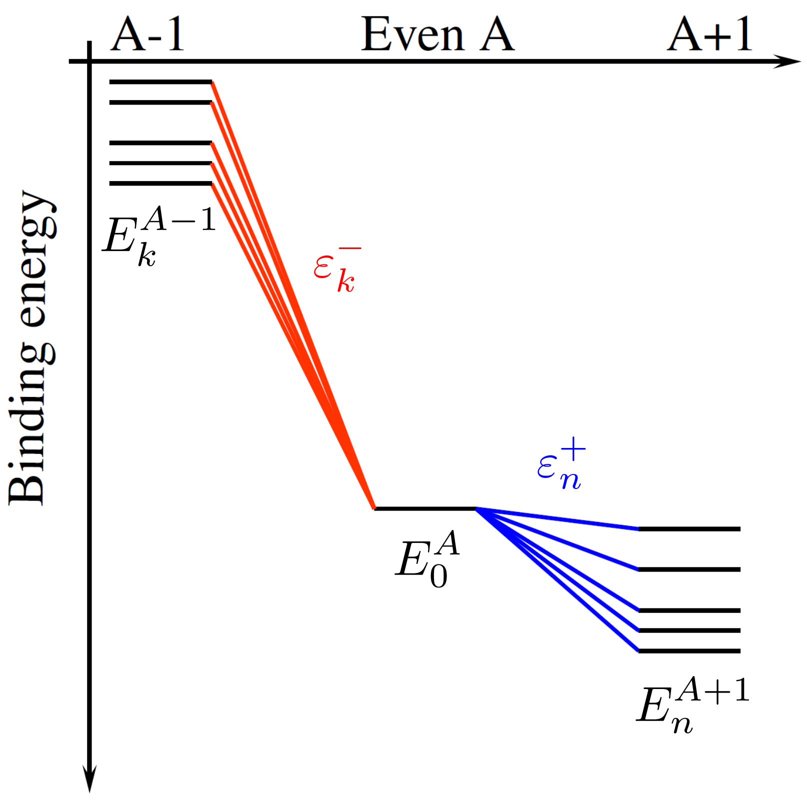
➪ Exact GF display a spectral representation

$$g_{\alpha\beta}(\omega) = \sum_n \frac{(\mathcal{X}_\alpha^n)^* \mathcal{X}_\beta^n}{\omega - \varepsilon_n^+ + i\eta} + \sum_k \frac{\mathcal{Y}_\alpha^k (\mathcal{Y}_\beta^k)^*}{\omega - \varepsilon_k^- - i\eta}$$

Separation energies

$$\varepsilon_n^+ = E_n^{A+1} - E_0^A$$

$$\varepsilon_k^- = E_0^A - E_k^{A-1}$$



Spectral representation

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

Transition amplitudes

$$\mathcal{X}^n_\alpha = \langle \Psi^{\text{A+1}}_n | a^\dagger_\alpha | \Psi^{\text{A}}_0 \rangle$$
$$\mathcal{Y}^k_\alpha = \langle \Psi^{\text{A-1}}_k | a_\alpha | \Psi^{\text{A}}_0 \rangle$$

Separation energies

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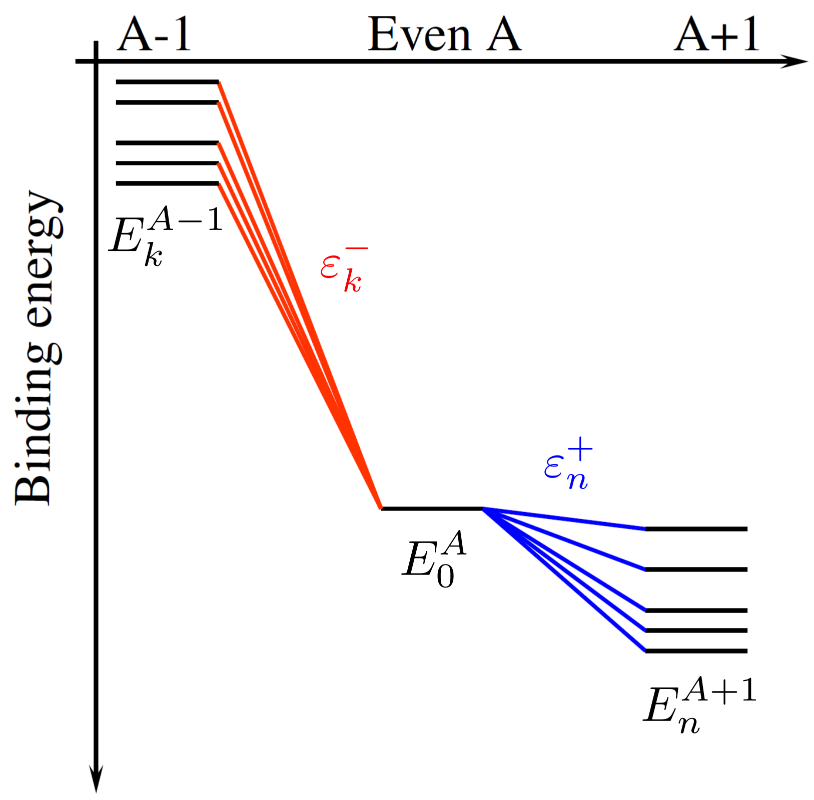

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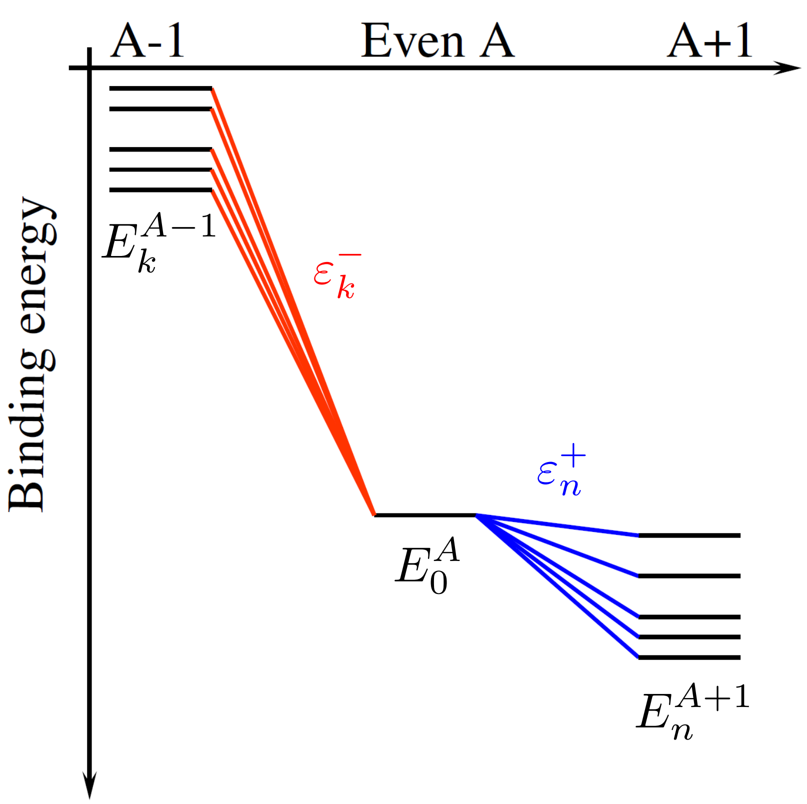
Separation energies

$$\varepsilon_n^+ = E_n^{A+1} - E_0^A$$
$$\varepsilon_k^- = E_0^A - E_k^{A-1}$$

Spectroscopic factors

$$SF_n^+ = \sum_{\alpha \in \mathcal{H}_1} |\mathcal{X}_\alpha^n|^2$$
$$SF_k^- = \sum_{\alpha \in \mathcal{H}_1} |\mathcal{Y}_\alpha^k|^2$$



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Numerator + denominator

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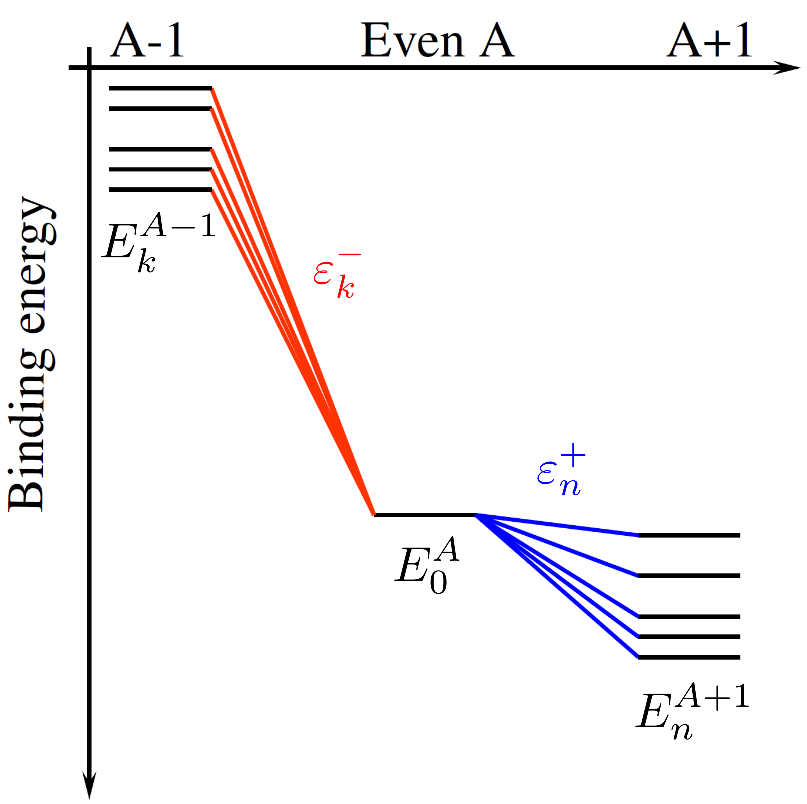

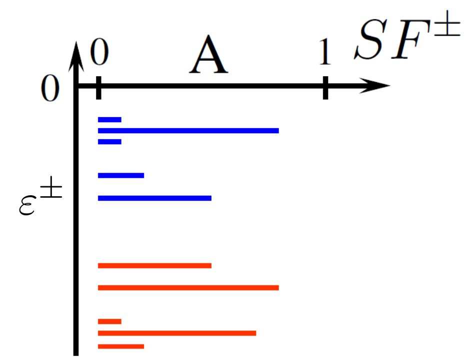

Spectral strength distribution

$$\mathcal{S}(\omega) = \sum_{n \in \mathcal{H}_{A+1}} SF_n^+ \, \delta(\omega - \varepsilon_n^+) + \sum_{k \in \mathcal{H}_{A-1}} SF_k^- \, \delta(\omega - \varepsilon_k^-)$$

Spectral representation

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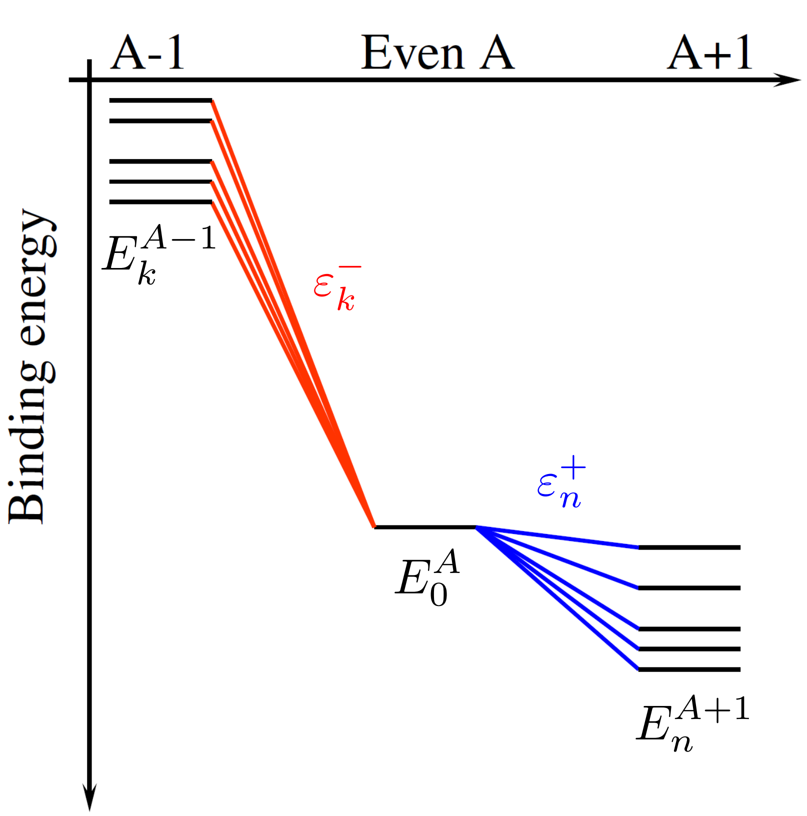

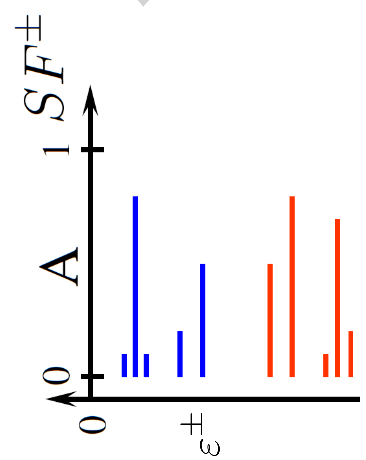

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Spectral representation

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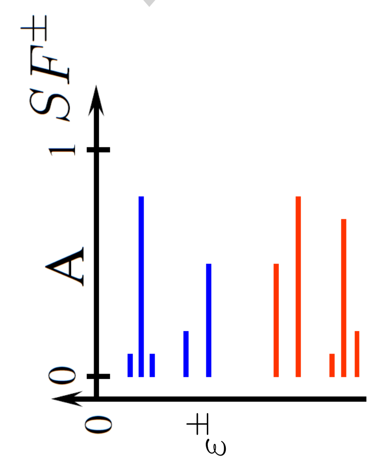
Numerator + denominator



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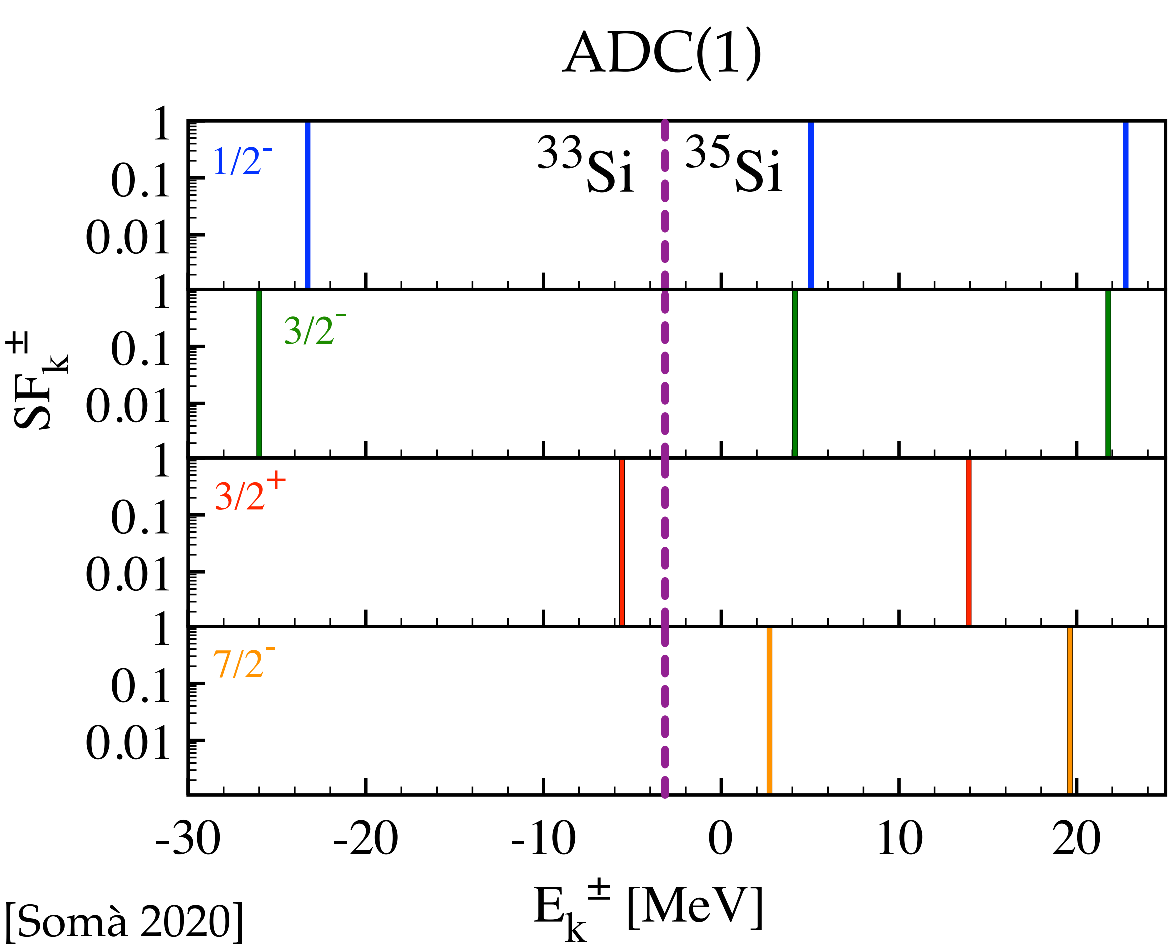

[Somà 2020]

Spectral strength distribution

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Spectral representation

➪ Exact GF display a spectral representation

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Separation energies

$$\varepsilon_n^+ = E_n^{A+1} - E_0^A$$
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Numerator + denominator

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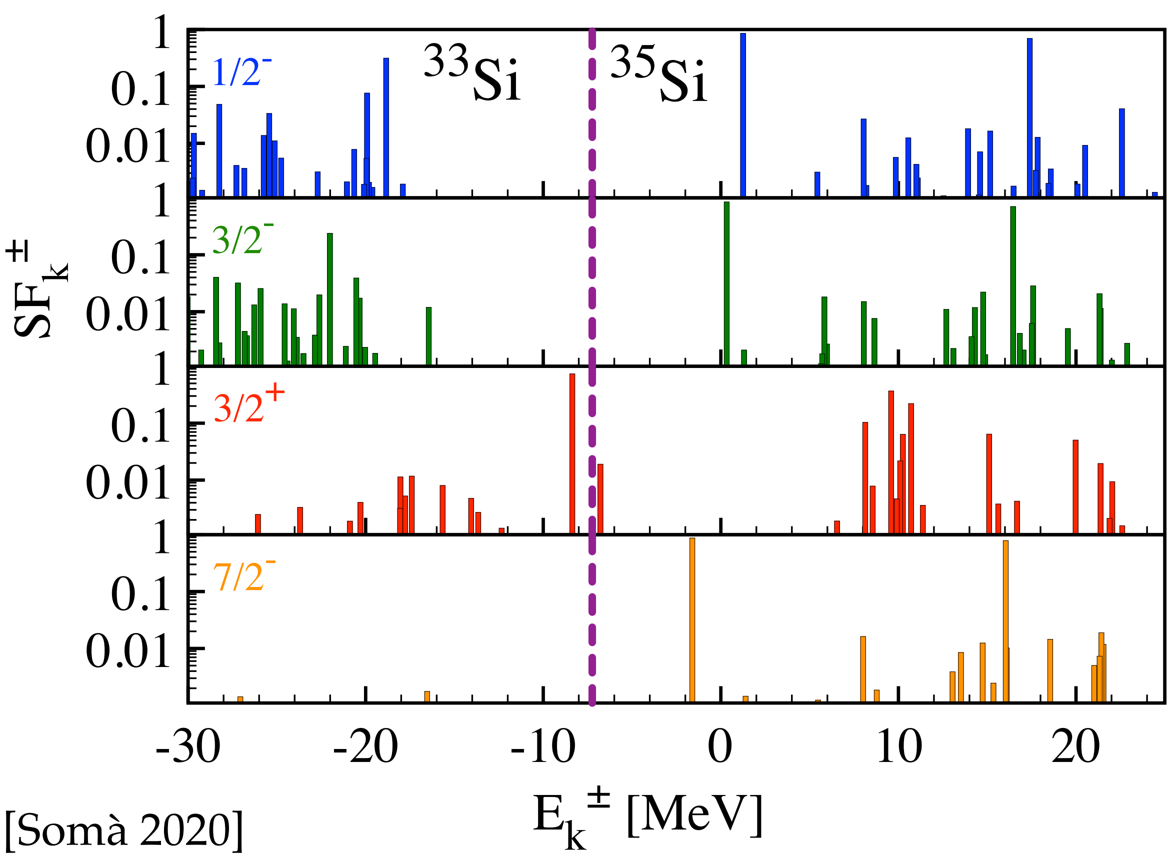
ADC(2)



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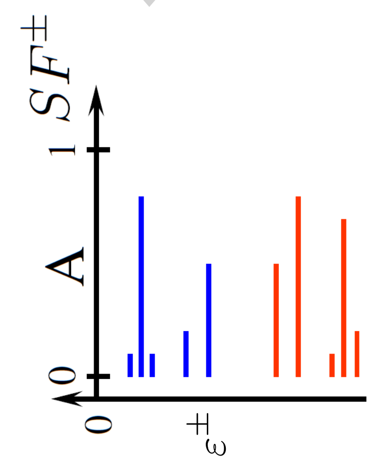

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Separation energies

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Numerator + denominator

Spectroscopic factors

$$SF_n^+ = \sum_{\alpha \in \mathcal{H}_1} |\mathcal{X}_\alpha^n|^2$$
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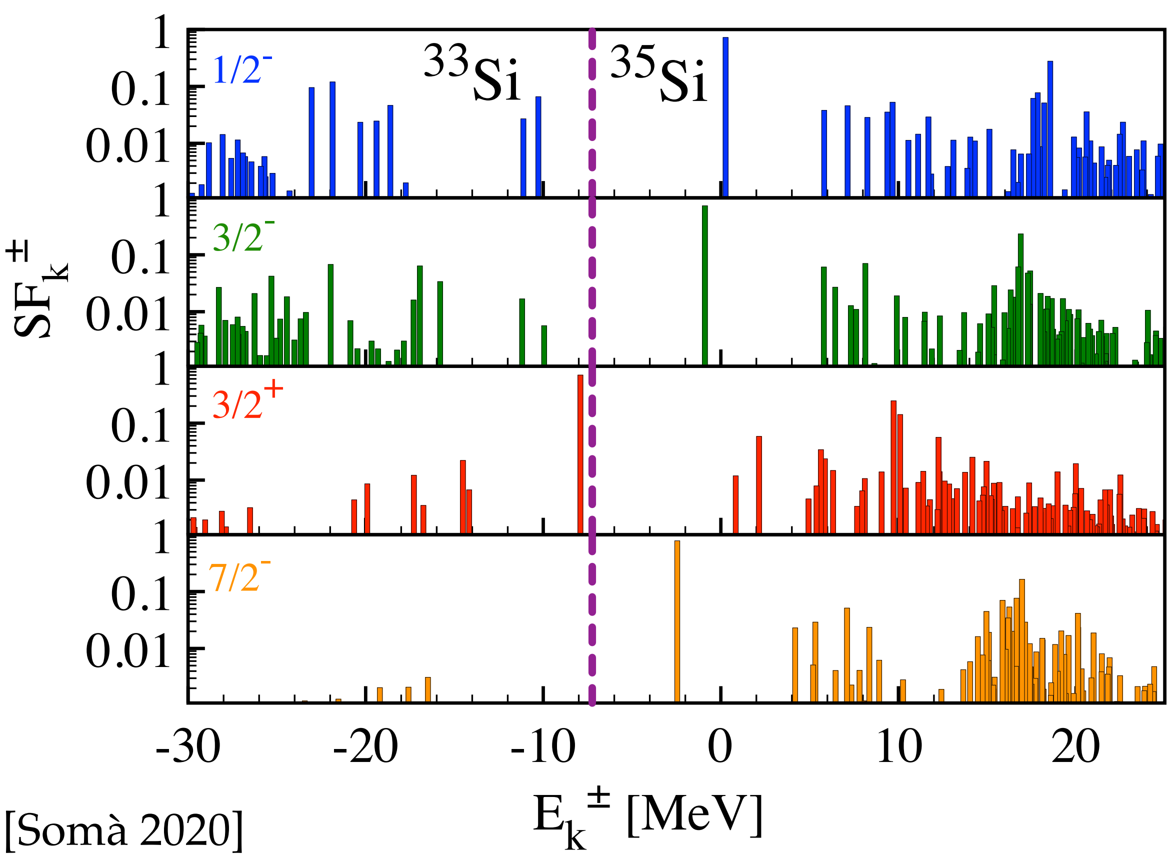
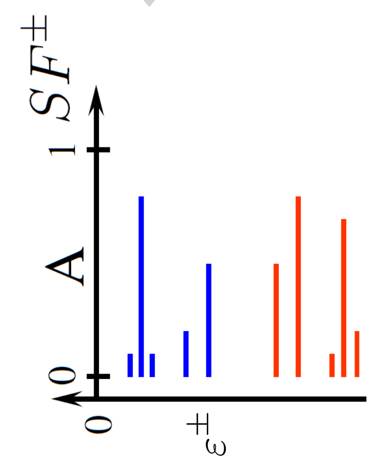
ADC(3)



[Somà 2020]



Spectral strength distribution

$$\mathcal{S}(\omega) = \sum_{n \in \mathcal{H}_{A+1}} SF_n^+ \, \delta(\omega - \varepsilon_n^+) + \sum_{k \in \mathcal{H}_{A-1}} SF_k^- \, \delta(\omega - \varepsilon_k^-)$$

Connection with experiments: direct reactions

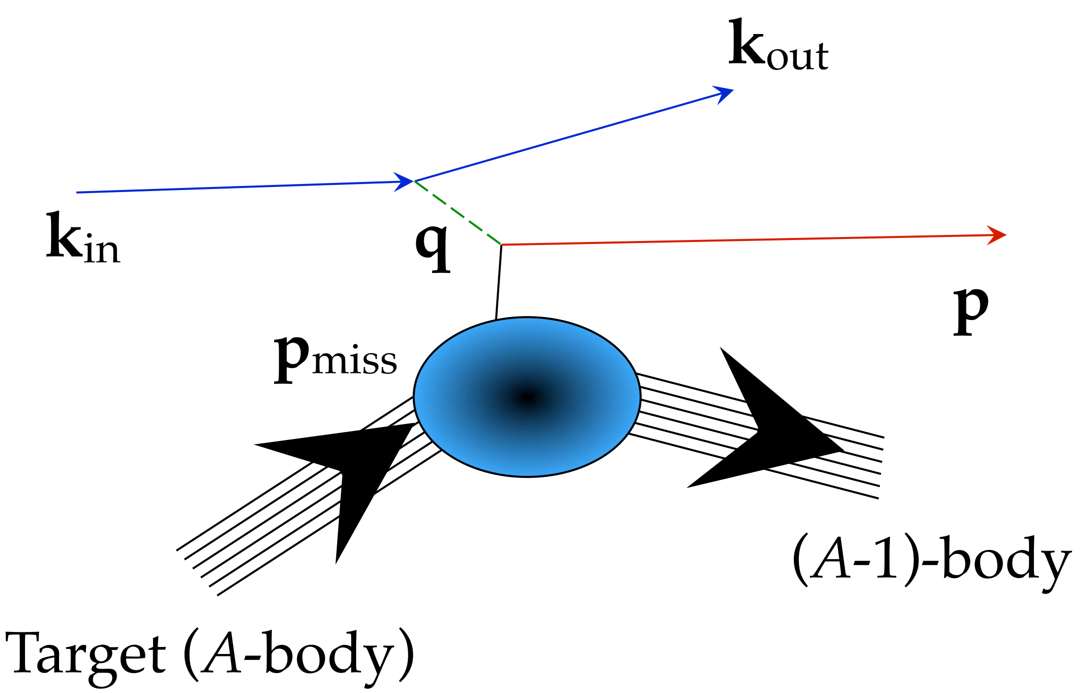
- Basic idea: spectroscopy via **direct knock-out reactions**
  - External probe transferring energy ω and momentum $\mathbf{q}$
  - Cross section $d\sigma \sim \sum_f \delta(\omega + E_i - E_f)\ |\langle \Psi_f | R(\mathbf{q}) | \Psi_i \rangle|^2$ with $R(\mathbf{q}) = \sum_{\mathbf{p}} a^\dagger_{\mathbf{p}}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

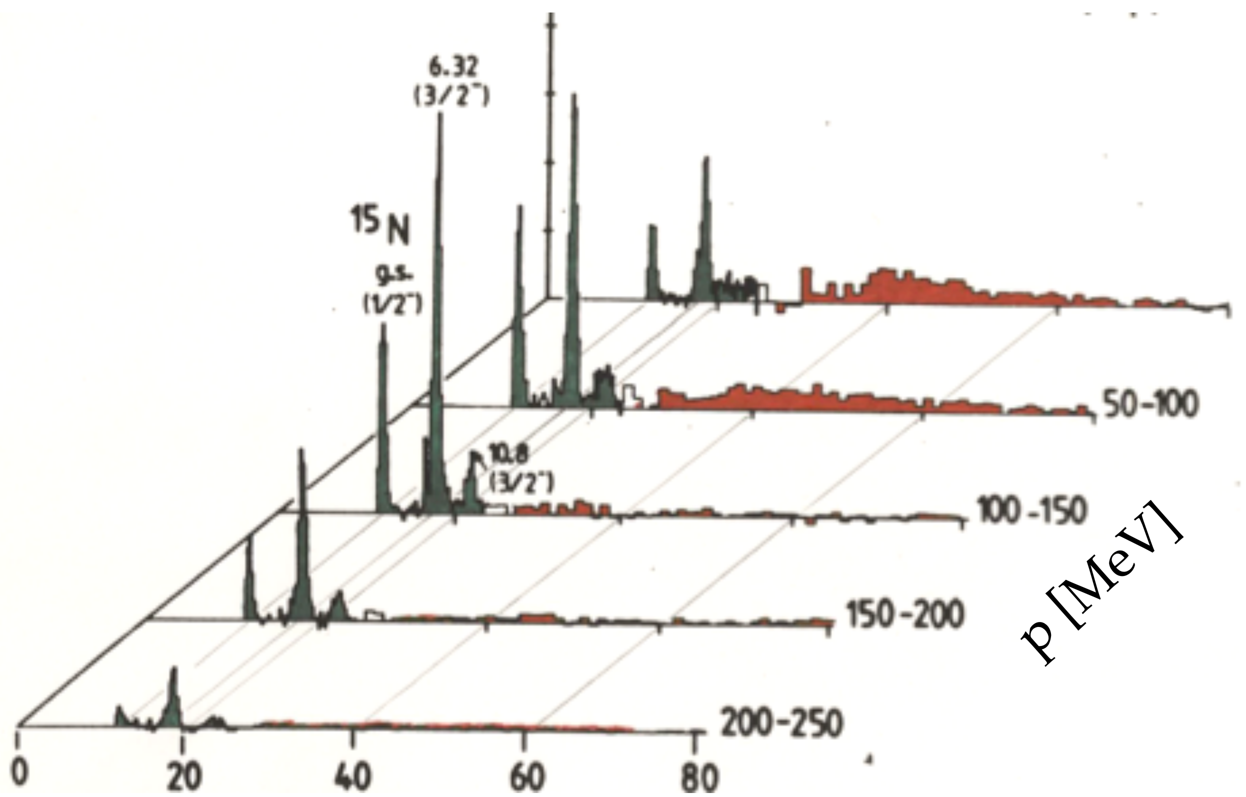
$$d\sigma \sim \sum_n \delta(E_{miss} - E_0^A + E_n^{A-1})\ \left|\langle \Psi_n^{A-1} | a_{\mathbf{p}_{miss}} | \Psi_0^A \rangle\right|^2$$
$$= S_{\mathbf{p}_{miss}}(E_{miss})$$



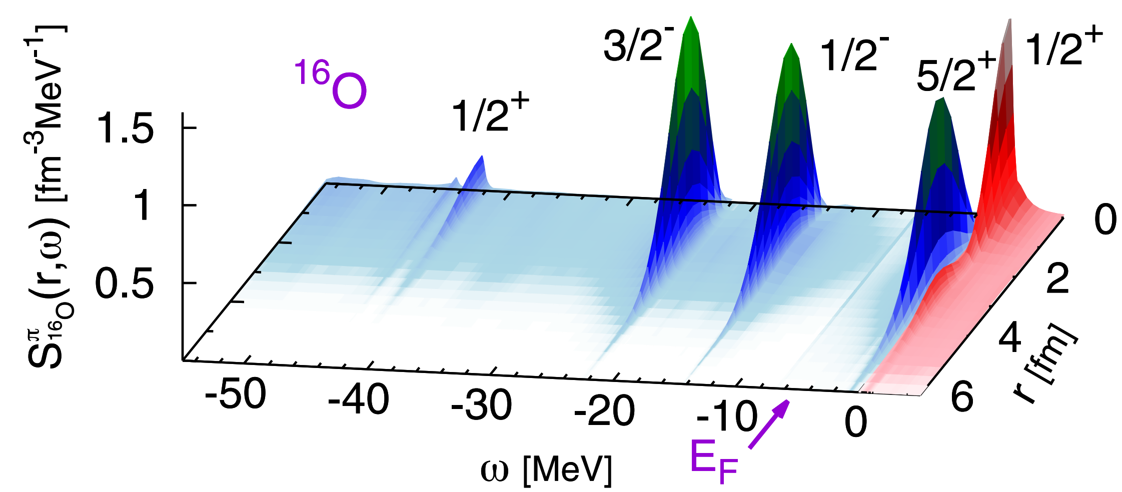
- Two assumptions
  - **Impulse approximation** (all energy transferred to one nucleon)
  - **No final state interactions**

Connection with experiments: direct reactions

⦿ Example: electron scattering



ω [MeV] [Mougey *et al.* 1980]



[Cipollone, Barbieri, Navrátil 2015]

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

GF calculations with chiral 2N+3N forces

However, keep in mind that

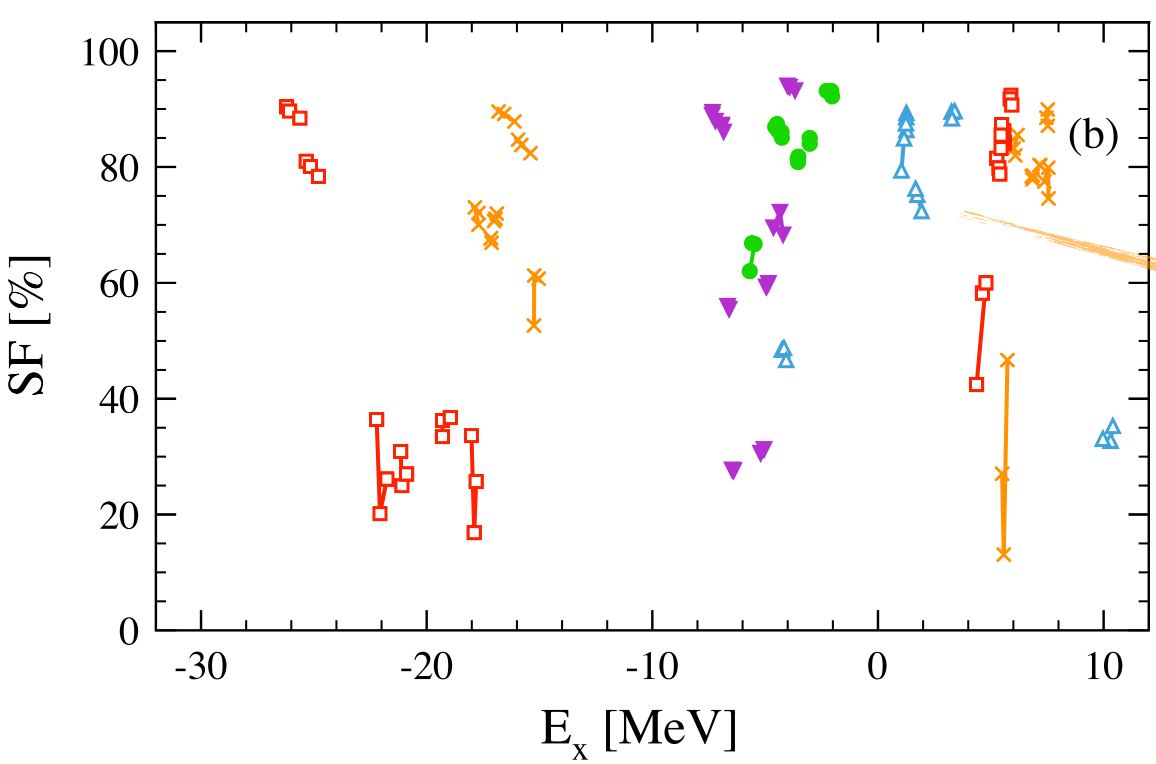
- Separation energies (position of the peaks in ω) are **observable** quantities
- Spectroscopic factors (height of the peaks) are **non-observable**

Observables vs non-observables

- Spectroscopic factors characterise how "correlated" the wave function is
  - SF close to 100% → all s.p. strength in one state → ~ independent particle picture
  - Low SF → Fragmented strength → highly correlated w.f. ≠ independent particle picture

This can be quantitatively discussed **only within a given model at a given resolution scale**

- Non-observability of spectroscopic factors
  - Can be mathematically proven
  - Was shown in actual GF calculations - in a limited interval of the res. scale ($\lambda \in$ [1.88, 2.23] fm^{-1})



[Duguet, Hergert, Holt, Somà 2015]

Scale dependence visible but not huge

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

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

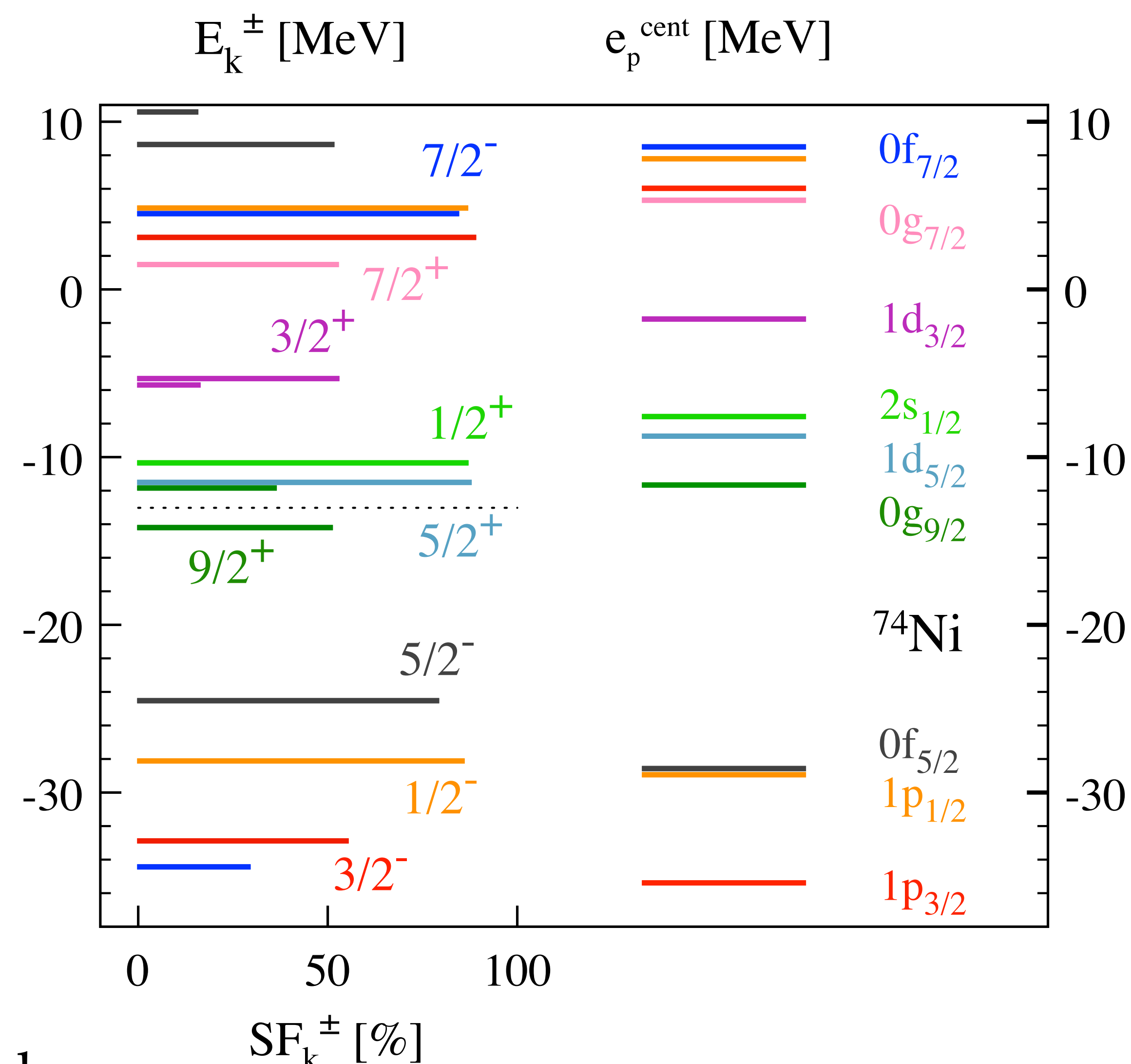
➟ Diagonalise

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

➟ 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]

Effective single-particle energies

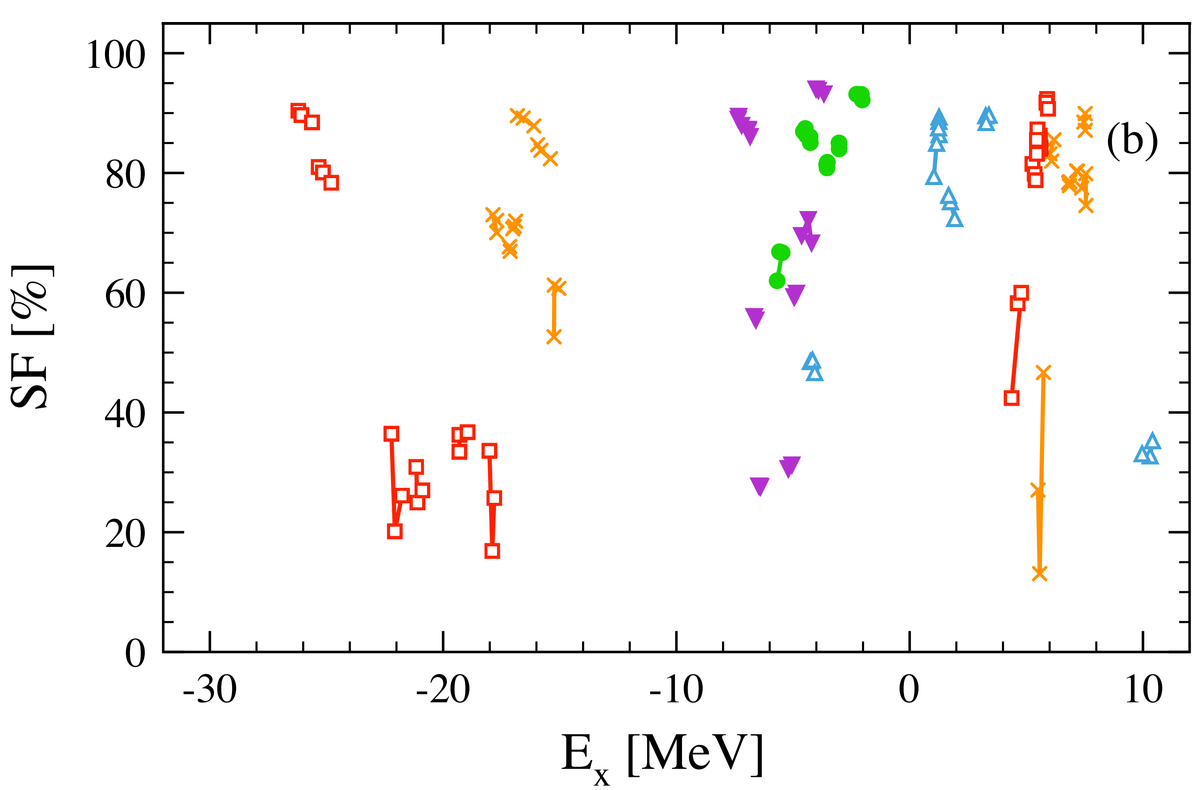
- Still, this decomposition is scale-dependent

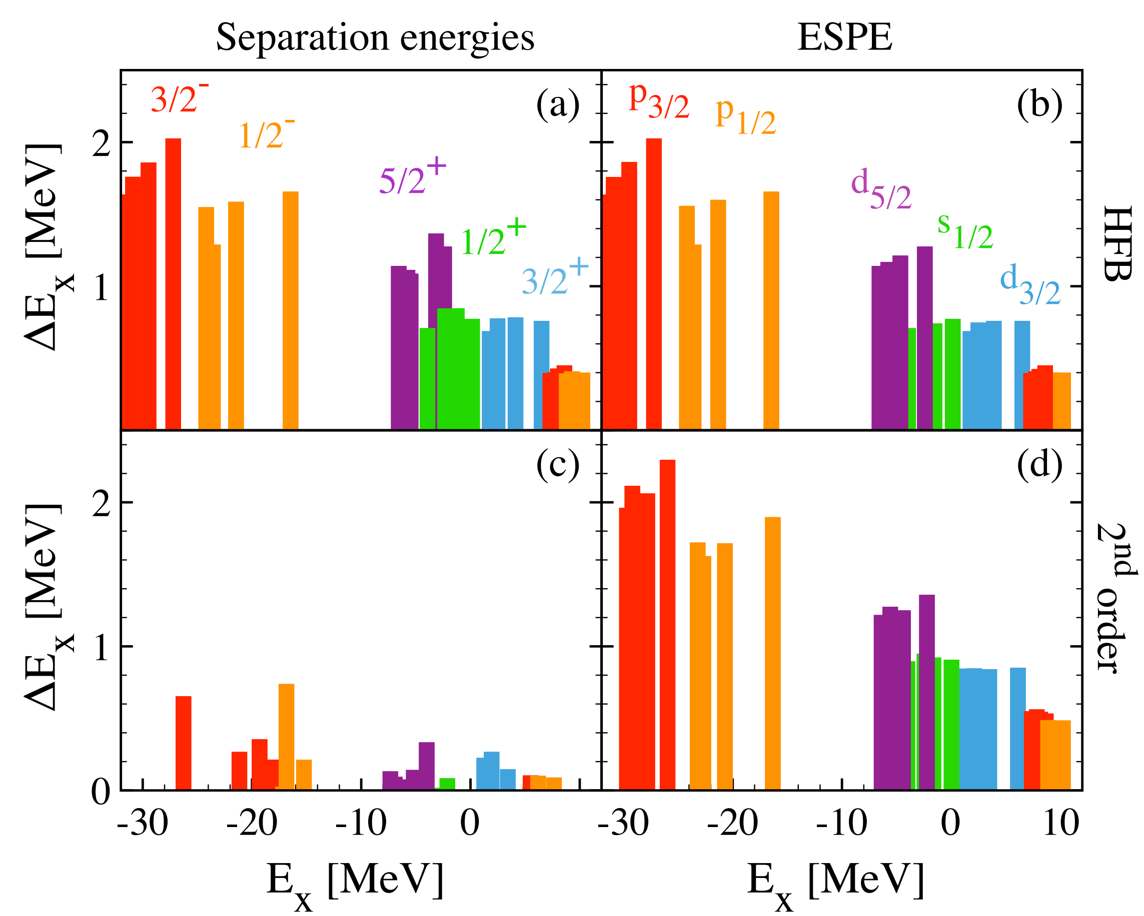
$$\underbrace{E^+_\mu}_{\text{invariant under } U(\lambda)} \equiv \underbrace{\sum_p s^{+pp}_\mu(\lambda) e^{\text{cent}}_p(\lambda)}_{\text{varies under } U(\lambda)} + \underbrace{\sum_{pq} s^{+pq}_\mu(\lambda) \Sigma^{\text{dyn}}_{qp}(E^+_\mu;\lambda)}_{\text{varies under } U(\lambda)}$$

(many-body observable; single-particle components; correlations)

➟ Also reconstructed ESPEs are **non-observable** quantities

- This can be again seen in actual GF calculations



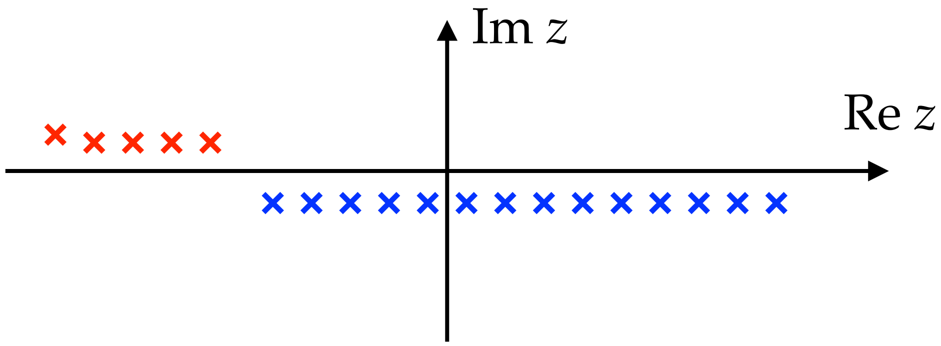


[Duguet, Hergert, Holt, Somà 2015]

Spectral representation: *finite* vs *infinite* systems

⊙ Recall the Källén-Lehmann representation

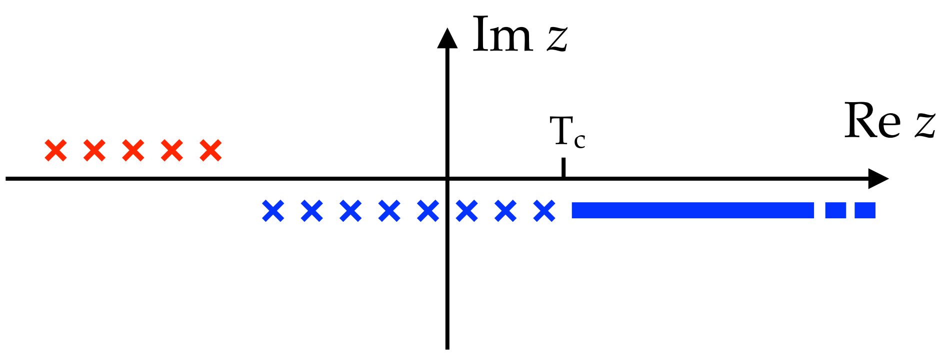
$$G_{ab}(z) = \sum_{\mu} \frac{\langle \Psi_0^A | a_a \,|\, \Psi_\mu^{A+1} \rangle \langle \Psi_\mu^{A+1} \,|\, a_b^\dagger | \Psi_0^A \rangle}{z - E_\mu^+ + i\eta} + \sum_{\nu} \frac{\langle \Psi_0^A | a_b^\dagger \,|\, \Psi_\nu^{A-1} \rangle \langle \Psi_\nu^{A-1} \,|\, a_a | \Psi_0^A \rangle}{z -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



with

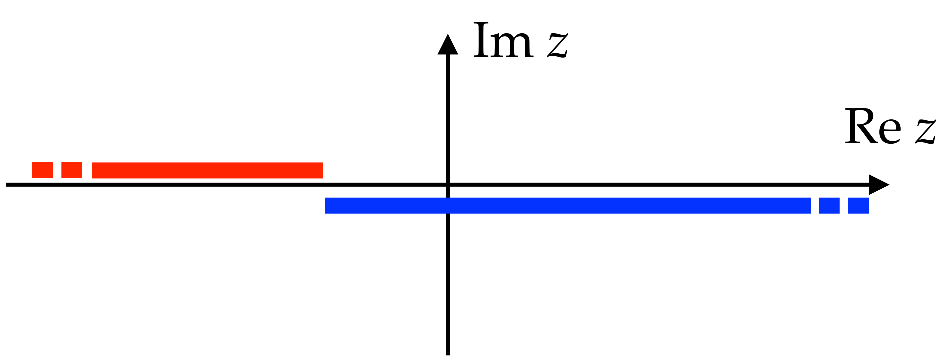
$$E_\mu^+ \equiv E_\mu^{A+1} - E_0^A$$
$$E_\nu^- \equiv E_0^A - E_\nu^{A-1}$$

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



⊙ Generally, 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

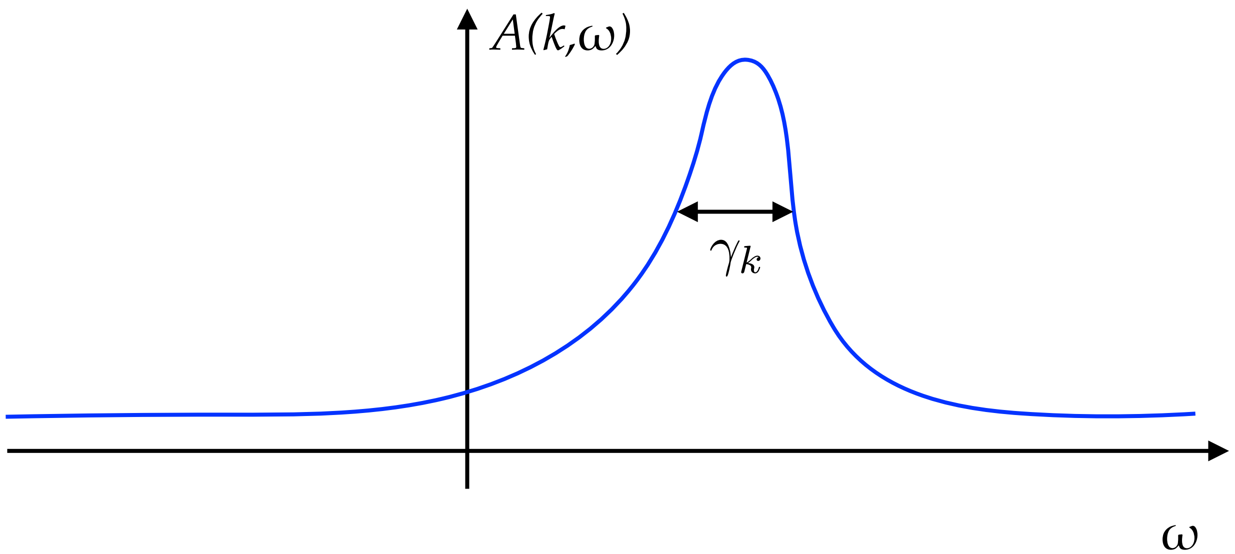
➟ Isolated poles no longer meaningful

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

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

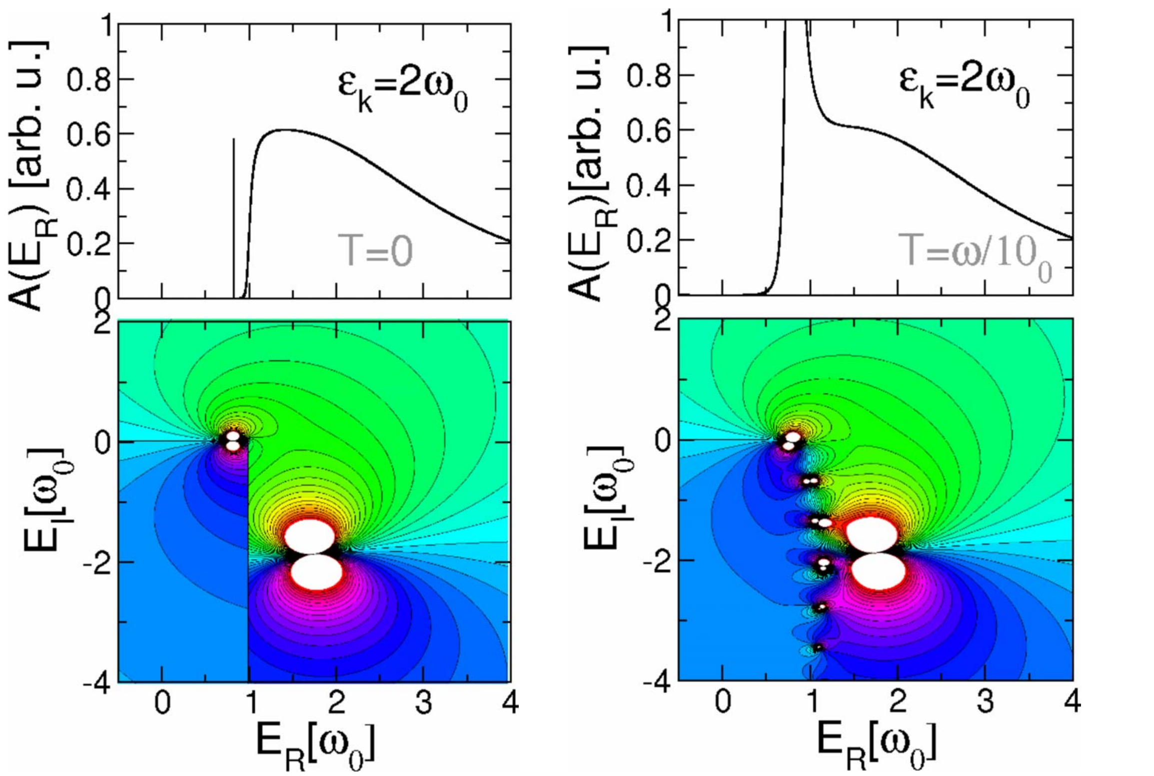
$$G^{-1}(k,z) = z - \frac{k^2}{2m} - \Sigma(k,z) \longrightarrow z_k = \varepsilon_k + i\gamma_k$$

Quasiparticle pole

- In practice, one needs to perform an analytic continuation of the self-energy

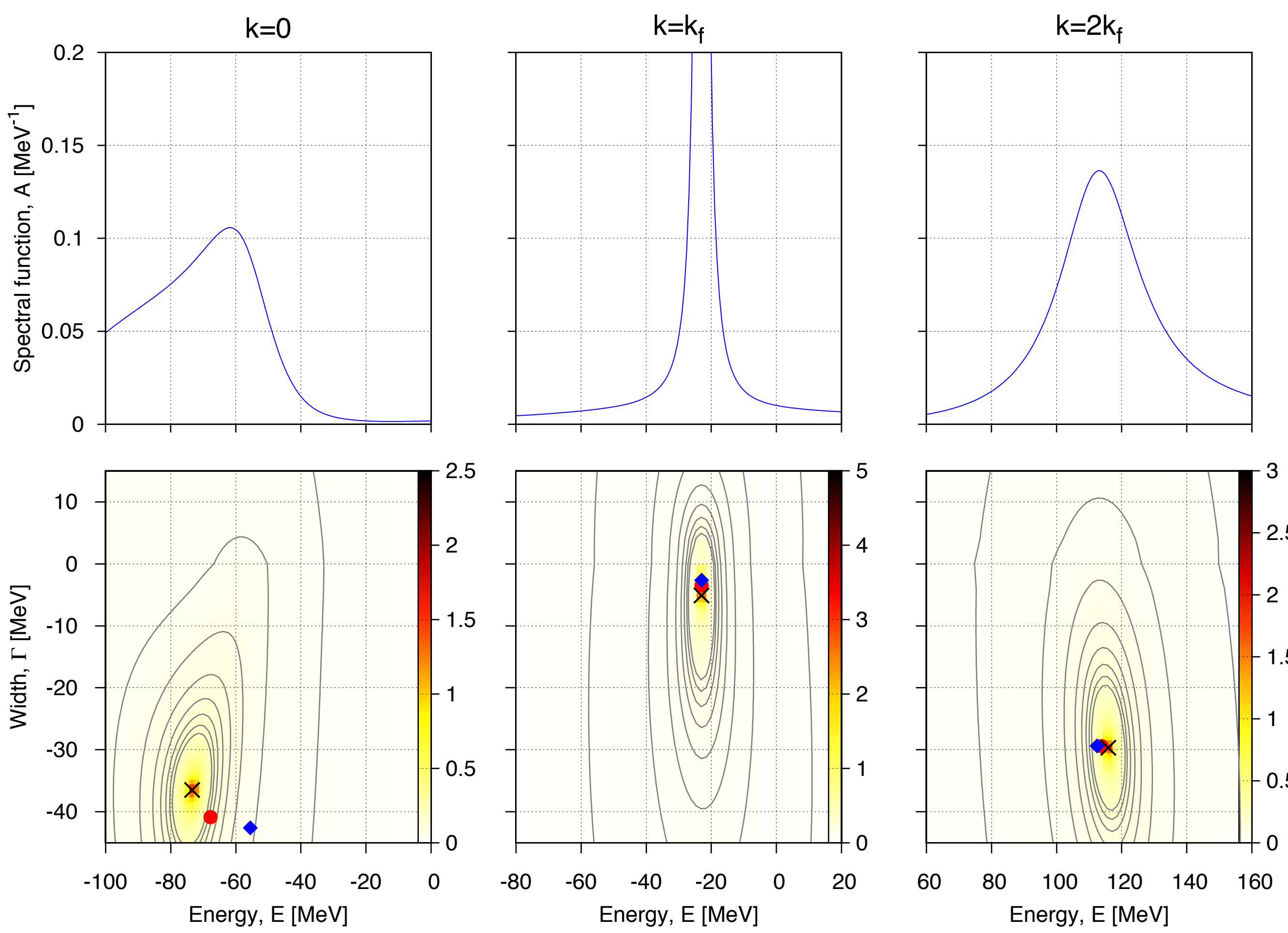
$$z(k) = \frac{k^2}{2m} + \text{Re}\tilde{\Sigma}(k, z(k)) + i\text{Im}\ \tilde{\Sigma}(k, z(k))$$

Electron-phonon Einstein model



[Eiguren, Ambrosch-Draxl & Echenique 2009]

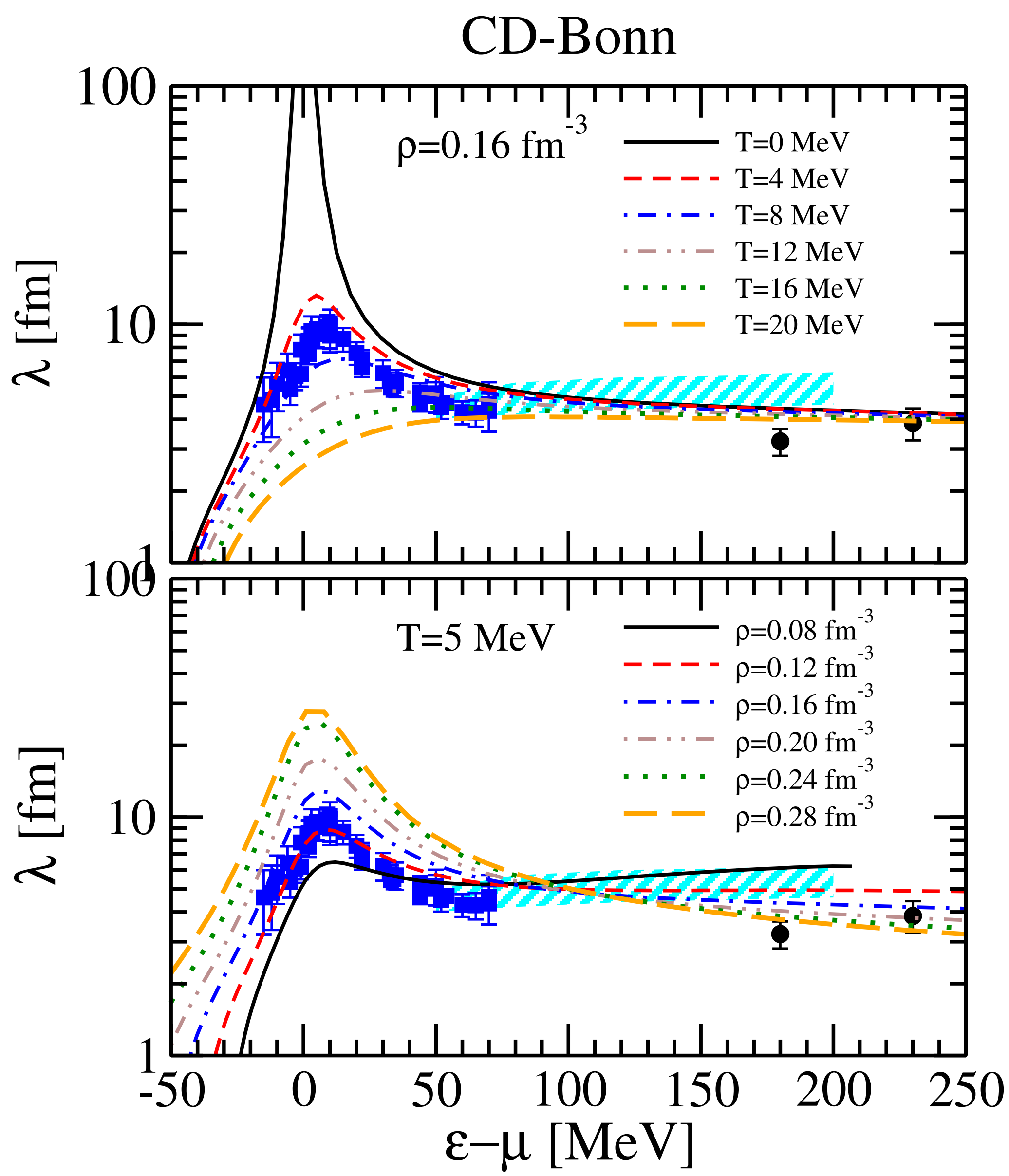
Symmetric nuclear matter



[Rios & Somà 2012]

Nucleon mean free path

⦿ Mean free path computed from quasiparticle lifetime and (group) velocity $\lambda_k = \frac{v_k}{\gamma_k} = \frac{\partial_k \varepsilon_k}{\gamma_k}$

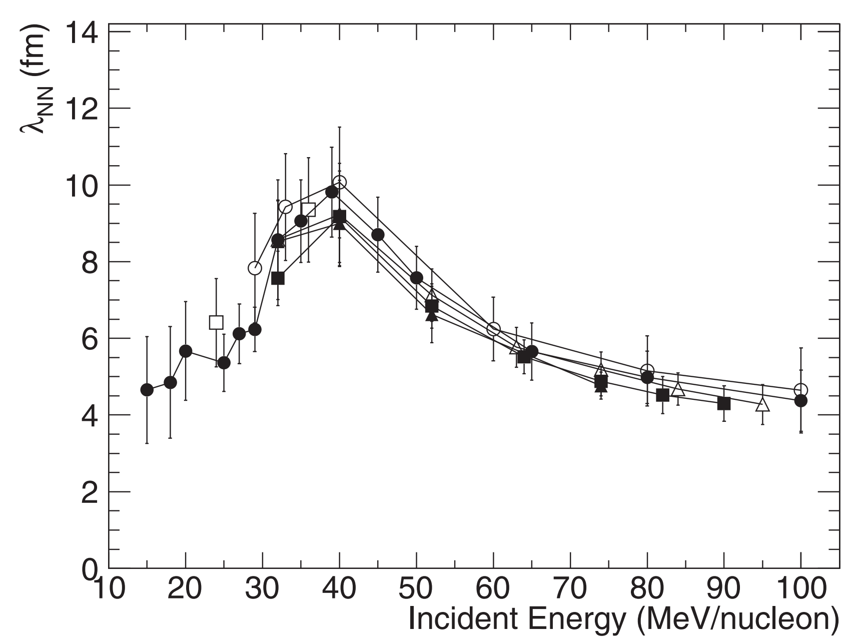


[Rios & Somà 2012]

○ Mean-free path extracted from "nuclear stopping"

○ Heavy-ion collisions

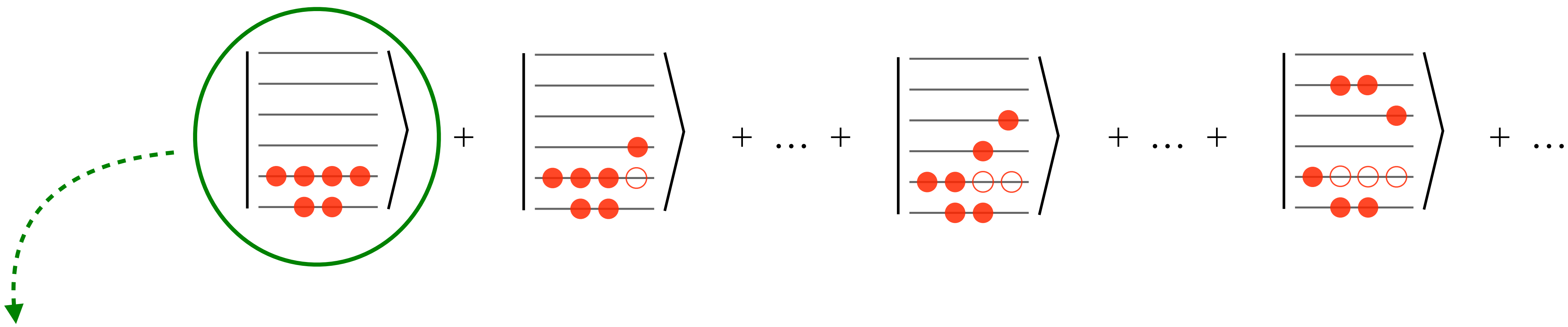
○ INDRA collaboration at GANIL



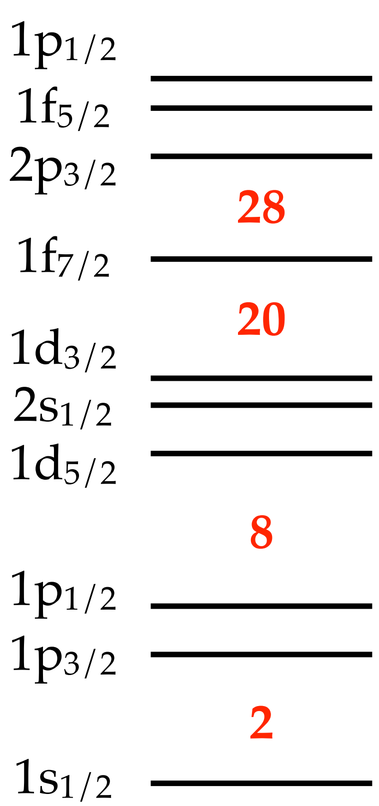
[Lopez *et al.* 2014]

Closed- vs. open-shell systems

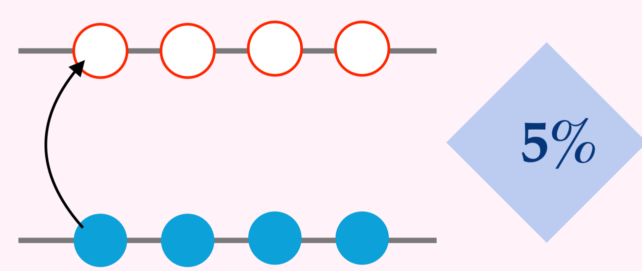
- In practice: the reference state varies with N & Z



Fill single-particle levels



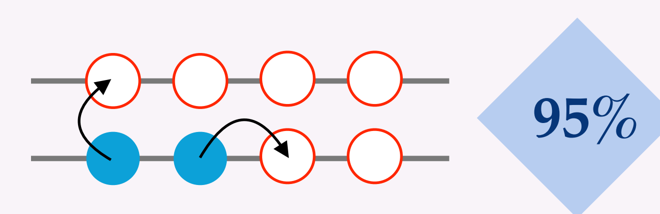
Closed-shell systems



Larger energy gap,
excitations hindered,
enhanced stability

Clear ph hierarchy,
expansion **well defined**

Open-shell systems

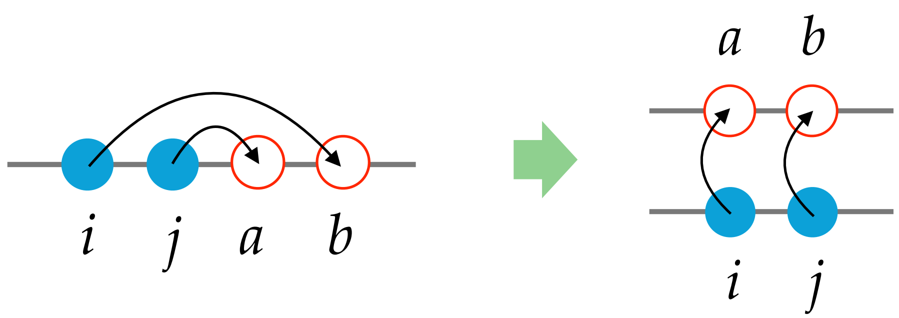


Smaller (→ 0) energy gap,
excitations enabled,
lesser stability

No ph hierarchy,
expansion **ill defined**

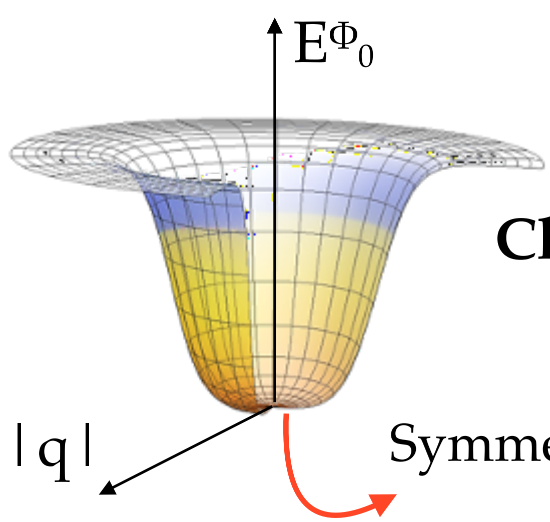
Symmetry breaking

⦿ Idea: reopen gap via **symmetry breaking** **(→ $G_{\text{Ham}} \neq G_{\text{wf}}$)**



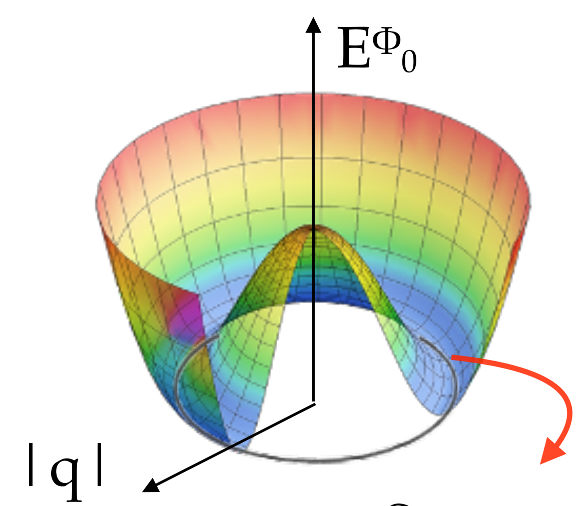
$$\langle \Phi_0 | Q | \Phi_0 \rangle = q \equiv |q| e^{i \arg(q)}$$

Order parameter



Closed-shell systems

Symmetry-conserving minimum



Open-shell systems

Symmetry-breaking minimum

Physical symmetry	*Group*	*Correlations*
Rotational inv.	SU(2)	Deformation
Particle-number	$U(1)_N \times U(1)_Z$	Superfluidity

Singly open-shell ➪ Sufficient to **break U(1)**

Doubly open-shell ➪ Necessary to **break SU(2)**

✔ **Advantage:** polynomial scaling (N^α) ✗ **Prices to pay:** N increases + symmetries must be restored

Gorkov Green's functions

Pairing correlations ➪

$$E_0^{A\pm 2n}(Z\pm 2n, N) - E_0^{A}(Z,N) \approx \pm\ 2n\mu_Z$$
$$E_0^{A\pm 2n}(Z, N\pm 2n) - E_0^{A}(Z,N) \approx \pm\ 2n\mu_N$$

Degeneracy associated to creating / annihilating pairs

Hamiltonian → Grand-canonical potential

$$\Omega \equiv H - \mu_Z Z - \mu_N N$$

G.s. wave function in equilibrium with a reservoir of Cooper pairs

Symmetry-breaking wave function

$$|\Psi_0\rangle = \sum_A^{\text{even}} |\Psi_0^A\rangle$$

SOVIET PHYSICS JETP VOLUME 34(7), NUMBER 3 SEPTEMBER, 1958

ON THE ENERGY SPECTRUM OF SUPERCONDUCTORS

L. P. GOR'KOV

Institute for Physical Problems, Academy of Sciences, U.S.S.R.

Submitted to JETP editor November 18, 1957

J. Exptl. Theoret. Phys. (U.S.S.R.) **34**, 735-739 (March, 1958)

A method is proposed, based on the mathematical apparatus of quantum field theory, for the calculation of the properties of a system of Fermi particles with attractive interaction.

Generalised one-body GFs

$$\mathrm{i}\, g^{11}_{\alpha\beta}(t-t') \equiv \langle\Psi_0|\ T[a_\alpha(t)a^\dagger_\beta(t')]\ |\Psi_0\rangle$$
$$\mathrm{i}\, g^{12}_{\alpha\beta}(t-t') \equiv \langle\Psi_0|\ T[a_\alpha(t)\bar{a}_\beta(t')]\ |\Psi_0\rangle$$
$$\mathrm{i}\, g^{21}_{\alpha\beta}(t-t') \equiv \langle\Psi_0|\ T[\bar{a}^\dagger_\alpha(t)a^\dagger_\beta(t')]\ |\Psi_0\rangle$$
$$\mathrm{i}\, g^{22}_{\alpha\beta}(t-t') \equiv \langle\Psi_0|\ T[\bar{a}^\dagger_\alpha(t)\bar{a}_\beta(t')]\ |\Psi_0\rangle$$

Nambu notation

$$\mathrm{i}\,\mathbf{g}_{\alpha\beta}(t-t') \equiv \langle\Psi_0|T\left\{\mathbf{A}_\alpha(t)\mathbf{A}^\dagger_\beta(t')\right\}|\Psi_0\rangle = \mathrm{i}\begin{pmatrix} g^{11}_{\alpha\beta}(t-t') & g^{12}_{\alpha\beta}(t-t') \\ g^{21}_{\alpha\beta}(t-t') & g^{22}_{\alpha\beta}(t-t') \end{pmatrix}$$

Gorkov Green's functions

Gorkov equation

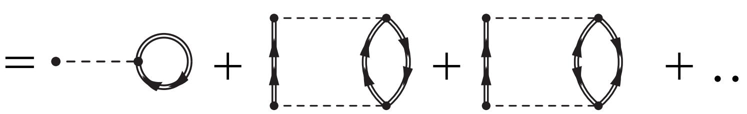
$$\mathbf{g}_{\alpha\beta}(\omega) = \mathbf{g}_{0\,\alpha\beta}(\omega) + \sum_{\gamma\,\delta} \mathbf{g}_{0\,\alpha\gamma}(\omega)\, \boldsymbol{\Sigma}^{\star}_{\gamma\delta}(\omega)\, \mathbf{g}_{\gamma\beta}(\omega)$$

Self-energy matrix

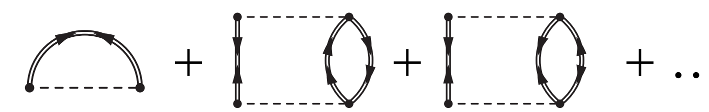
$$\boldsymbol{\Sigma}^{\star}_{\alpha\beta}(\omega) \equiv \begin{pmatrix} \Sigma^{\star\,11}_{\alpha\beta}(\omega) & \Sigma^{\star\,12}_{\alpha\beta}(\omega) \\ \Sigma^{\star\,21}_{\alpha\beta}(\omega) & \Sigma^{\star\,22}_{\alpha\beta}(\omega) \end{pmatrix}$$

Perturbative expansion

$\Sigma^{\star\,11}_{\alpha\beta}(\omega) =$



$\Sigma^{\star\,21}_{\alpha\beta}(\omega) =$



[Somà, Duguet, Barbieri 2011]

Observables

$$\langle \Psi_0 | O | \Psi_0 \rangle = \sum_{\alpha\beta} o_{\alpha\beta}\, \rho_{\beta\alpha} \qquad \text{where} \qquad \rho_{\alpha\beta} \equiv \langle \Psi_0 | c^{\dagger}_{\beta} c_{\alpha} | \Psi_0 \rangle = \frac{1}{\pi} \int_{-\infty}^{0} \operatorname{Im} g^{11}_{\alpha\beta}(\omega)\, d\omega$$

➪ Generalised Koltun sum rule holds

$$\Omega_0 = \frac{1}{2\pi} \int_{-\infty}^{0} d\omega \sum_{\alpha\beta} \left[t_{\alpha\beta} - \mu\delta_{\alpha\beta} + \omega\delta_{\alpha\beta} \right] \operatorname{Im} g^{11}_{\beta\alpha}(\omega)$$

Spectral representation

$$\mathbf{g}_{\alpha\beta}(\omega) = \sum_{k} \left\{ \frac{\mathbf{X}^{k}_{\alpha}\, \mathbf{X}^{k\dagger}_{\beta}}{\omega - \omega_k + i\eta} + \frac{\mathbf{Y}^{k}_{\alpha}\, \mathbf{Y}^{k\dagger}_{\beta}}{\omega + \omega_k - i\eta} \right\}$$

✗ **Missing step:** symmetry restoration

- Correct particle number *on average*
- Observables "contaminated"
- Effect depends on nucleus and observable

Algebraic diagrammatic construction

Gorkov self-energy has the general form

$$\Sigma^{\star}_{\alpha\beta}(\omega) = -\mathbf{U} + \Sigma^{(\infty)}_{\alpha\beta} + \tilde{\Sigma}_{\alpha\beta}(\omega)$$

Dynamical part has also a spectral representation

$$\tilde{\Sigma}_{\alpha\beta}(\omega) = \sum_k \left\{ \frac{\mathbf{M}^k_\alpha \, \mathbf{M}^{k\dagger}_\beta}{\omega - E_k + i\eta} + \frac{\mathbf{N}^k_\alpha \, \mathbf{N}^{k\dagger}_\beta}{\omega + E_k - i\eta} \right\} \equiv \tilde{\Sigma}^+_{\alpha\beta}(\omega) + \tilde{\Sigma}^-_{\alpha\beta}(\omega)$$

$$\tilde{\Sigma}^+_{\alpha\beta}(\omega) = \mathbf{M}_\alpha \left(\omega \mathbf{1} - \mathbf{E}\right)^{-1} \mathbf{M}^\dagger_\beta$$

Expand in perturbation

$$\tilde{\Sigma}^+_{\alpha\beta}(\omega) = \tilde{\Sigma}^{+\,(1)}_{\alpha\beta}(\omega) + \tilde{\Sigma}^{+\,(2)}_{\alpha\beta}(\omega) + \dots$$

Algebraic diagrammatic construction (ADC) postulates

$$\tilde{\Sigma}^{+\,\mathrm{ADC}}_{\alpha\beta}(\omega) = \mathbf{C}_\alpha \left(\omega \mathbf{1} - \mathbf{W} - \mathbf{P}\right)^{-1} \mathbf{C}^\dagger_\beta$$

[Schirmer *et al.* 1983]

Expand in perturbation

$$\mathbf{P} = \mathbf{P}^{(1)} + \mathbf{P}^{(2)} + \dots$$

$$\mathbf{C}_\alpha = \mathbf{C}^{(1)}_\alpha + \mathbf{C}^{(2)}_\alpha + \dots$$

Match **ADC(n)** to **n-th** order perturbation theory

$$\tilde{\Sigma}^{+\,\mathrm{ADC}}_{\alpha\beta}(\omega) = \mathbf{C}_\alpha \left(\omega \mathbf{1} - \mathbf{W}\right)^{-1} \sum_{n=0}^{\infty} \left\{ \mathbf{P} \left(\omega \mathbf{1} - \mathbf{W}\right)^{-1} \right\}^n \mathbf{C}^\dagger_\beta$$

➪ **ADC: re-organisation of the perturbative series**

- ○ Systematic set of approximations ADC(n)
- ○ Infinite partial resummations [from ADC(3)]
- ○ Analytic structure preserved ← causality

Gorkov ADC

- ○ ADC(2) derived & implemented

  [Somà, Duguet, Barbieri 2011]

- ○ ADC(3) derived

  [Barbieri, Duguet, Somà 2022]

Algebraic diagrammatic construction

⊙ **ADC → rewrite Gorkov equation as an energy-independent eigenvalue problem**

$$\mathbf{g}_{\alpha\beta}(\omega) = \mathbf{g}_{0\,\alpha\beta}(\omega) + \sum_{\gamma\,\delta} \mathbf{g}_{0\,\alpha\gamma}(\omega)\,\mathbf{\Sigma}^{\star}_{\gamma\delta}(\omega)\,\mathbf{g}_{\gamma\beta}(\omega)$$

Exploit analytic structure of $\mathbf{g}$

$$\mathbf{g}_{\alpha\beta}(\omega) = \sum_k \left\{ \frac{\mathbf{X}^k_\alpha\,\mathbf{X}^{k\dagger}_\beta}{\omega - \omega_k + \mathrm{i}\eta} + \frac{\mathbf{Y}^k_\alpha\,\mathbf{Y}^{k\dagger}_\beta}{\omega + \omega_k - \mathrm{i}\eta} \right\}$$

$$\omega_k \mathbf{X}^k_\alpha = \sum_\beta \mathbf{\Sigma}_{\alpha\beta}(\omega)\mathbf{X}^k_\beta$$

Energy-**dependent** eigenvalue problem

Exploit analytic structure of $\mathbf{\Sigma}$

$$\tilde{\mathbf{\Sigma}}^{+\,\mathrm{ADC}}_{\alpha\beta}(\omega) = \mathbf{C}_\alpha \left(\omega\mathbf{1} - \mathbf{W} - \mathbf{P}\right)^{-1} \mathbf{C}^\dagger_\beta$$

$$\omega_k \begin{pmatrix} \mathbf{X}^k \\ \mathbf{Z}^k \end{pmatrix} = \begin{pmatrix} \mathbf{\Sigma}^\infty & \mathbf{C} \\ \mathbf{C}^\dagger & \mathbf{W}+\mathbf{P} \end{pmatrix} \begin{pmatrix} \mathbf{X}^k \\ \mathbf{Z}^k \end{pmatrix} \equiv \mathbf{\Xi} \begin{pmatrix} \mathbf{X}^k \\ \mathbf{Z}^k \end{pmatrix}$$

(Hermitian) energy-**independent** eigenvalue problem

$$\mathbf{\Sigma}^\infty = \mathbf{\Sigma}^\infty(\mathbf{X})$$

$$\mathbf{C} = \mathbf{C}(\mathbf{X},\omega)$$

$$\mathbf{W} = \mathbf{W}(\omega)$$

$$\mathbf{P} = \mathbf{P}(\omega)$$

➟ Iterative solution

➟ Matrix dimensions increase at every iteration

Implementation: practical steps

1. **Derive working equations**
   - From diagrams to algebraic expressions

2. **Choose (one-body) basis → rewrite working equation in this basis**
   - Symmetries of the problem may be exploited to devise *reduced* basis

3. **Implement numerical code**
   - Usually in C++ or Fortran

4. **Get 2N & 3N interaction matrix elements**
   - Non-trivial task, very recently public routines becoming available

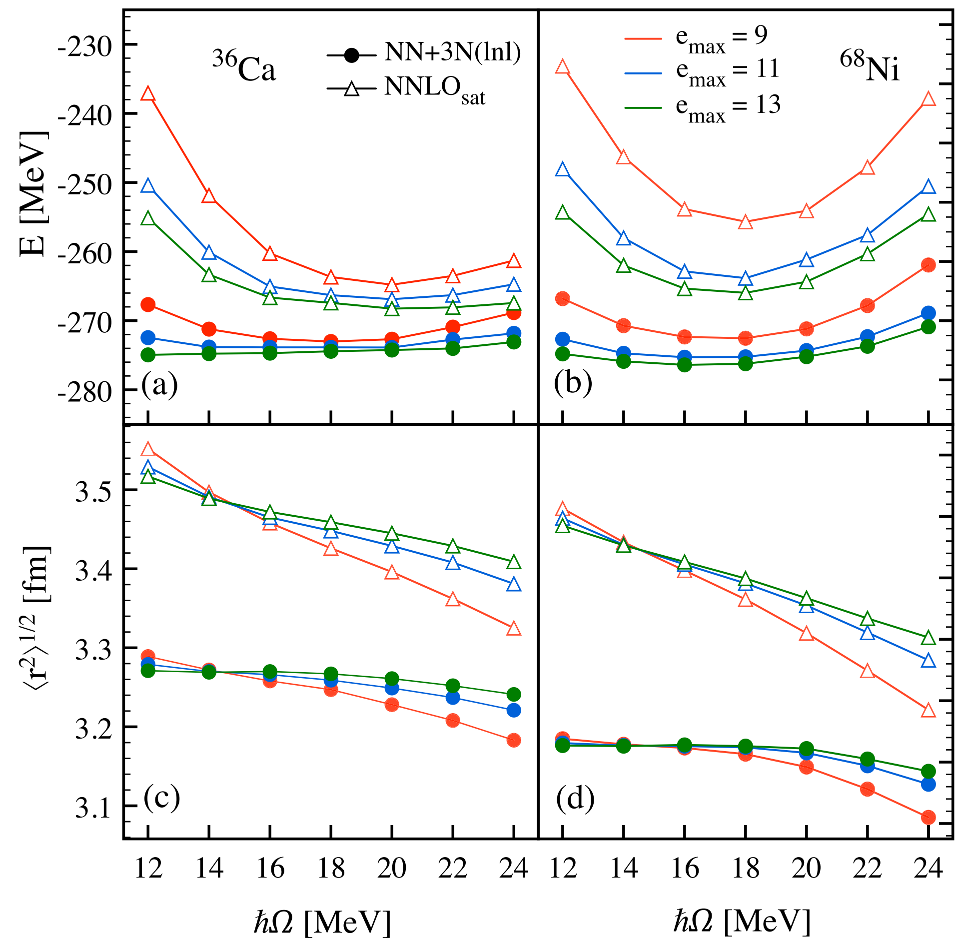
5. **Benchmark & optimise**
   - Test against different implementation
   - Parallelisation to exploit high-performance computing resources
   - Optimisation usually method-specific

Uncertainties

- **From basis & many-body truncations**
  - Truncation of one-body Hilbert space

Typically according to energy of basis states

$$e = 2n + \ell \leqslant e_{\max}$$



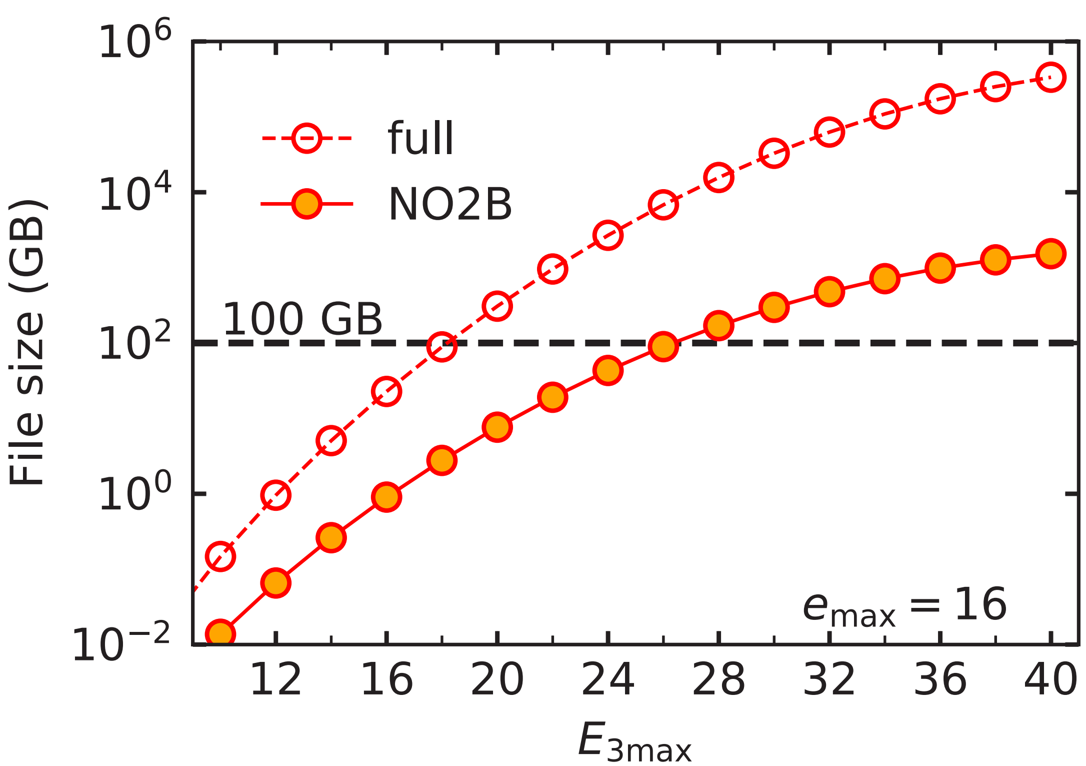
[Somà *et al.* 2020]

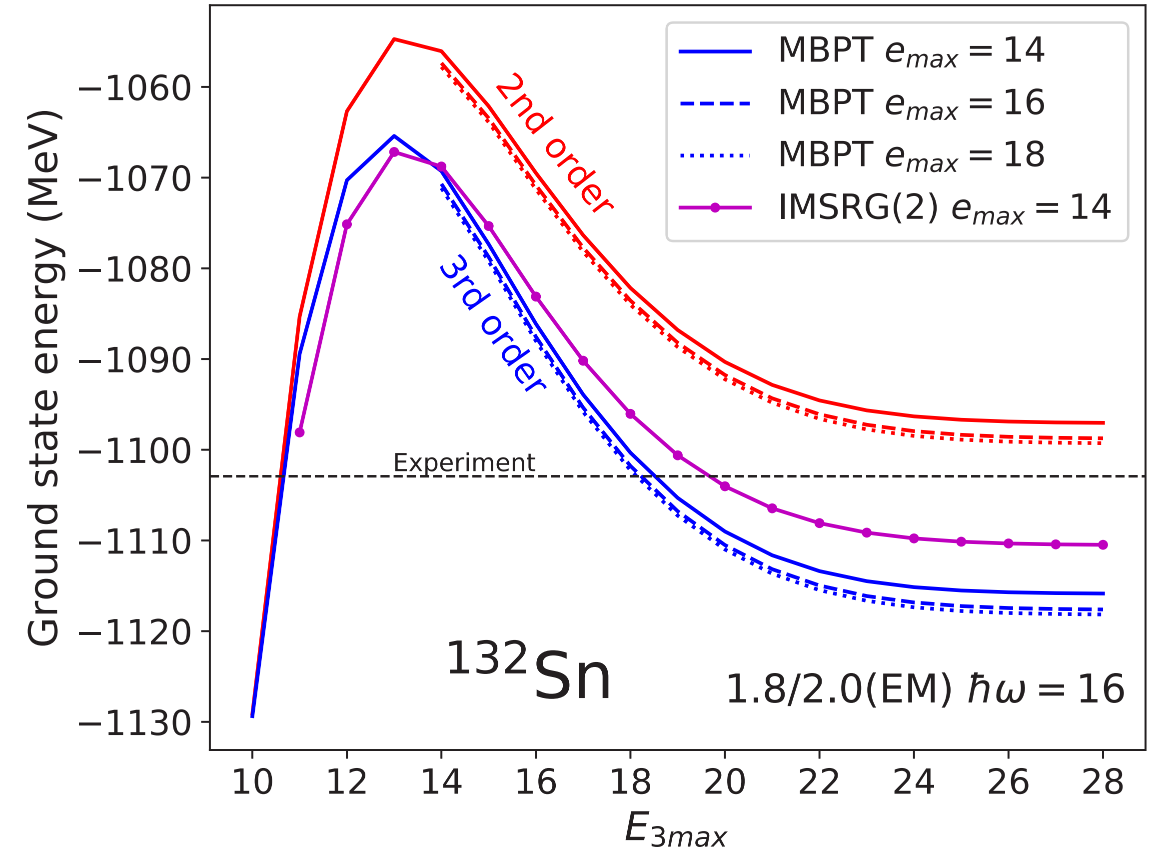
Uncertainties

- **From basis & many-body truncations**
  - Truncation of one-body Hilbert space
  - Truncation of three-body matrix elements

Additional truncation necessary

$e_1 + e_2 + e_3 \leqslant E_{3\max} < 3\, e_{\max}$

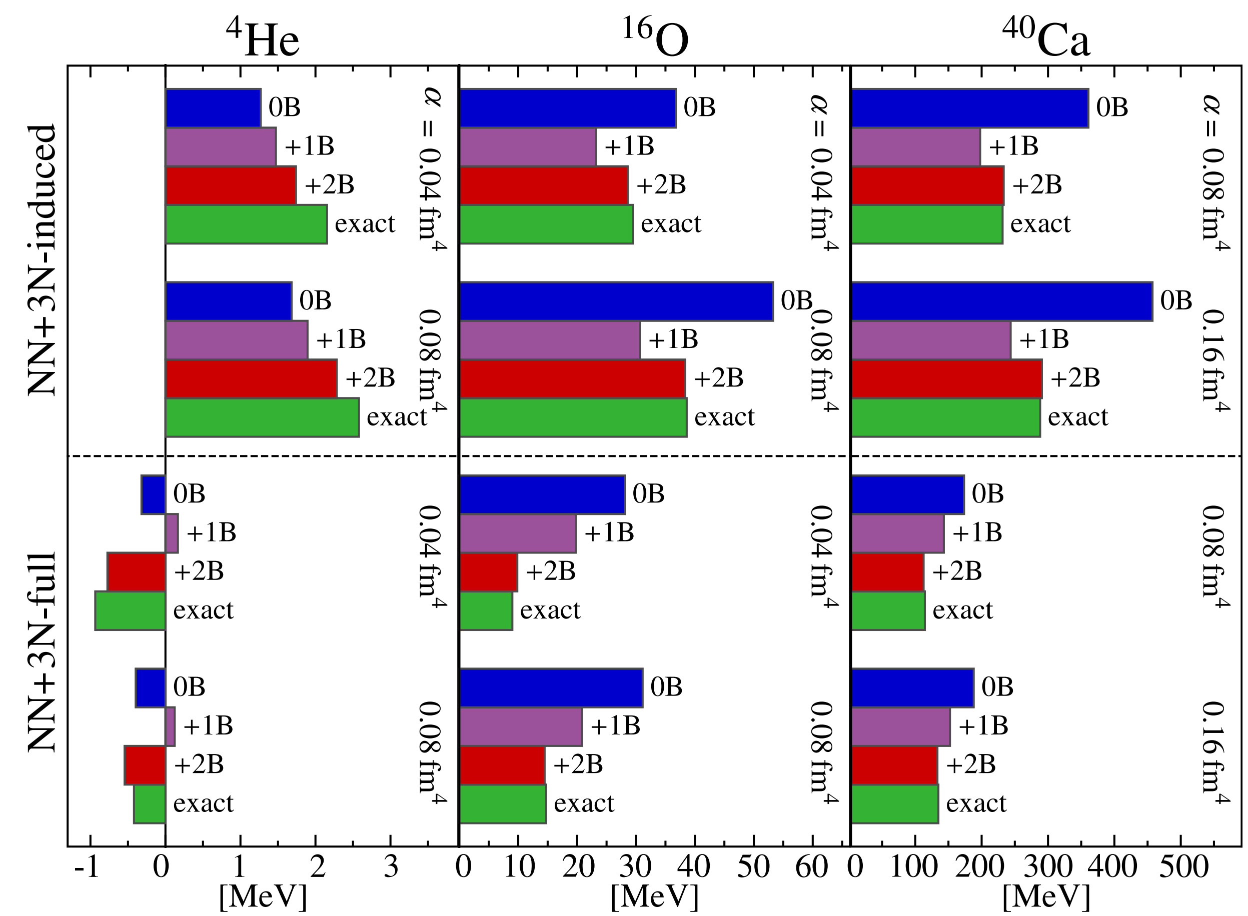




[Miyagi *et al.* 2022]

Uncertainties

- **From basis & many-body truncations**
  - Truncation of one-body Hilbert space
  - Truncation of three-body matrix elements
  - Approximate treatment of 3N forces

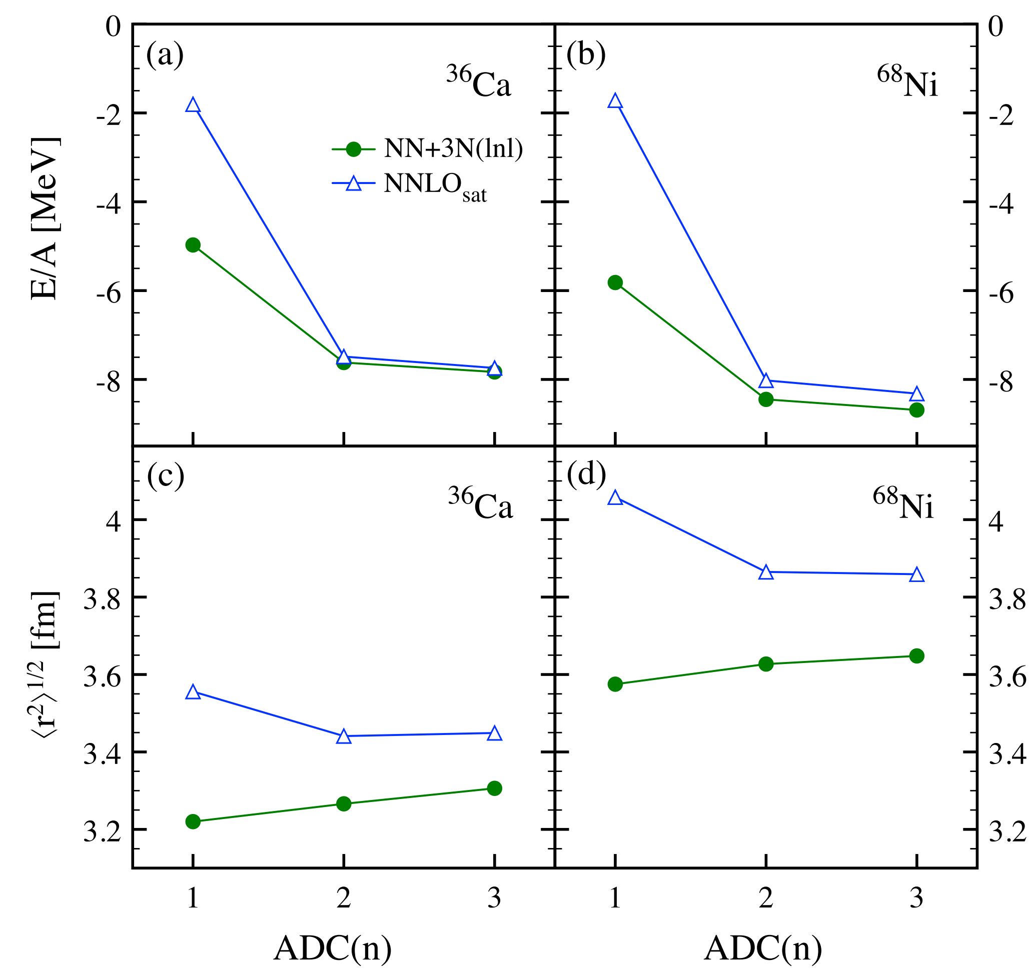


[Roth *et al.* 2012]

Uncertainties

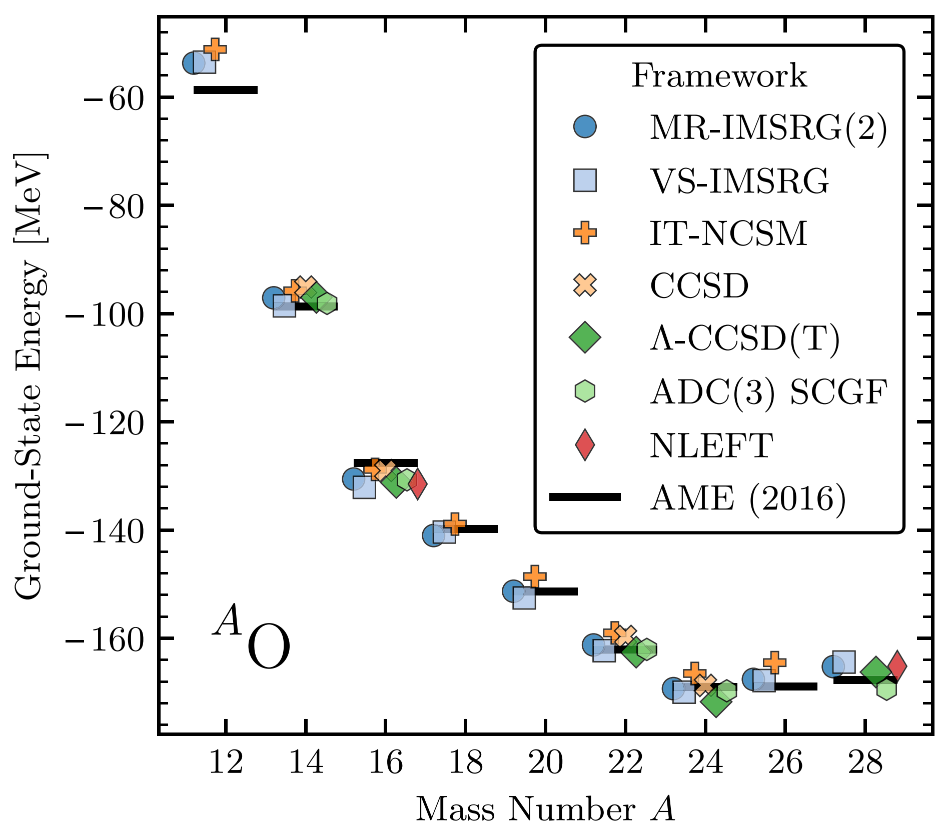
- **From basis & many-body truncations**
  - Truncation of one-body Hilbert space
  - Truncation of three-body matrix elements
  - Approximate treatment of 3N forces
  - Truncation of self-energy expansion

From higher orders



[Somà *et al.* 2020]

From other methods

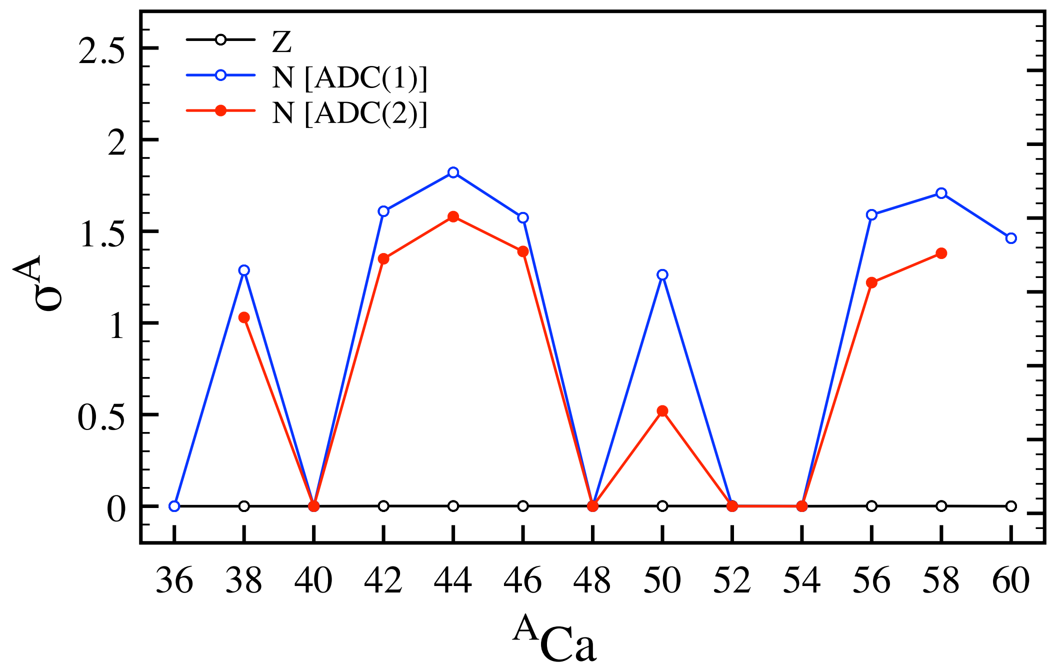


[Drischler, Bogner 2021]

Uncertainties

- ⦿ **From basis & many-body truncations**
  - ○ Truncation of one-body Hilbert space
  - ○ Truncation of three-body matrix elements
  - ○ Approximate treatment of 3N forces
  - ○ Truncation of self-energy expansion
  - ○ Symmetry breaking

Particle-number variance



[Somà *et al.*, unpublished]

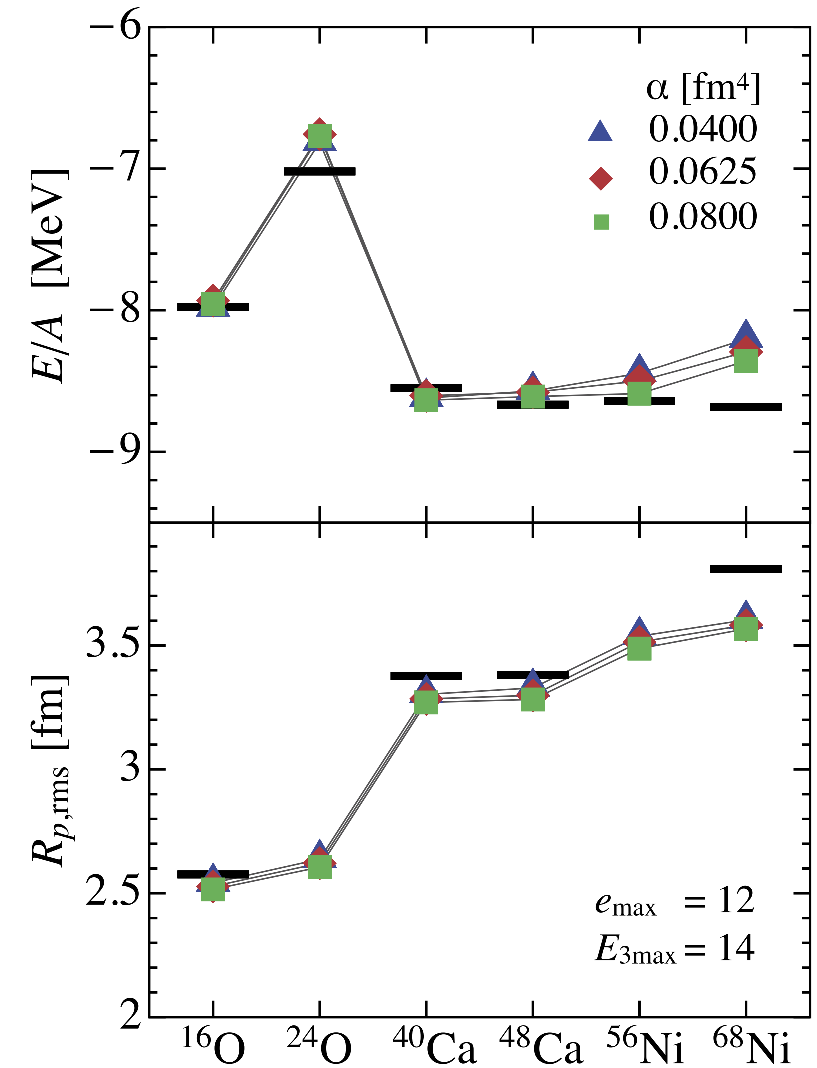
Model-independent estimate

$$\Delta E = \frac{1}{8a}\langle \Delta N^2 \rangle + \frac{1}{8b}\langle \Delta Z^2 \rangle + \frac{1}{4c}\langle \Delta N \Delta Z \rangle$$

[Papenbrock 2022]

Uncertainties

- **From basis & many-body truncations**
  - Truncation of one-body Hilbert space
  - Truncation of three-body matrix elements
  - Approximate treatment of 3N forces
  - Truncation of self-energy expansion
  - Symmetry breaking
  - Non-unitarity of SRG transformation



[Hüther *et al.* 2020]

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Few percent each ➡ Total ~ 5 - 10%

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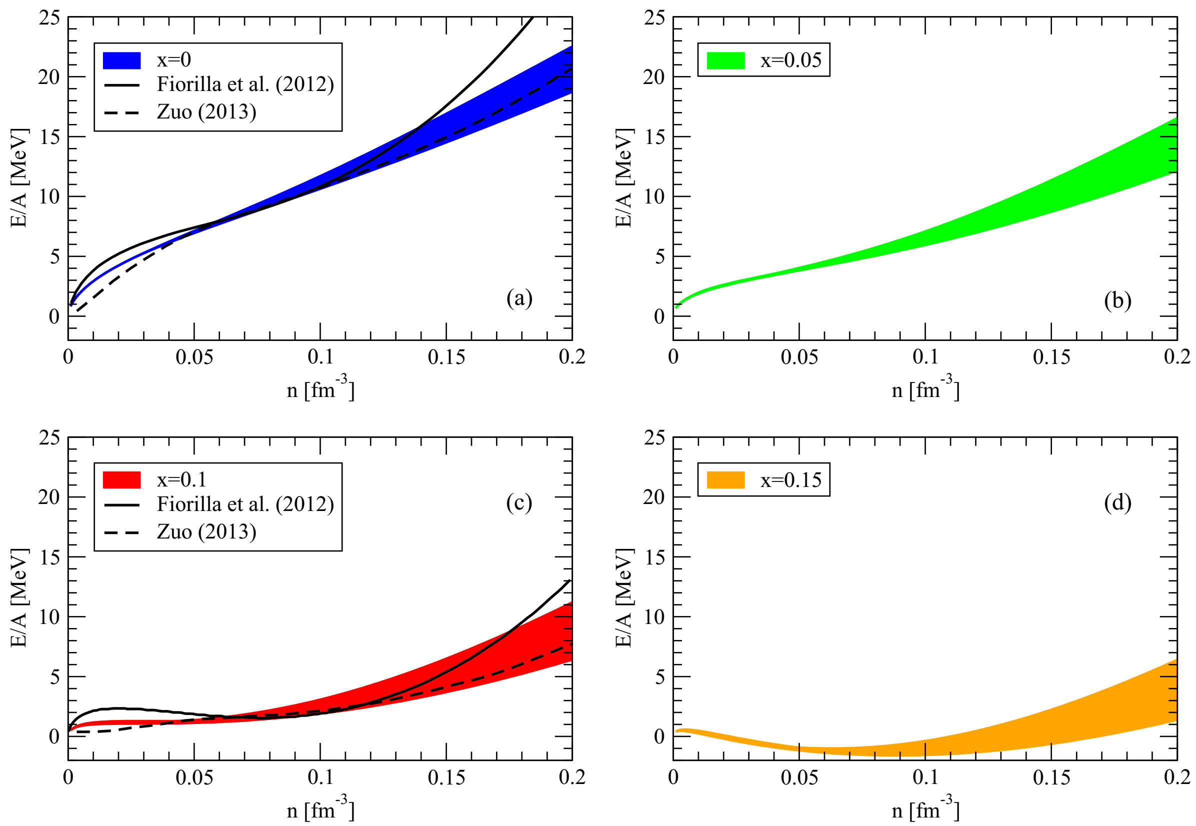
- **From the input Hamiltonian**
  - Past
    - ➪ Test different input interactions (not systematic)



[Drischler *et al.* 2014]

Uncertainties

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- ○ **Past**
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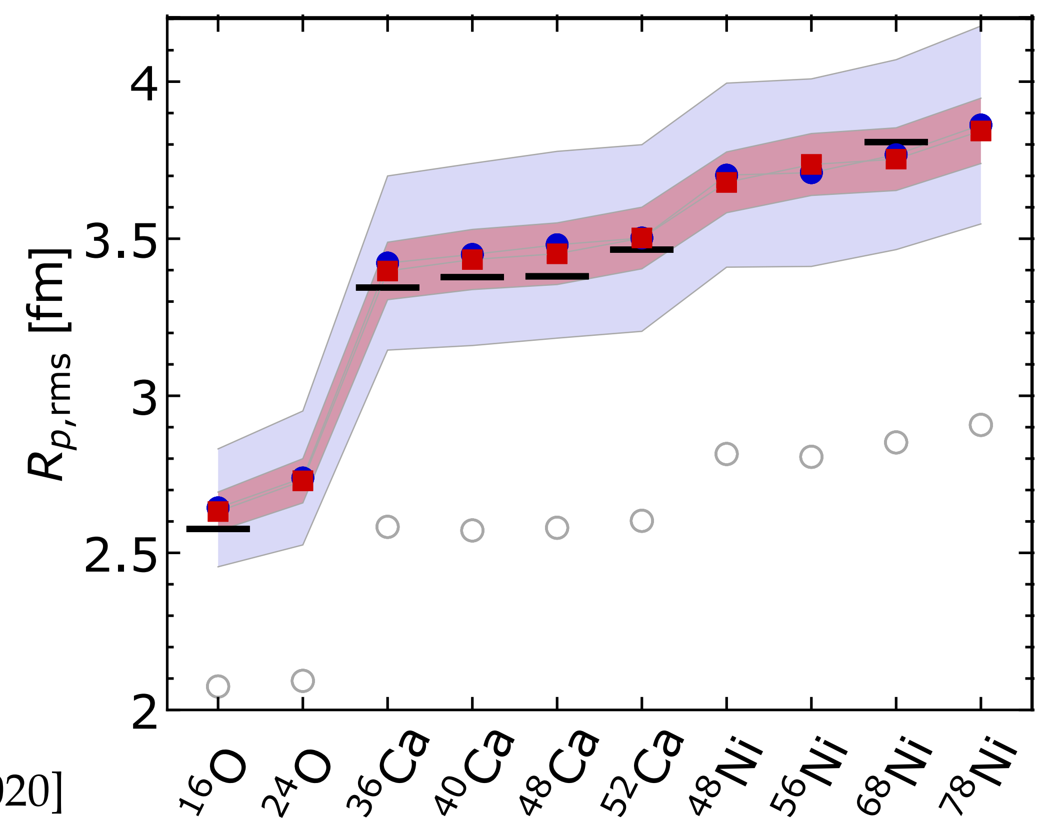
- ○ **Present**
  - ➪ Hamiltonians in WPC available at different orders



[Hüther *et al.* 2020]

Uncertainties

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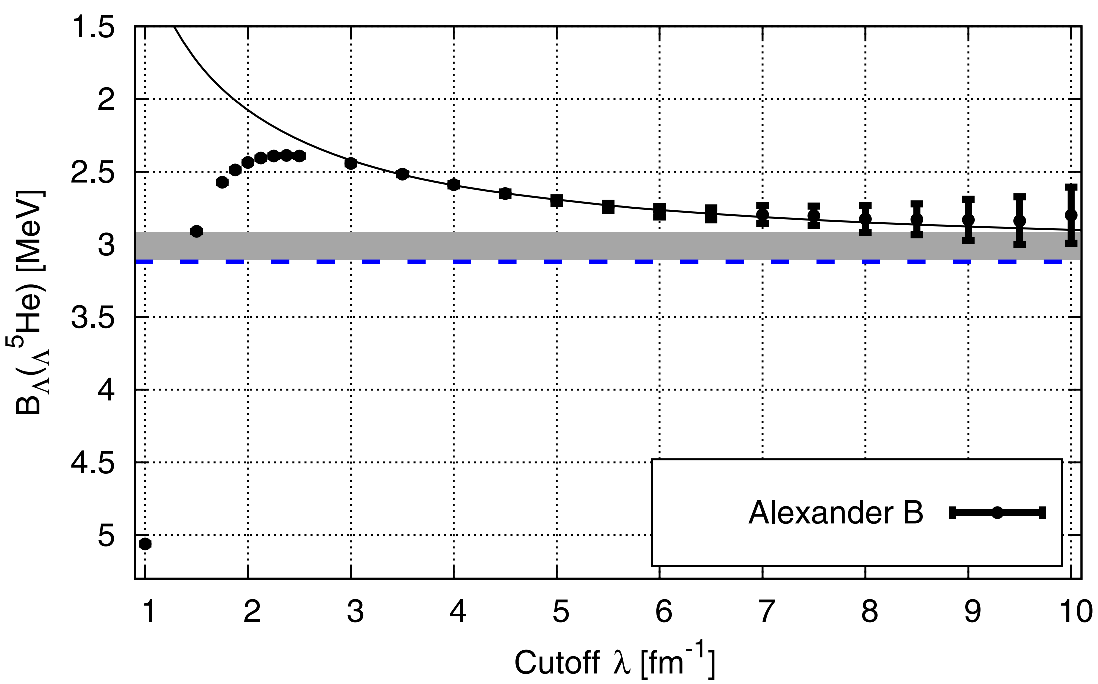
  - **Future**
    - ➪ Renormalisable Hamiltonians → EFT truncation error
    - ➪ Interplay between many-body & renormalisation

[Contessi, Barnea, Gal 2018]



Uncertainties

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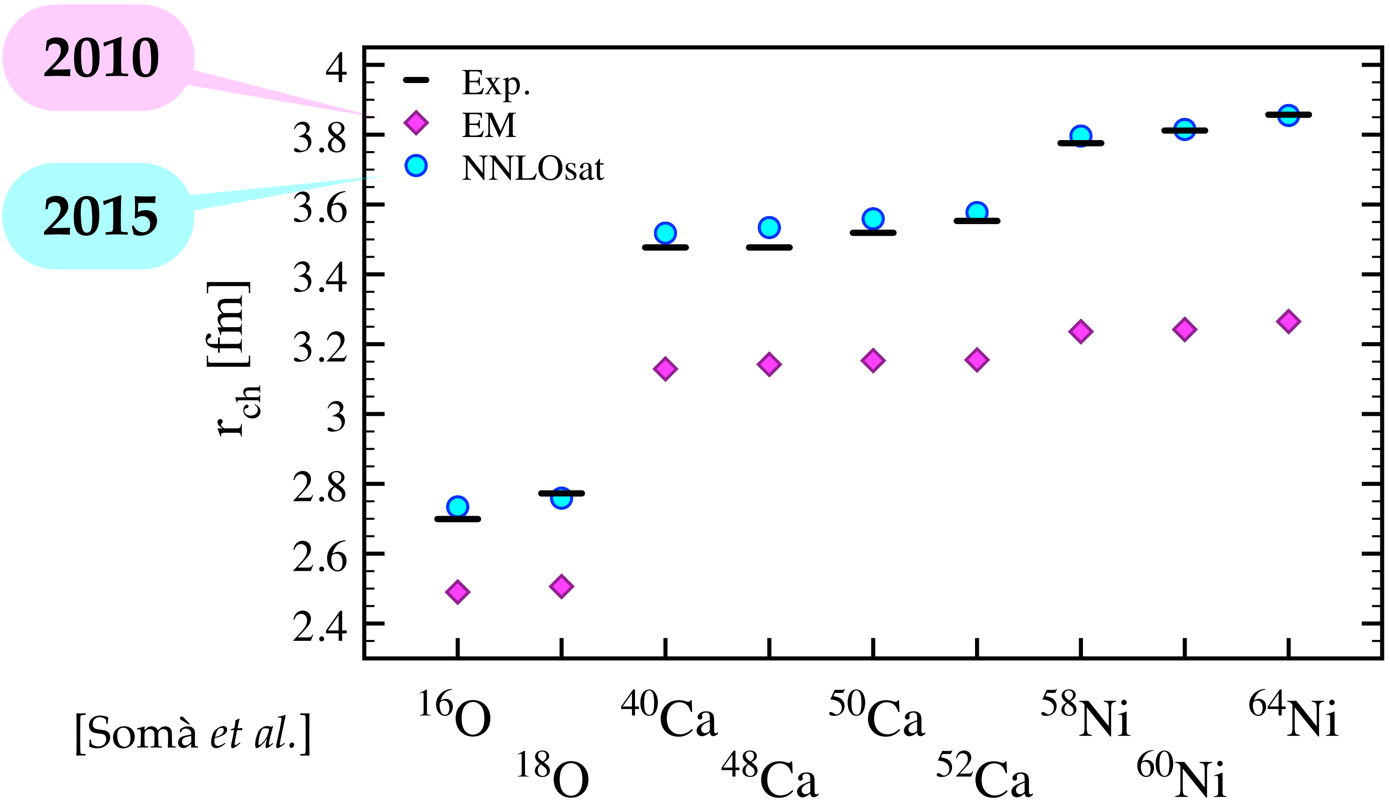
Few percent each ➡ Total ~ 5 - 10%

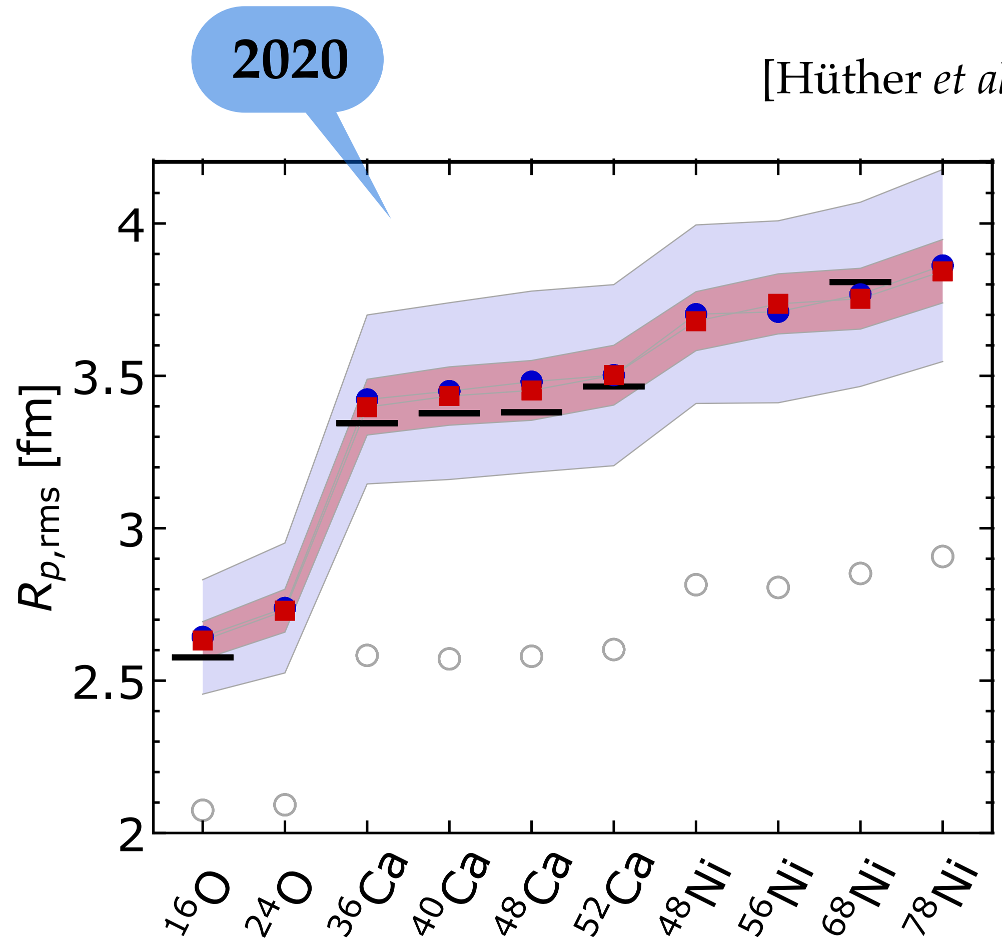
- **From the input Hamiltonian**
  - **Past**
    - ➪ Test different input interactions (not systematic)
  - **Present**
    - ➪ Hamiltonians in WPC available at different orders ➡ Estimates ~ 5 - 10%
  - **Future**
    - ➪ Renormalisable Hamiltonians → EFT truncation error
    - ➪ Interplay between many-body & renormalisation

Accuracy of chiral potentials

⦿ **Accuracy of chiral potentials steadily improving**



[Somà *et al.*]



[Hüther *et al.* 2020]

Rms deviations approaching phenomenological approaches

○ Ground-state energies → rms deviation around 3 MeV (~ **1-1.5%**)

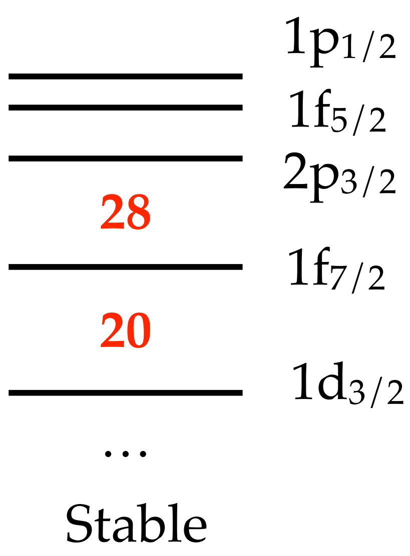
(cf. ~1 MeV in energy density functionals)

○ Charge radii → rms deviation around 0.02 fm (~ **0.5-1%**)

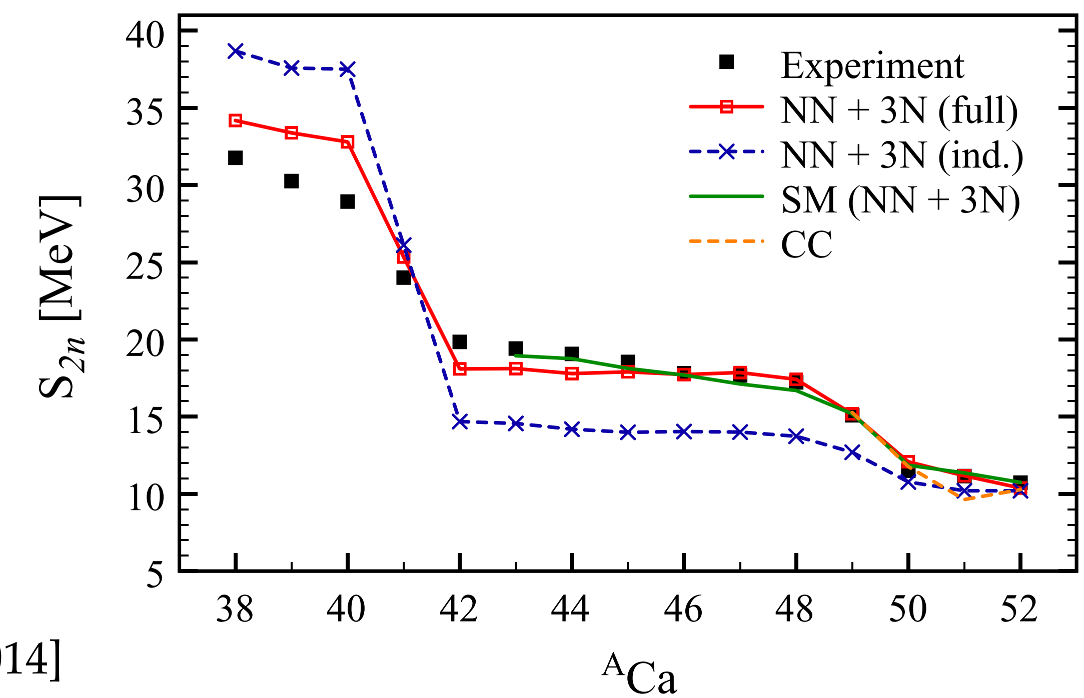
(similar in energy density functionals)

Magic numbers

- Magic numbers: extra-stable combinations of N & Z



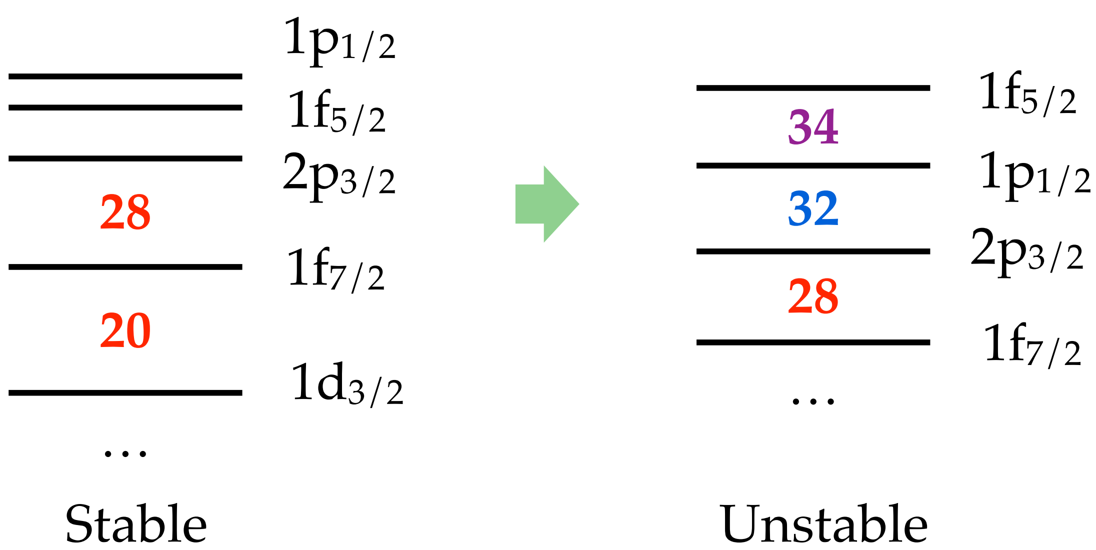
$$S_{2n}(N,Z) \equiv |E(N,Z)| - |E(N-2,Z)|$$



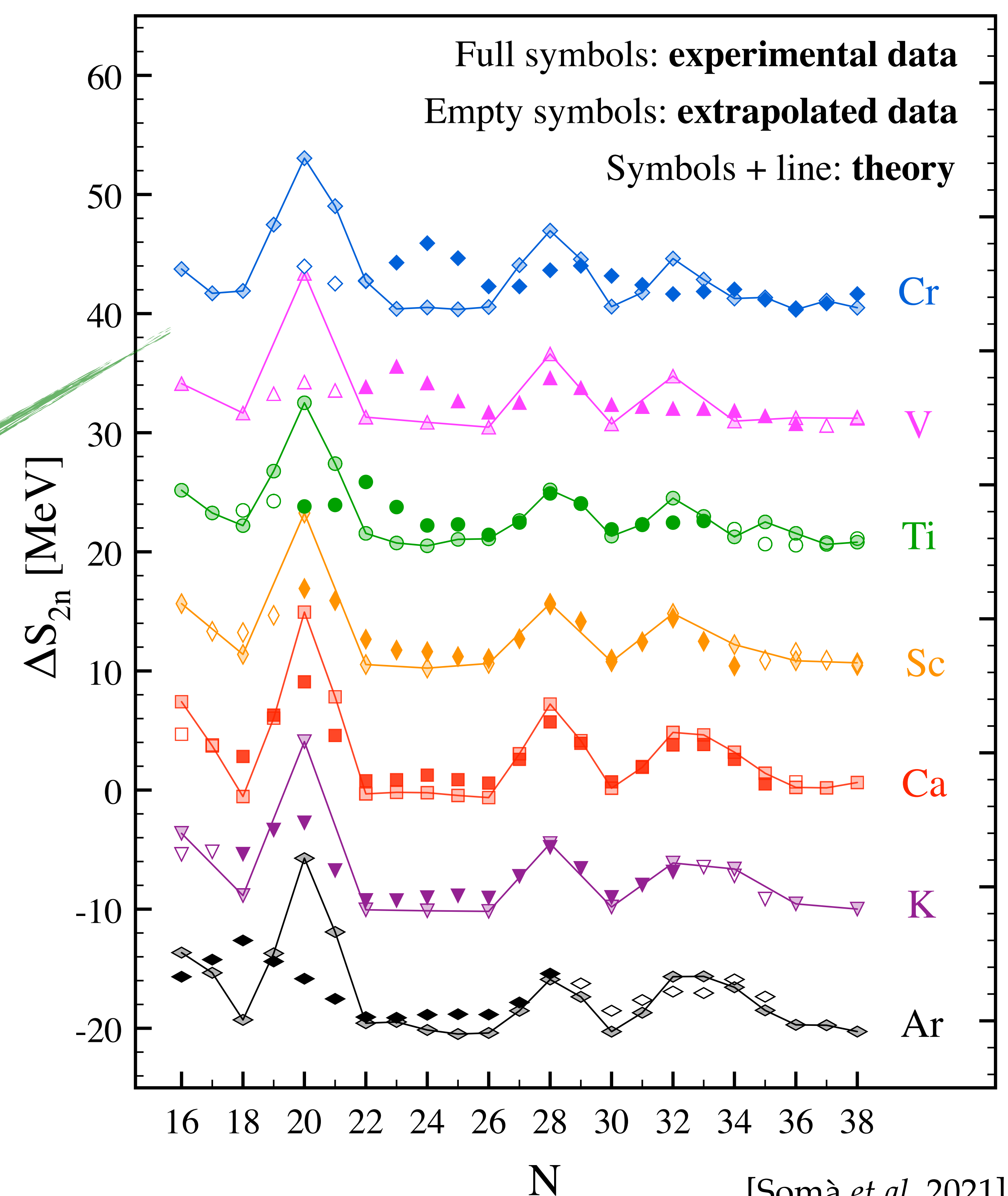
[Somà *et al.* 2014]

Magic numbers

- Magic numbers: extra-stable combinations of N & Z

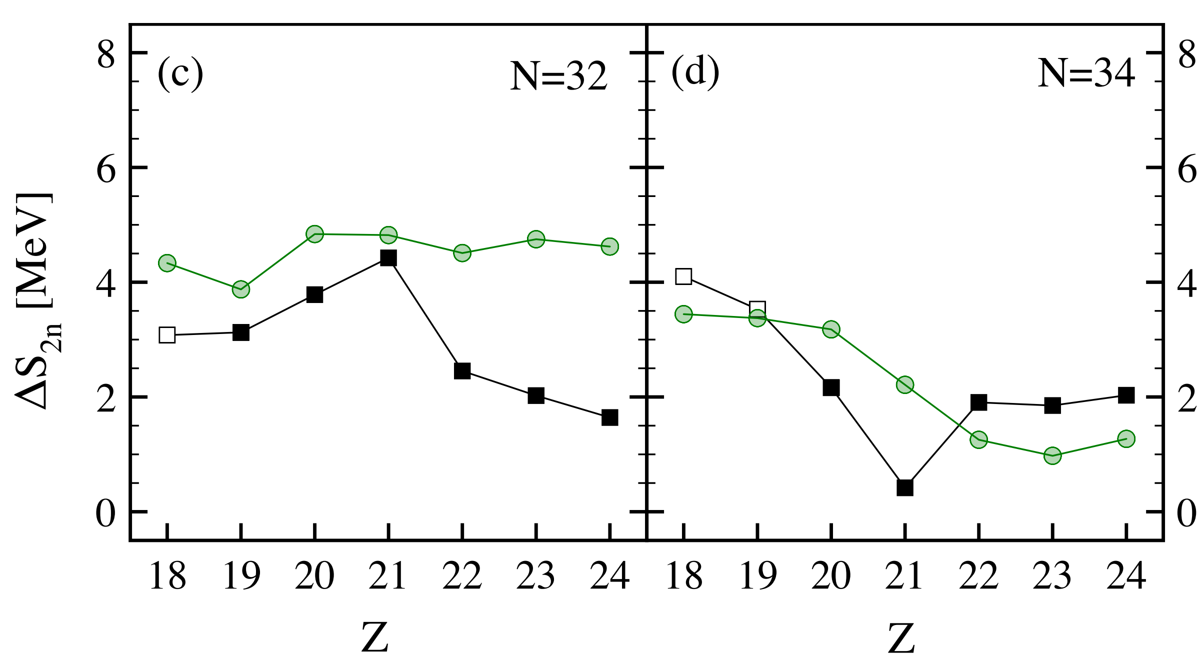


$$\Delta_{2n}(N,Z) \equiv S_{2n}(N,Z) - S_{2n}(N+2,Z)$$



➪ **Magic numbers emerge "ab initio"**

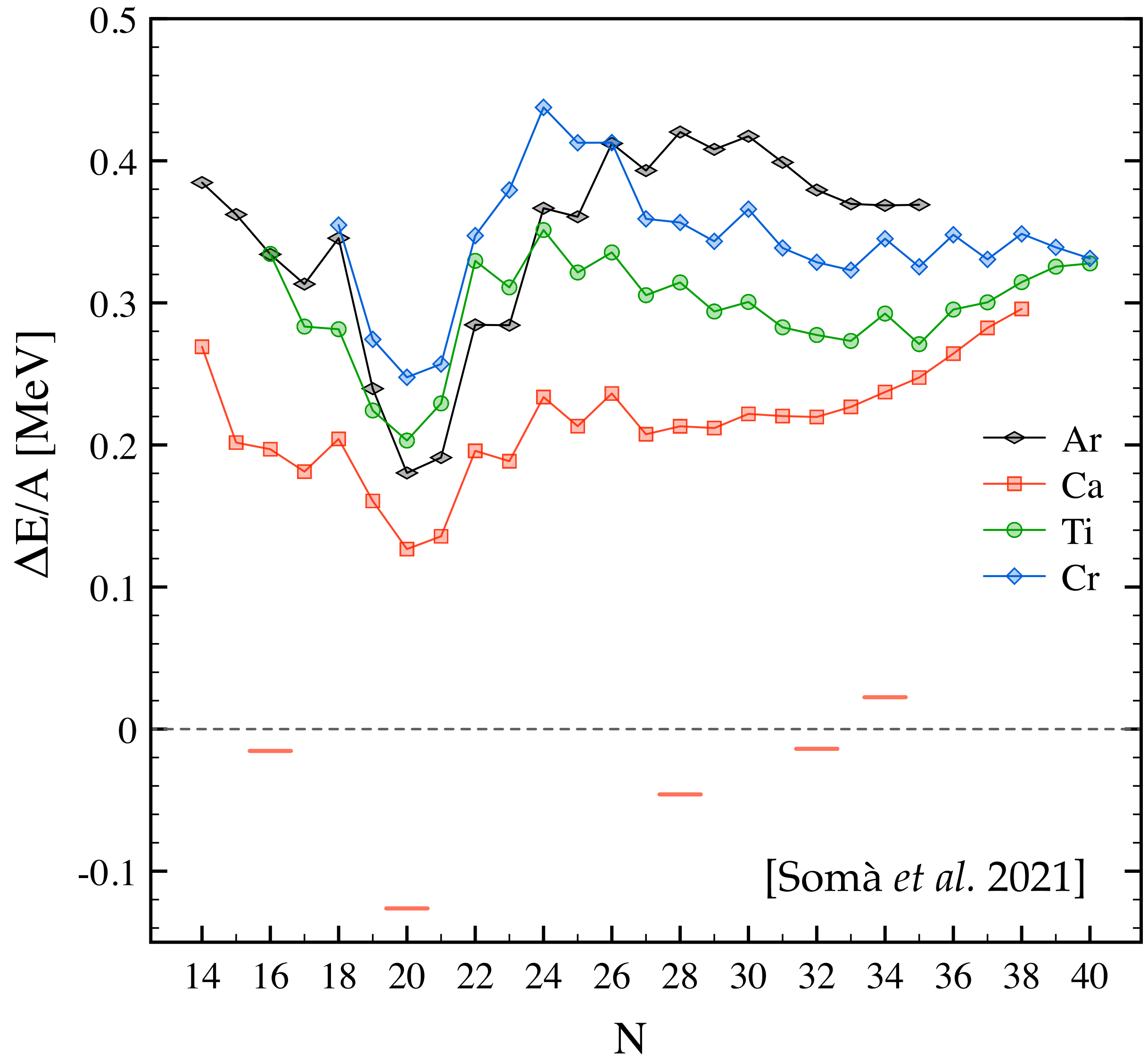
➪ Their evolution qualitatively captured

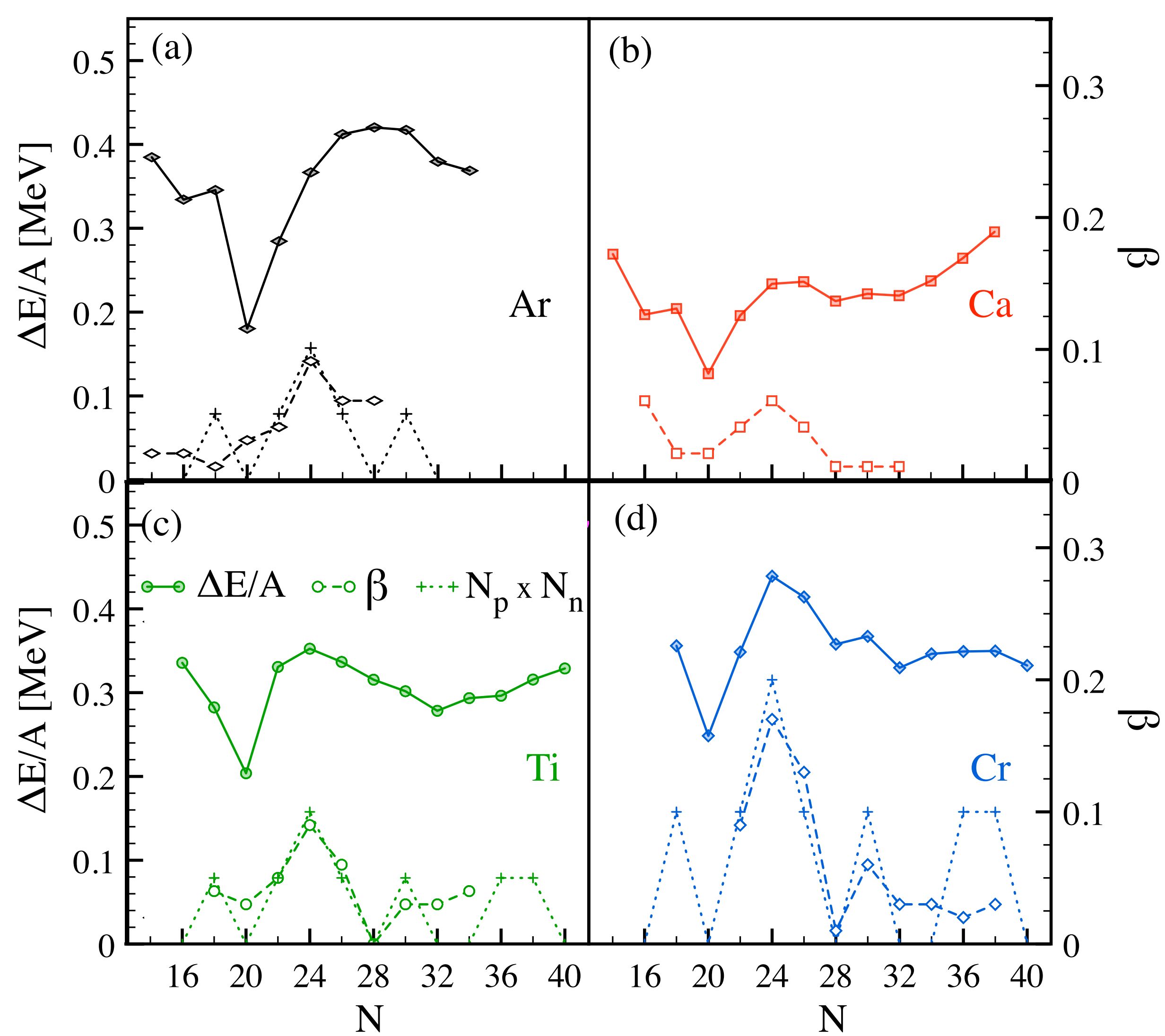


[Somà *et al.* 2021]

Footprint of deformation

⦿ Reproduction of data deteriorates when moving away from (semi-)magic systems





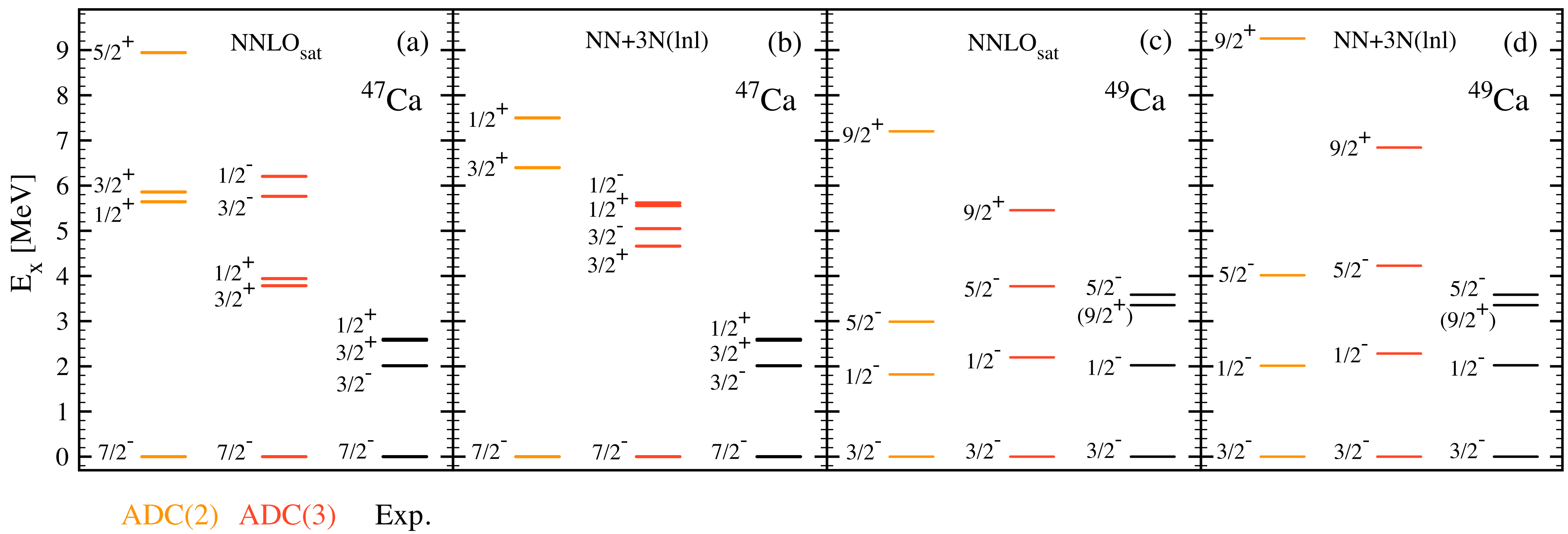
Behaviour consistent throughout isotopic chains

Correlation with measures of deformation

➪ Extension to SU(2)-breaking scheme required for doubly open-shell nuclei

Spectroscopy of mid-mass nuclei

⦿ Odd-even neighbours reached via one-nucleon addition / removal (example: ^{48}Ca)



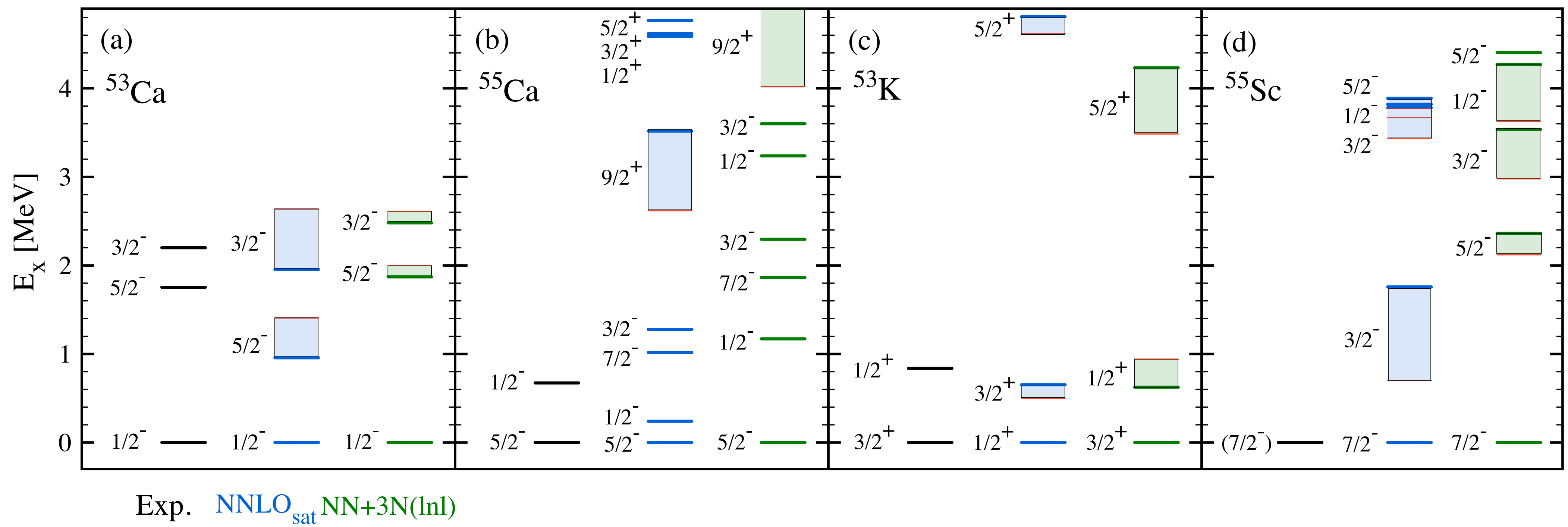
[Somà *et al.* 2020]

➟ Qualitative difference in the two channels driven by deficiency of interaction

➟ ADC(3) only partially corrects for it

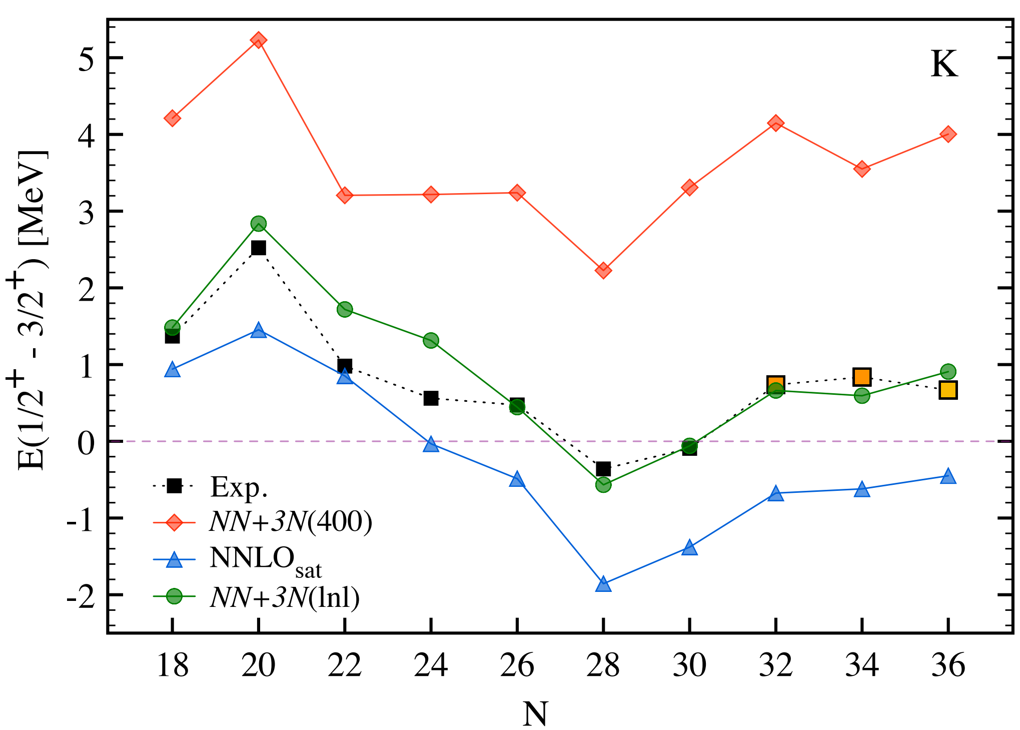
Spectroscopy of mid-mass nuclei

⊙ Odd-even neighbours reached via one-nucleon addition / removal (example: ^{54}Ca)



[Somà *et al.* 2020]

Evolution of ground- & first excited state

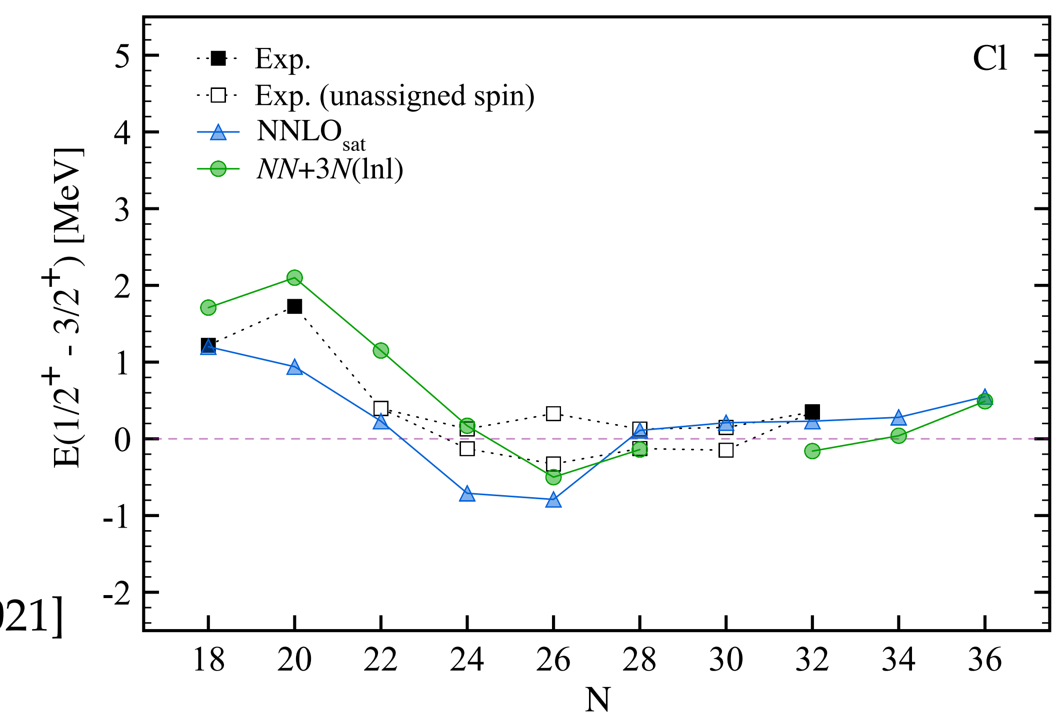


[Sun *et al.* 2020]

[Koiwai *et al.* 2022]

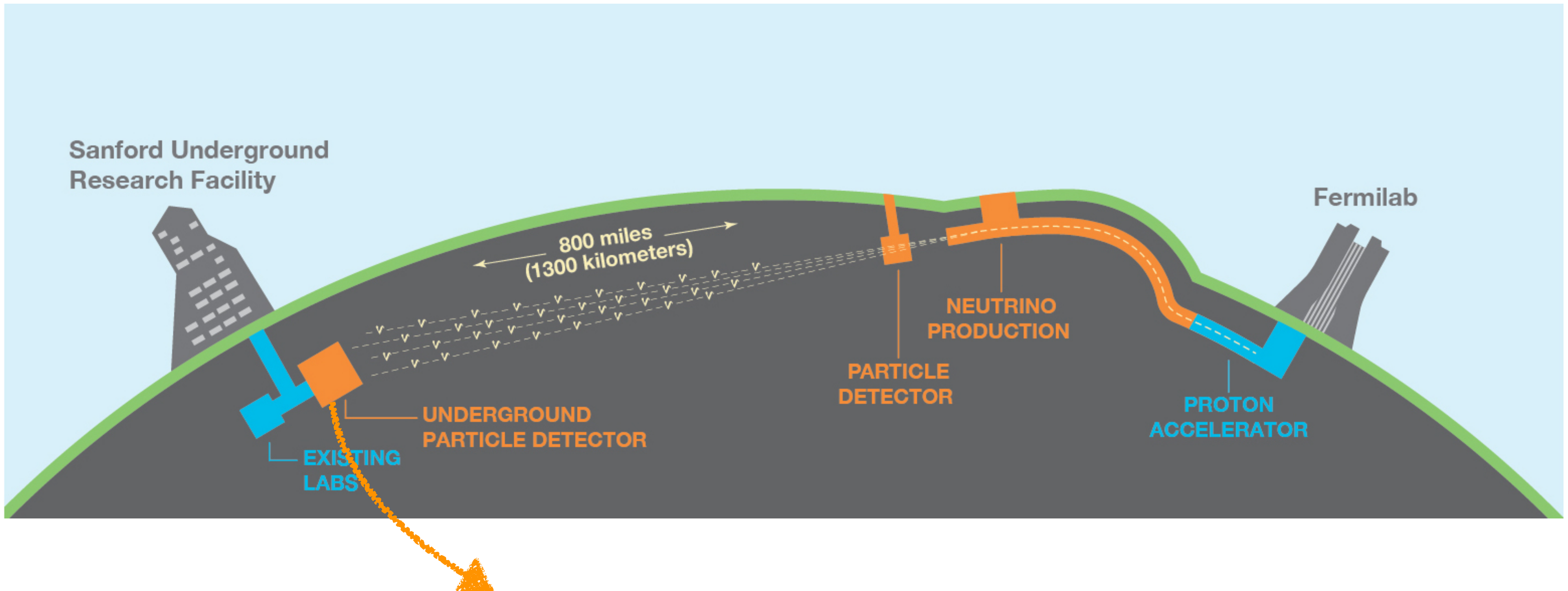
[Linh *et al.* 2021]

Extension to Cl chain



Lepton-nucleus scattering

⦿ Modelling **neutrino-^{40}Ar cross section** crucial for next-gen neutrino experiments (e.g. DUNE)

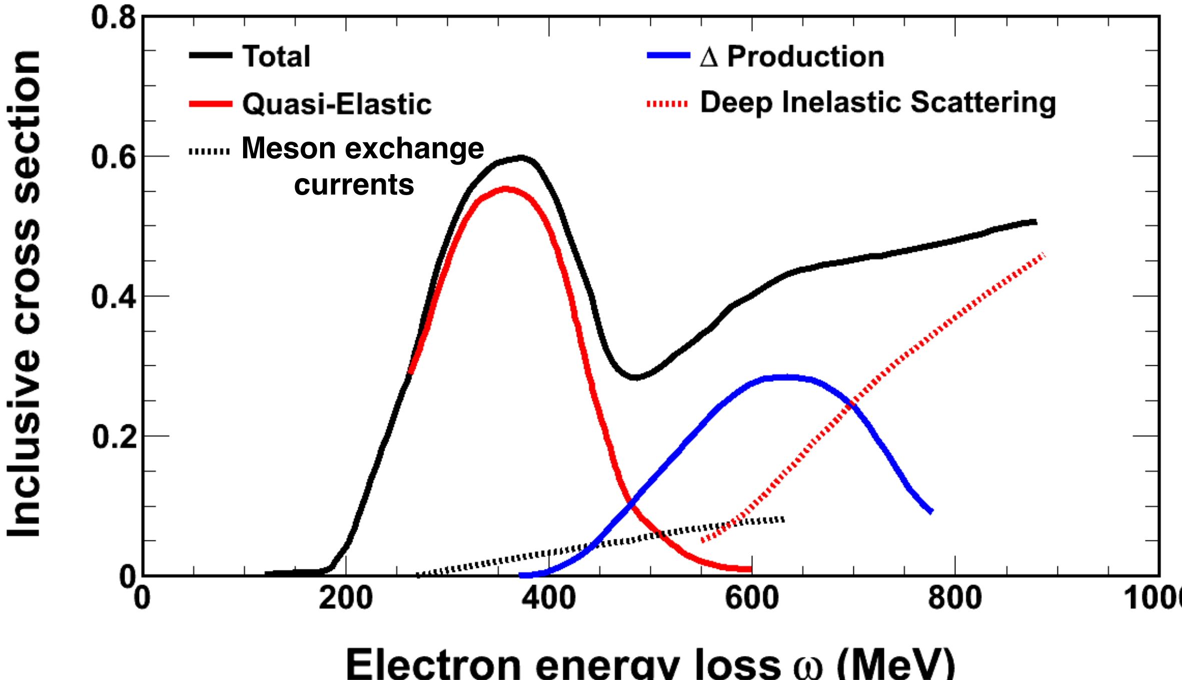


Liquid argon time-projection chambers

➪ Cross section needed over a large energy range

➪ Different processes to be modelling

➪ Nuclear structure input needed

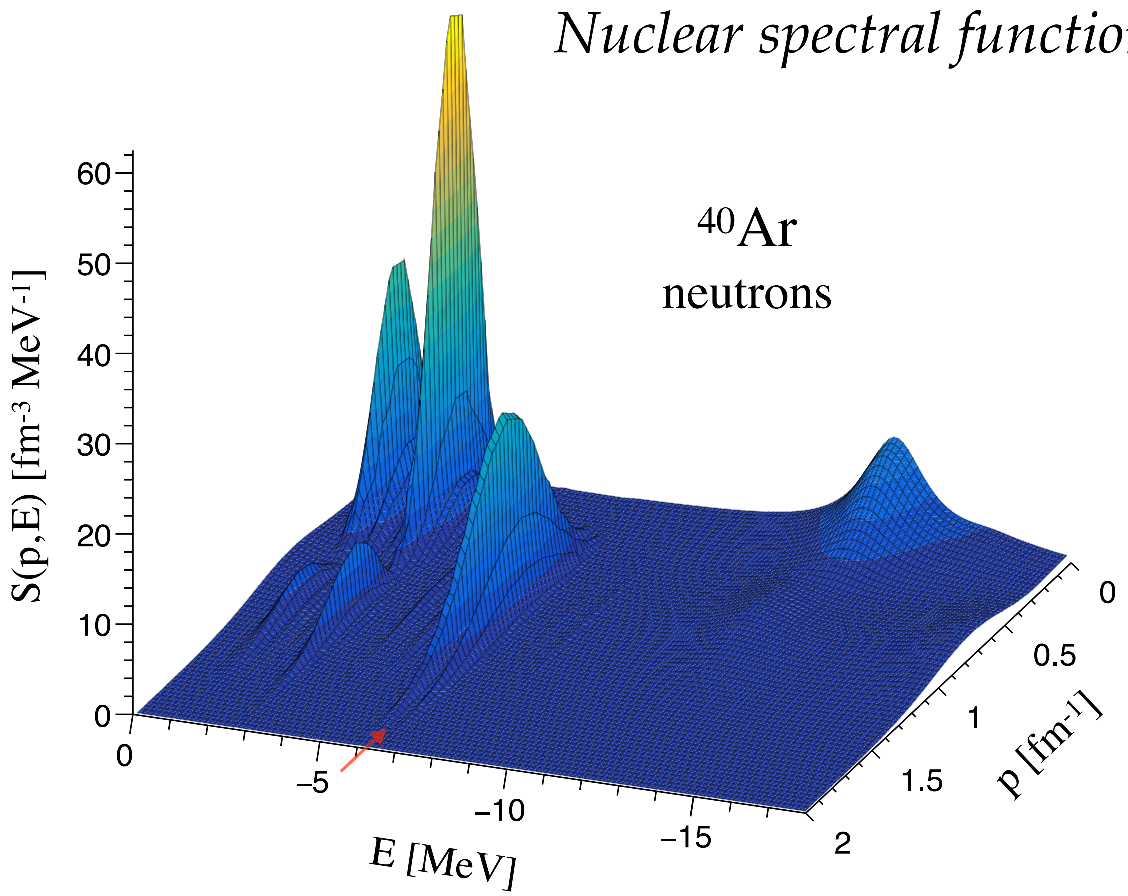


[*Figure*: N. Rocco]

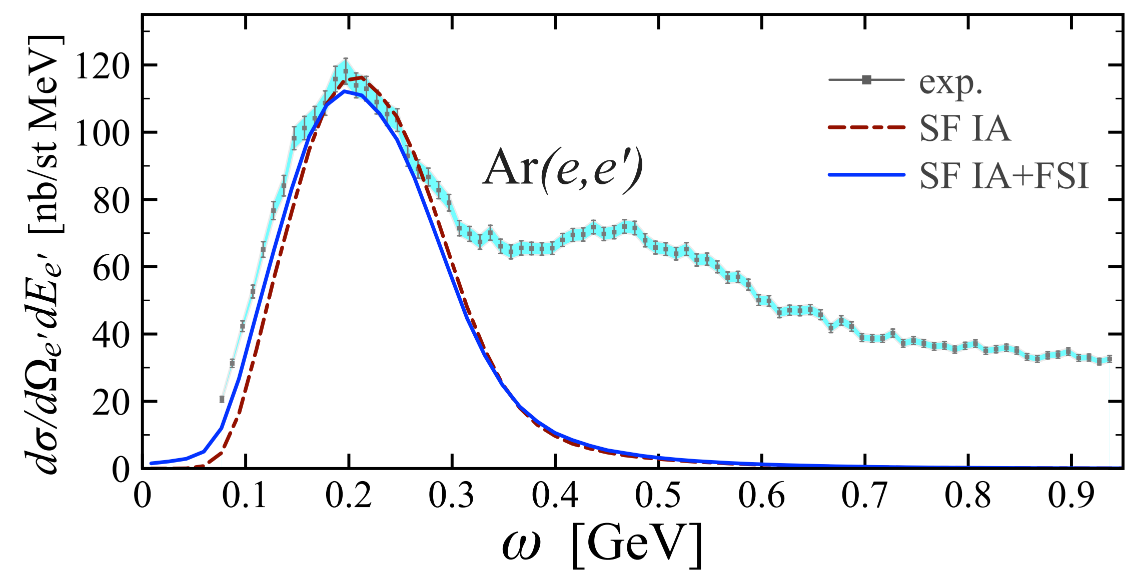
Lepton-nucleus scattering

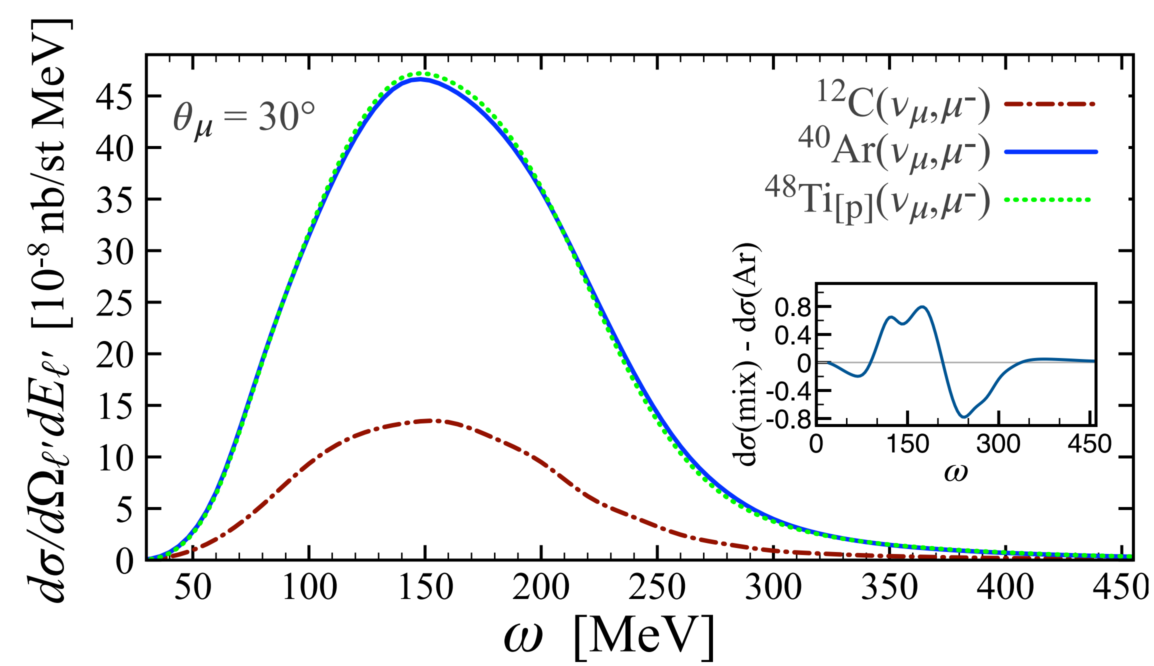
- Modelling **neutrino-^{40}Ar cross section** crucial for next-gen neutrino experiments (e.g. DUNE)
- Quasielestic peak $\rightarrow$ Impulse approximation $|\Psi_f^A\rangle \rightarrow |\mathbf{p}'\rangle \otimes |\Psi_n^{A-1}\rangle$
  - ➪ Reaction process ≈ Incoherent scattering on nucleons weighted by spectral function

Nuclear spectral function



[Barbieri *et al.* 2019]

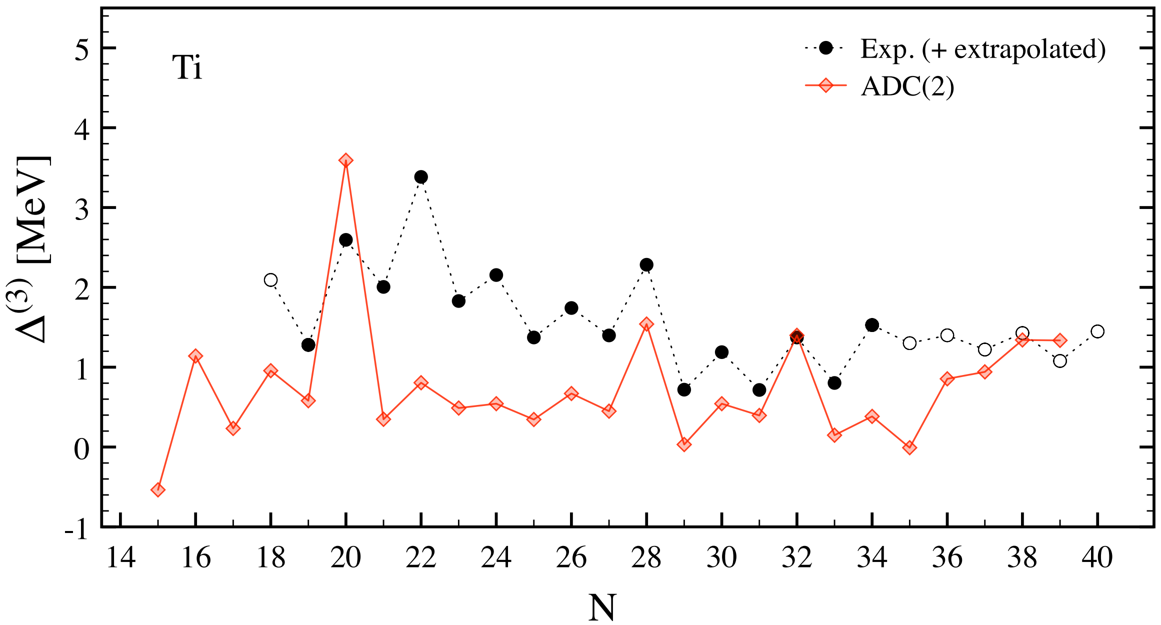




1. Tested on JLAB data (e$^-$ scattering)
2. Applied to σ_{ch} for 1 GeV neutrinos

Perspectives

- **What is the microscopic origin of nuclear superfluidity?**
  - How much is accounted for at lowest order (i.e., how collective is it)?



[Somà *et al.* 2021]

→ ADC(2): lowest order + coupling to 1p1h

→ Pairing strength too low compared to data

Gorkov ADC(3)

- Coupling to collective fluctuations
- Equations derived [Barbieri, Duguet, Somà 2022]
- Computationally demanding
  - → Scaling increases to N⁶
  - → Gorkov matrix less sparse

- **How to access excited states of the *A*-body system?**

↓ Polarisation propagator

$$\Pi_{\gamma\delta,\alpha\beta}(\omega) = \sum_{n_\pi \neq 0} \frac{\langle \Psi_0^A | a_\delta^\dagger a_\gamma | \Psi_{n_\pi}^A \rangle \langle \Psi_{n_\pi}^A | a_\alpha^\dagger a_\beta | \Psi_0^A \rangle}{\hbar\omega - \left(E_{n_\pi}^A - E_0^A\right) + i\eta} + \Pi^-$$

Gorkov polarisation propagator

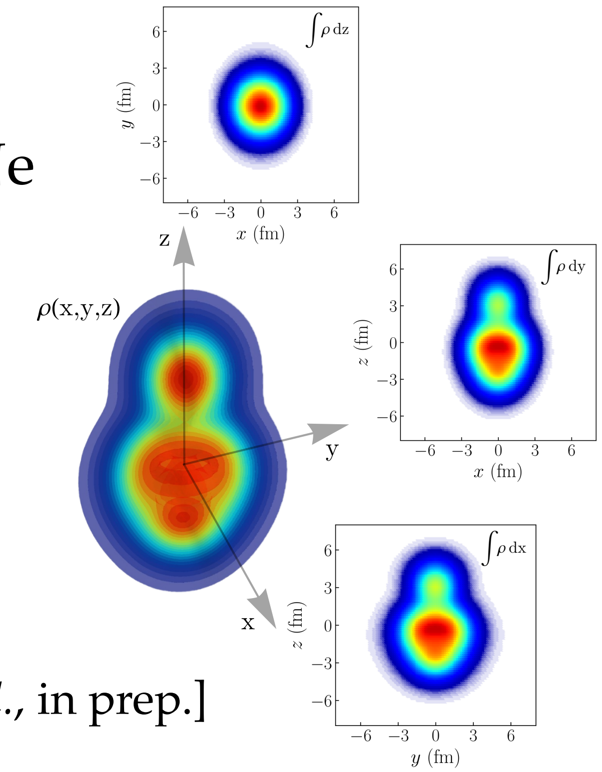
- Non-trivial extension
- Formal derivation in progress

[Stellin, Duguet, Somà, in prep.]

Perspectives

- **Doubly open-shell nuclei require breaking of rotational symmetry**
  - Routine in EDF calculations, few ab initio implementations

^{20}Ne



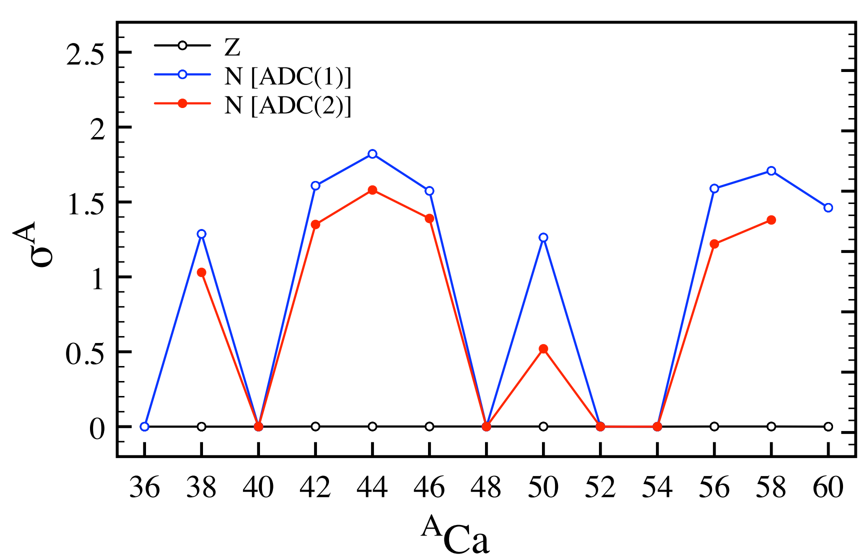
[Bally *et al.*, in prep.]

SU(2)-breaking (Gorkov) GFs

- Builds on CEA expertise
  - → Ab initio PGCM [Frosini *et al.* 2022]
- Computationally demanding (*m*-scheme)
  - → Exploit/develop optimisation tools
  - → Implementation on the way

[Scalesi *et al.*, in prep.]

- **Symmetry-restoration step still missing for GF theory**
  - U(1) → relatively small error, more problematic for SU(2)



[Somà *et al.*, unpublished]

Symmetry-restored GFs

- Yet to be formalised
- Differences to MBPT/CC pose challenge