



energie atomique • énergies alternatives

# Self-consistent Gorkov-Green's function calculations from Chiral-EFT interactions

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# Outline

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- ✱ Introduction and goals
- ✱ Elements of Green's function methods
- ✱ Preliminary results
- ✱ Outlook

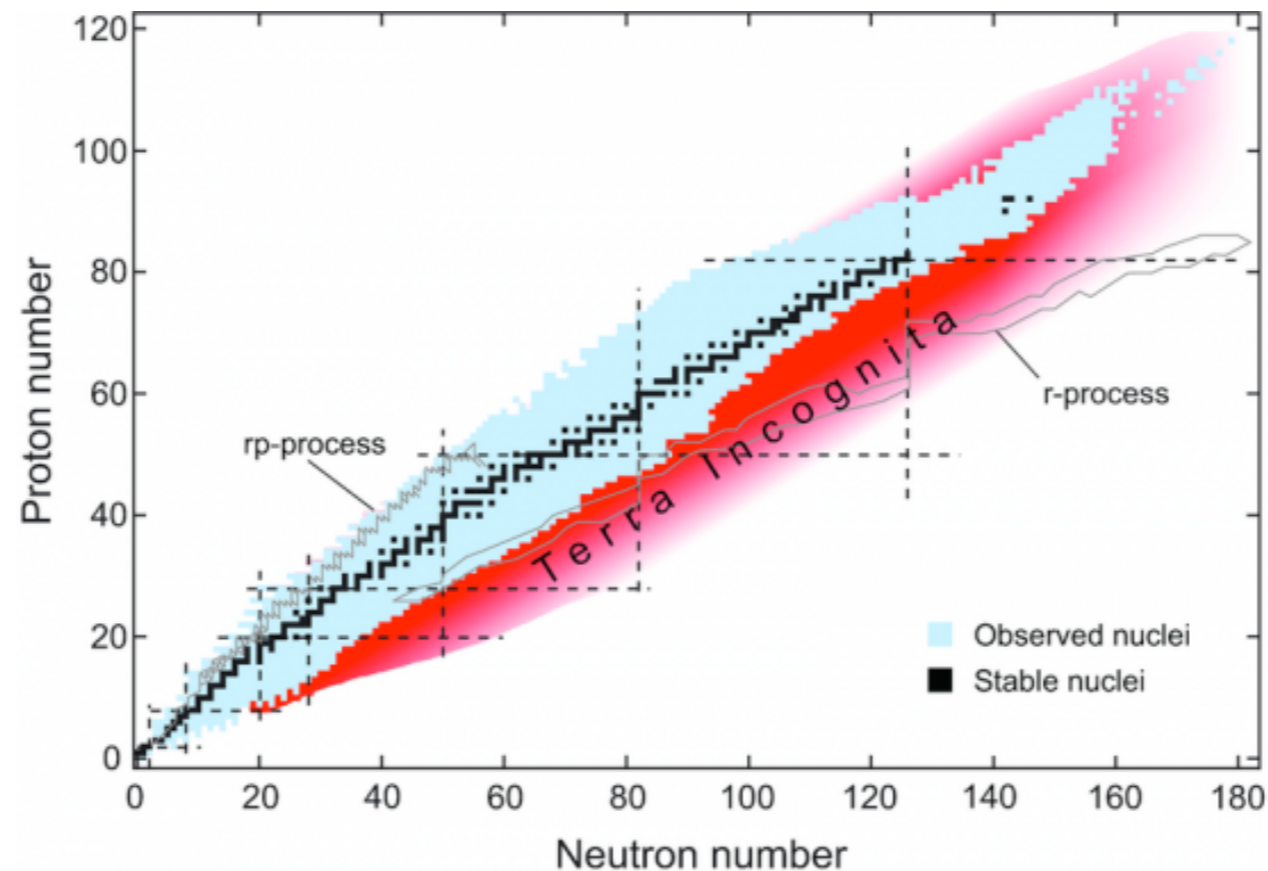
# Introduction and goals

# Goals

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- 1) Tackle finite-nuclei superfluidity in an ab-initio fashion
- 2) Revisit many-body techniques using low-momentum interactions
- 3) Study the effect of NNN forces
- 4) Connect with (non-empirical) energy density functionals

# Towards a unified description of nuclei



“Exact” methods (GFMC, NCSM, ...)



Ab-initio approaches (CC, SCGF, IM-SRG)



Shell model



SR and MR energy density functionals

# State-of-the-art ab-initio nuclear structure theory

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✱ Methods for an ab-initio description of medium-mass nuclei as of 2010

(1) Coupled-cluster [Dean, Papenbrock, Hagen, ...]

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⇒  ${}^3\text{He}$ ,  ${}^4\text{He}$ ,  ${}^{16}\text{O}$ ,  ${}^{40}\text{Ca}$  [Hagen *et al.* 2007]

⇒  ${}^{16}\text{O}$ ,  ${}^{22}\text{O}$ ,  ${}^{24}\text{O}$ ,  ${}^{28}\text{O}$  [Hagen *et al.* 2009]

(2) In-medium similarity renormalization group [Tsukiyama, Bogner, Schwenk]

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⇒  $^{16}\text{O}$ ,  $^{40}\text{Ca}$  [Barbieri, Dickhoff 2004]

⇒  $^{56}\text{Ni}$  [Barbieri, Hjorth-Jensen 2009]

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Dyson-Green's functions  Gorkov-Green's functions

# Low-momentum nuclear interactions

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→ Traditional “hard core” potentials

---

(1) Unconstrained

{ short-range  
low- $k$  - high- $k$  coupling

(2) Low- $k$   $\leftrightarrow$  high- $k$  couplings make  
N-body calculations **unbearable**

(3) Details of high- $k$  physics **irrelevant**  
to low-energy nuclear structure

# Low-momentum nuclear interactions

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(2) Low- $k$   $\leftrightarrow$  high- $k$  couplings make N-body calculations unbearable

(3) Details of high- $k$  physics irrelevant to low-energy nuclear structure

(1) Universal low- $k$  physics unchanged

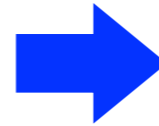
(2) Low- $k$   $\leftrightarrow$  high- $k$  decoupled

(3) High- $k$  physics screened out

# Low-momentum nuclear interactions

RG

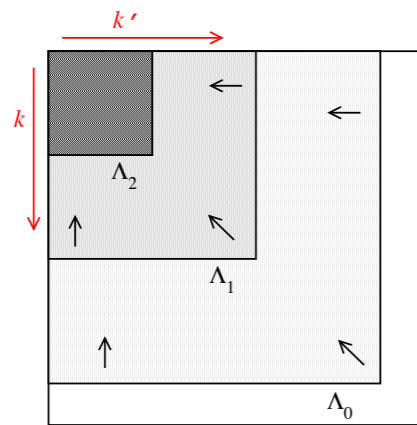
→ Traditional “hard core” potentials



→ “Soft” NN and NNN interactions

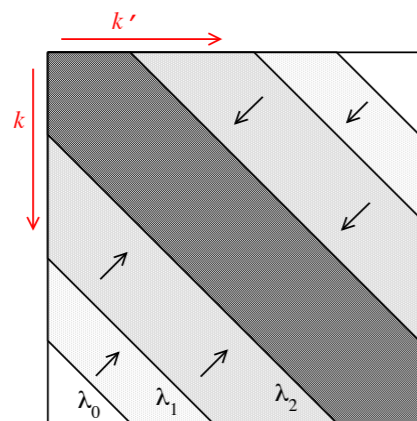
✱ Renormalization group transformations to decouple low and high momenta

(a)  $V_{\text{low-k}}$

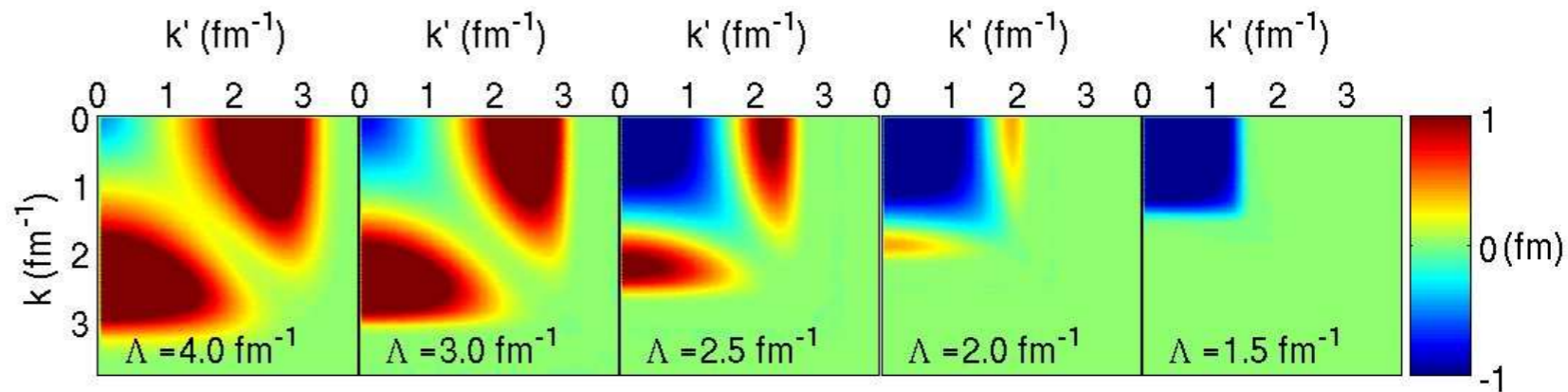


[Bogner, Furnstahl, Schwenk 2009]

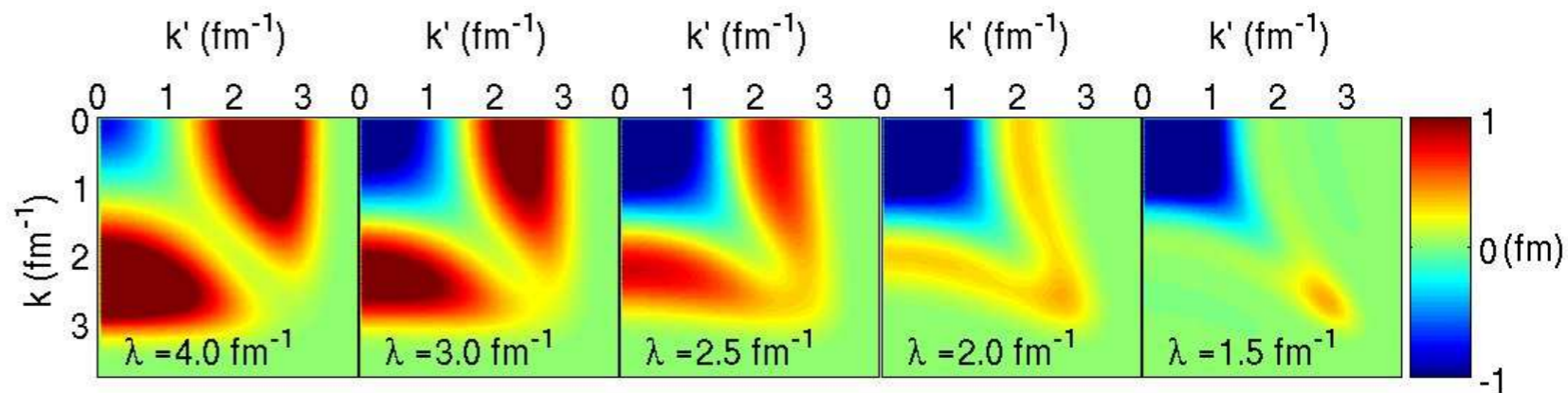
(b)  $V_{\text{SRG}}$



$N^3\text{LO}$  from EFT -  $^3S_1$  channel



(a)



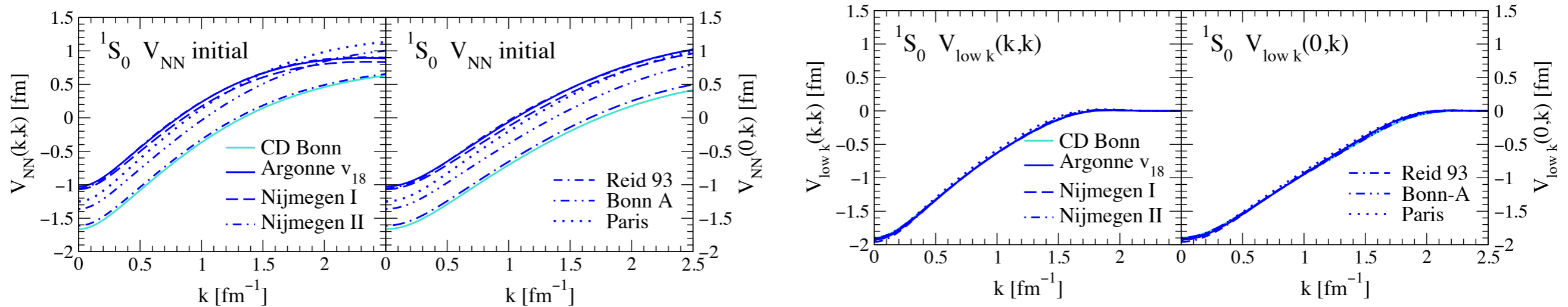
(b)

→ NN scattering phase-shifts and deuteron binding energy **conserved**



# Low-momentum nuclear interactions

## ✱ Universality

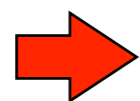


✱ RG transformations induce many-body forces

[Bogner, Furnstahl, Schwenk 2009]

✱ N-body observables are RG invariant if and only if

- 1) Induced N-body (e.g. 3-body) forces are kept
- 2) N-body calculation is exact

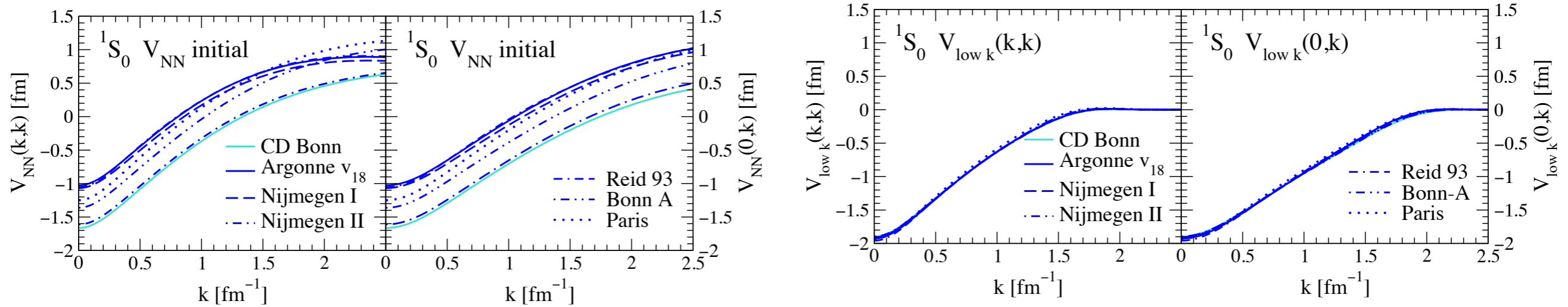


RG cutoff dependence helps tracking

- 1) Importance of omitted N-body forces
- 2) Incomplete N-body calculation

# Low-momentum nuclear interactions

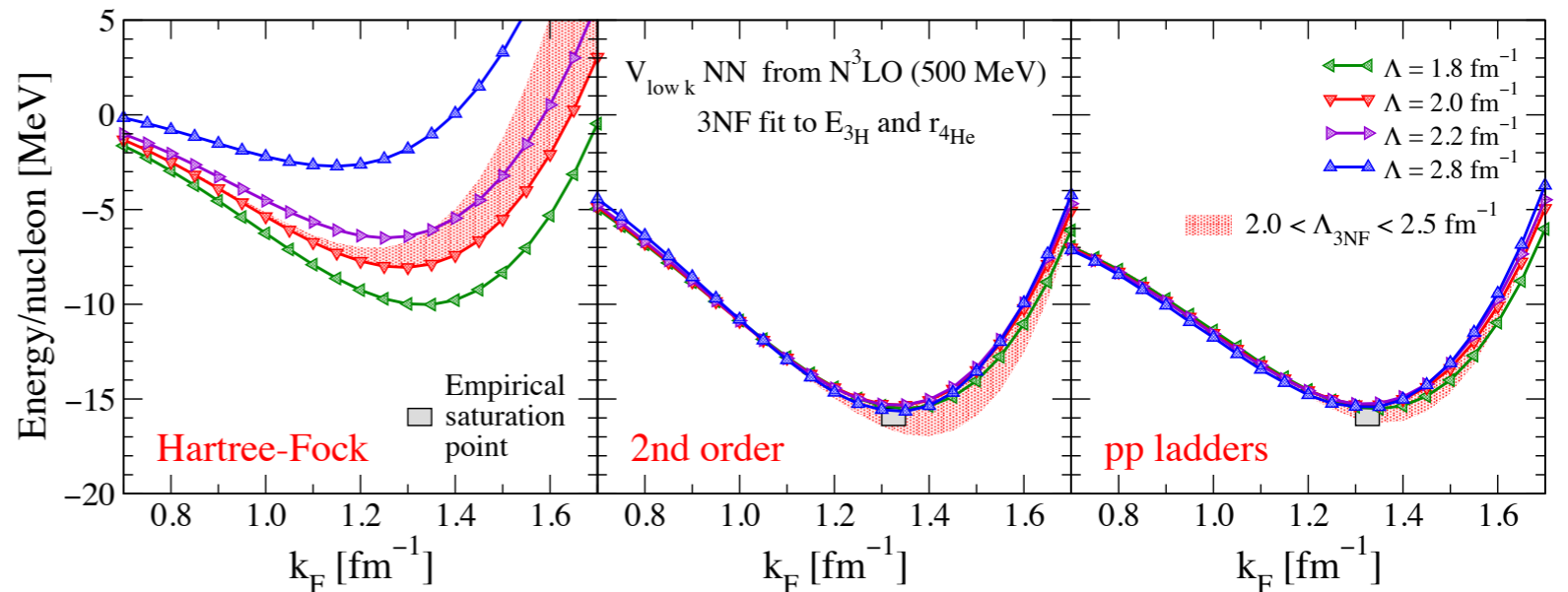
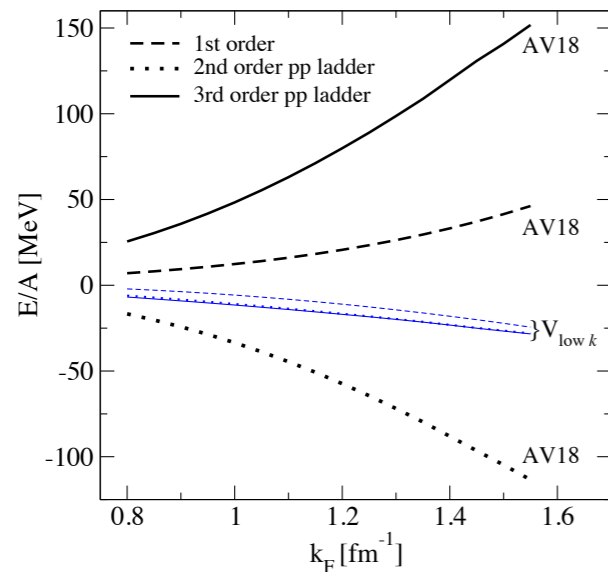
## ✱ Universality



[Bogner, Furnstahl, Schwenk 2009]

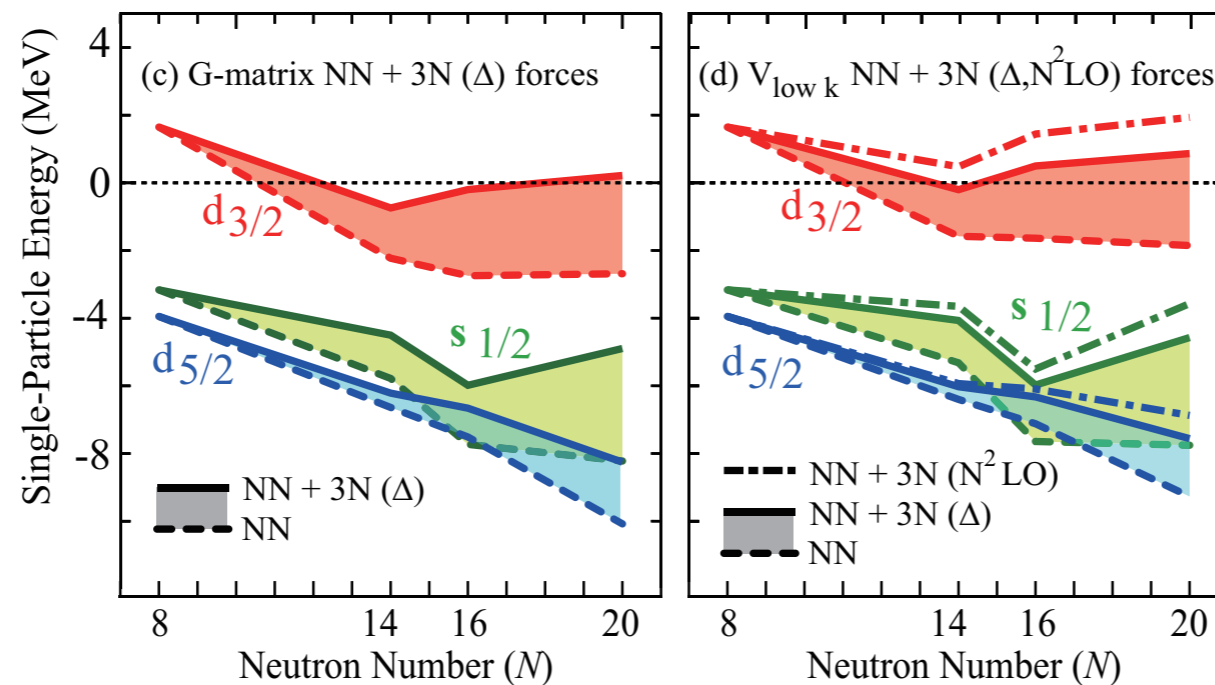
## ✱ Perturbativeness?

[Bogner, Furnstahl, Nogga, Schwenk 2009]



# Three-body forces

- ✱ Realistic microscopic calculations cannot avoid the use of NNN forces
  - Binding energies, saturation properties and radii
  - Shell evolution
  - Spin-orbit splitting
  - Three-nucleon scattering



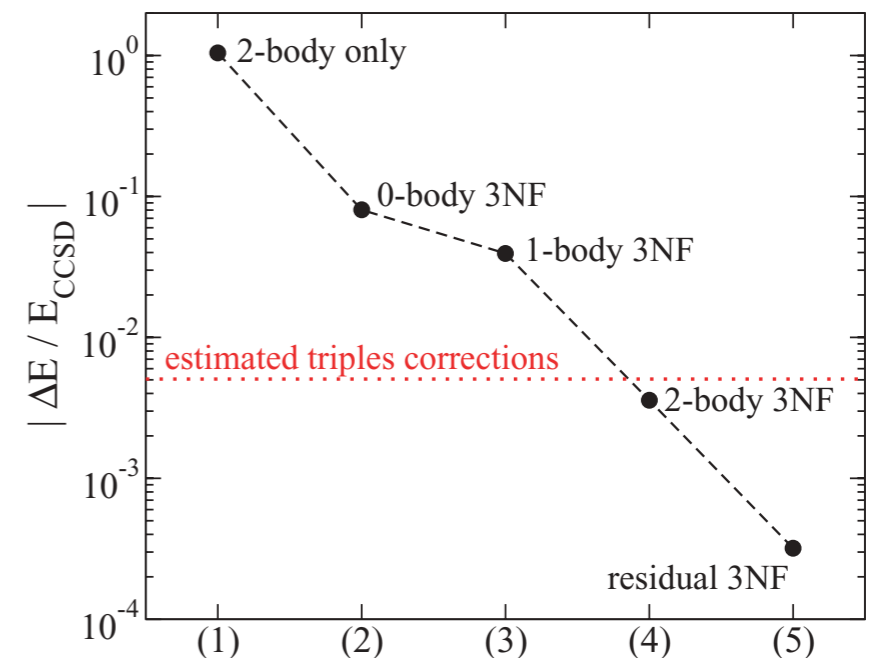
[Otsuka *et al.* 2010]

⇒ Dripline location in O isotopes ( $^{24}\text{O}$ ) possibly due to NNN physics

# Three-body forces

- ✱ Realistic microscopic calculations cannot avoid the use of NNN forces
  - Binding energies, saturation properties and radii
  - Shell evolution
  - Spin-orbit splitting
  - Three-nucleon scattering
- ✱ Currently: microscopic NNN interactions only in light systems and INM
  - Normal-ordered (average) part of NNN possibly sufficient

- ⇒ Coupled-cluster in  $^4\text{He}$  [Hagen *et al.* 2007]
- ⇒ SCGF in INM [Somà, Božek 2008]
- ⇒ Perturbation theory in INM [Hebeler, Schwenk 2009]



# Connection to *non-empirical* EDF

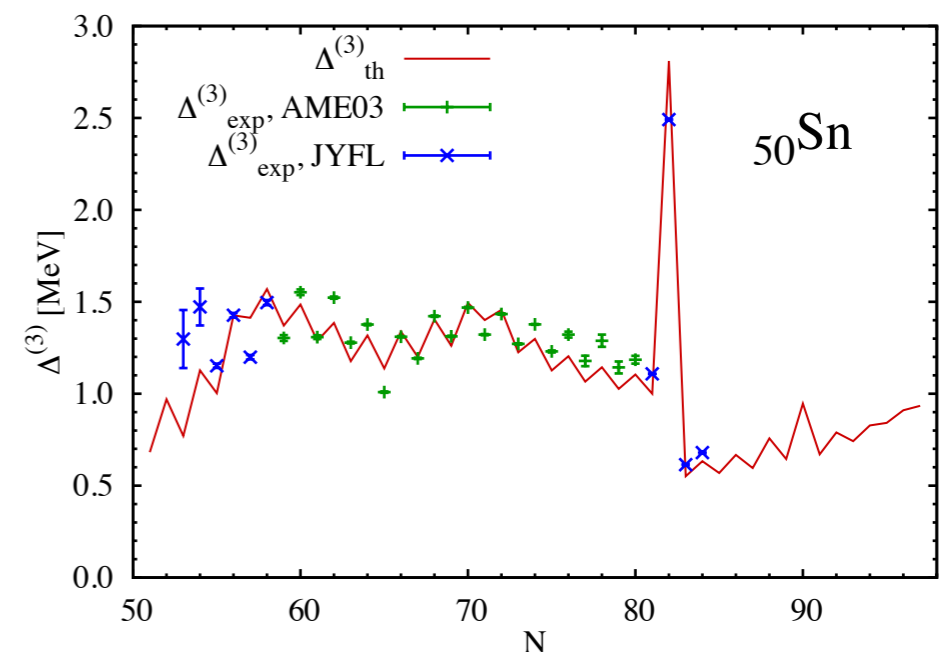
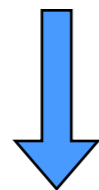
- ✱ Standard EDF parameterizations (e.g. Skyrme, Gogny, relativistic)
  - Successful in major shell where adjusted
  - Lack predictive power in new regions of interest



Efforts to extend and connect with more fundamental approaches

- ✱ Non-empirical EDF from low-momentum interactions

- Pairing channel [Duguet *et al.*]
- Particle-hole channel [Gebremariam *et al.*]



Benchmarks needed from many-body methods that share the same features

# Elements of Green's function methods

# Dyson Green's functions

- Many-body Hamiltonian

$$H \equiv T + V^{NN} + V^{NNN} \equiv \sum_{ab} t_{ab} a_a^\dagger a_b + \frac{1}{(2!)^2} \sum_{abcd} \bar{V}_{abcd}^{NN} a_a^\dagger a_b^\dagger a_d a_c + \frac{1}{(3!)^2} \sum_{abcdef} \bar{V}_{abcdef}^{NNN} a_a^\dagger a_b^\dagger a_c^\dagger a_f a_e a_d$$

- One-body propagator or Green's function

$$i G_{ab}(t, t') \equiv \langle \Psi_0^N | T \{ a_a(t) a_b^\dagger(t') \} | \Psi_0^N \rangle \equiv \begin{array}{c} a \\ \parallel \\ \blacktriangleright \\ \parallel \\ b \end{array}$$

- Heisenberg representation for creation/annihilation operators

$$a_b(t) = a_b^{(H)}(t) \equiv \exp[iHt] a_b \exp[-iHt]$$

$$a_b^\dagger(t) = [a_b^{(H)}(t)]^\dagger \equiv \exp[iHt] a_b^\dagger \exp[-iHt]$$

- Fourier transform to energy domain

$$G_{ab}(\omega) = \int d(t - t') e^{i\omega(t-t')} G_{ab}(t, t')$$

- Hierarchy of coupled equations between 1-body, 2-body, ... N-body propagators

# Observables (1)

## 1) Separation energy spectrum

$$G_{ab}(\omega) = \sum_k \frac{\chi_a^{k(N)*} \chi_b^{k(N)}}{\omega - E_k^{+(N)} + i\eta} + \sum_k \frac{\gamma_a^{k(N)} \gamma_b^{k(N)*}}{\omega - E_k^{-(N)} - i\eta}$$

Lehmann representation

where

$$\begin{cases} \chi_a^{k(N)} \equiv \langle \psi_k^{N+1} | a_a^\dagger | \psi_0^N \rangle \\ \gamma_a^{k(N)} \equiv \langle \psi_k^{N-1} | a_a | \psi_0^N \rangle \end{cases}$$

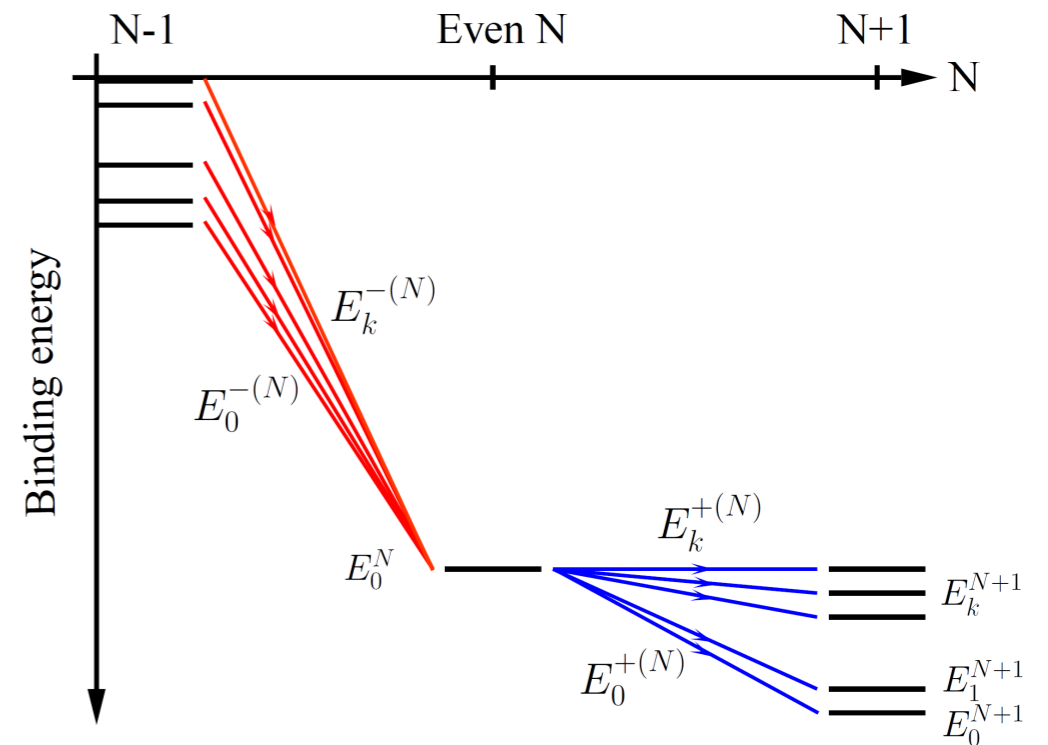
and

$$\begin{cases} E_k^{+(N)} \equiv E_k^{N+1} - E_0^N \\ E_k^{-(N)} \equiv E_0^N - E_k^{N-1} \end{cases}$$

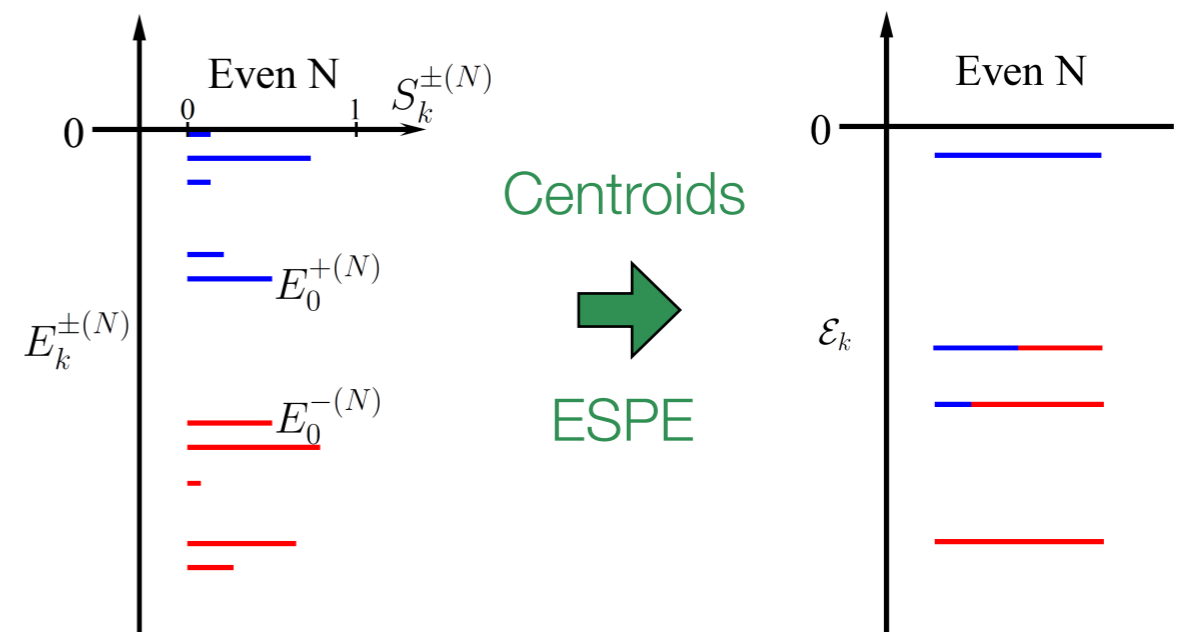
## 2) Spectroscopic factors

$$S_k^{N+1} \equiv \sum_a |\langle \psi_k^{N+1} | a_a^\dagger | \psi_0^N \rangle|^2 = \sum_a |\chi_a^{k(N)}|^2$$

$$S_k^{N-1} \equiv \sum_a |\langle \psi_k^{N-1} | a_a | \psi_0^N \rangle|^2 = \sum_a |\gamma_a^{k(N)}|^2$$



Separation energies





## Observables (2)

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3) One-body observables with  $\hat{O} = \sum_{ab} O_{ab} a_a^\dagger a_b$

$$\langle \hat{O} \rangle = \sum_{ab} \int \frac{d\omega}{2\pi} O_{ab} G_{ab}(\omega)$$

⇒ e.g. kinetic energy  $\langle \hat{T} \rangle = \sum_{ab} \int \frac{d\omega}{2\pi} t_{ab} G_{ab}(\omega)$

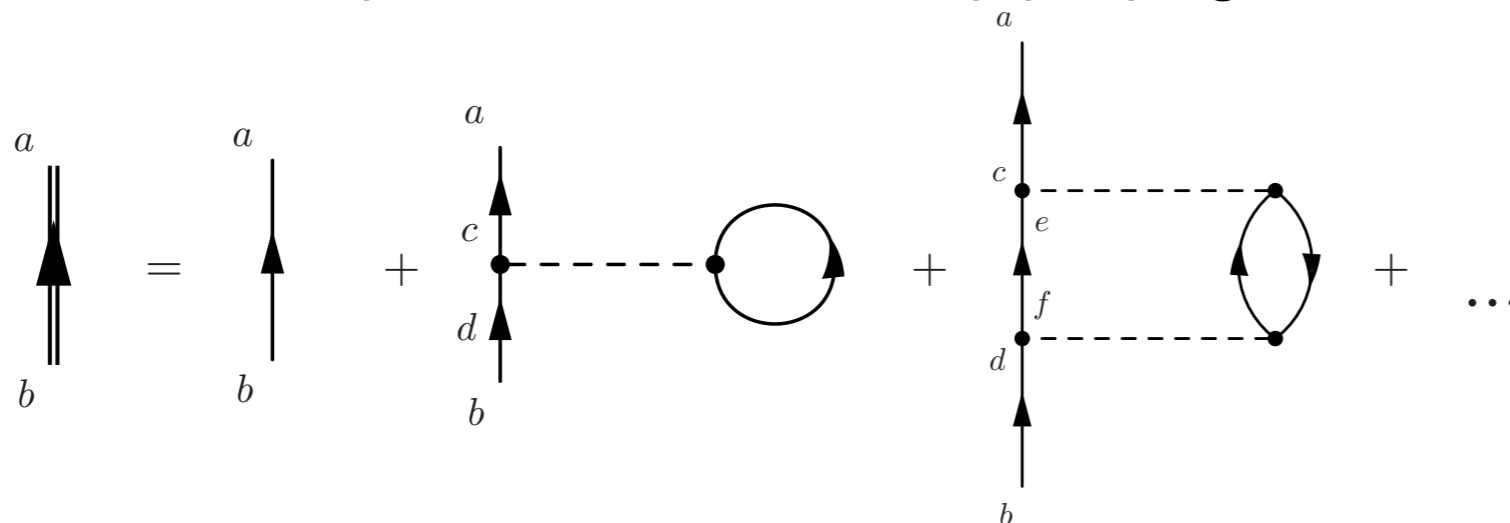
4) Koltun sum rule

$$\langle \hat{H} \rangle = E_0 = \sum_{ab} \int \frac{d\omega}{2\pi} [t_{ab} + \omega \delta_{ab}] G_{ab}(\omega)$$

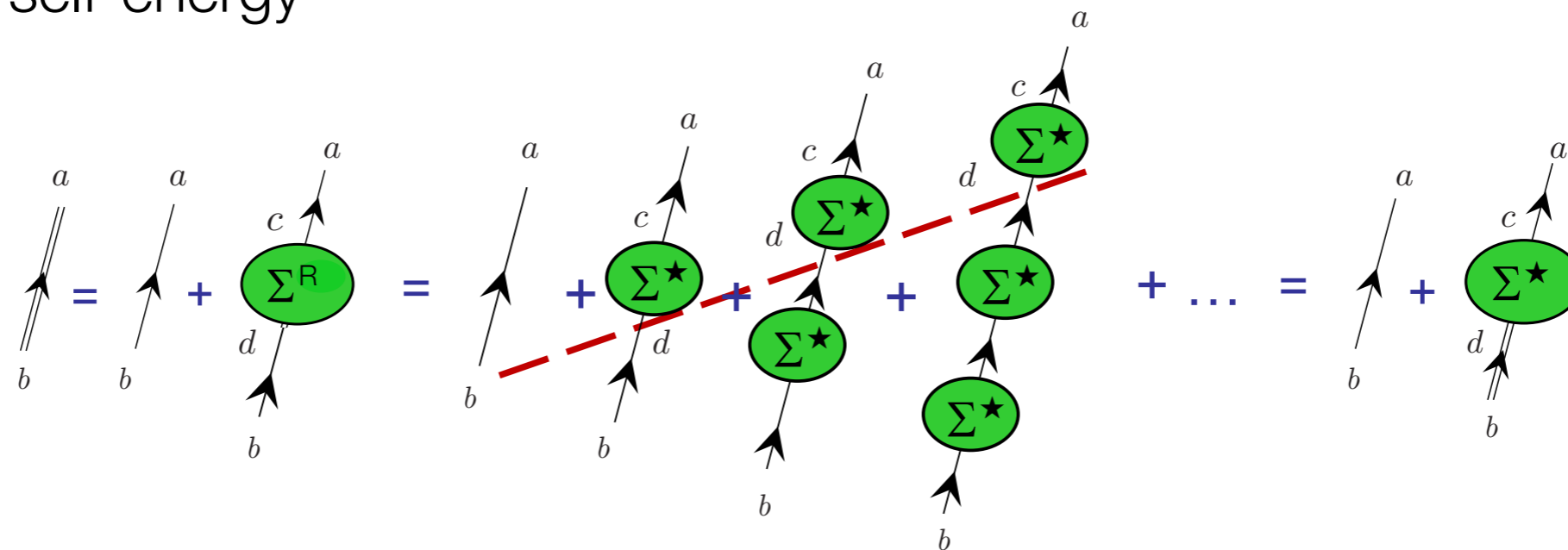
⇒ two-body observable computed from the one-body propagator

# Dyson equation & self-energy

✱ Perturbative expansion of one-body propagator



✱ Irreducible self-energy



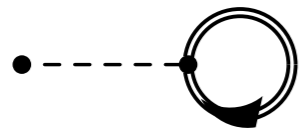
✱ Dyson equation

$$G_{ab}(\omega) = G_{ab}^{(0)}(\omega) + \sum_{cd} G_{ac}^{(0)}(\omega) \Sigma_{cd}^*(\omega) G_{db}(\omega)$$

# Solving Dyson equation

✱ Different approximations to the self-energy (**self-consistent** approaches)

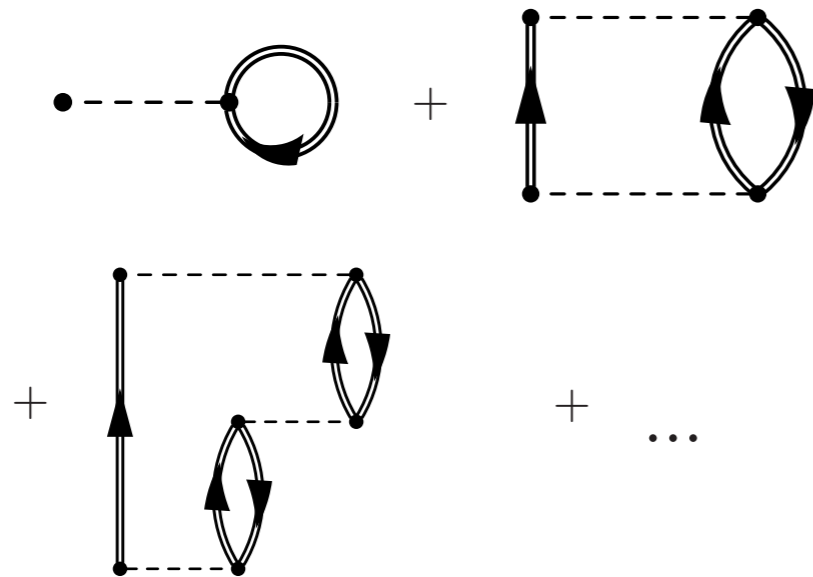
⇒ Hartree-Fock



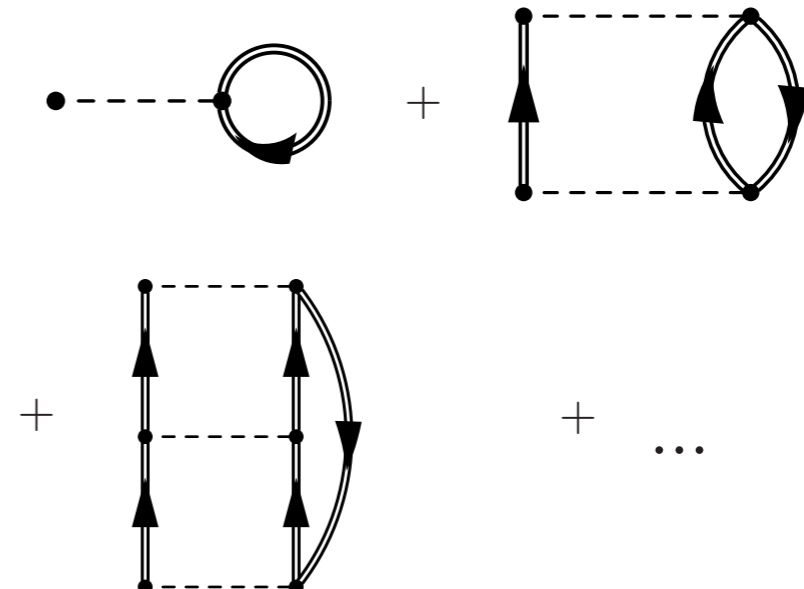
⇒ Second order



⇒ RPA



⇒ Ladder (or T-matrix)



➔ (Nearly) degenerate systems: **breakdown** of truncated expansions

↪ e.g. *pairing correlations*: approximation schemes face Cooper instability

➔ **Non-perturbative** treatment of such an instability needed

# Gorkov ansatz

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✱ Ansatz

$$\dots \approx E_0^{N+2} - E_0^N \approx E_0^N - E_0^{N-2} \approx \dots \approx 2\mu$$

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

→ Mixes various particle numbers

→ Introduce a “grand-canonical” potential  $\Omega = H - \mu N$

→  $|\Psi_0\rangle$  minimizes  $\Omega_0 = \langle \Psi_0 | \Omega | \Psi_0 \rangle$

under the constraint  $N = \langle \Psi_0 | N | \Psi_0 \rangle$

→  $\Omega_0 = \sum_{N'} |c_{N'}|^2 \Omega_0^{N'} \approx E_0^N - \mu N$

# Gorkov Green's functions and equations

✱ Set of 4 Green's functions

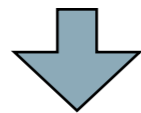
$$i G_{ab}^{11}(t, t') \equiv \langle \Psi_0 | T \{ a_a(t) a_b^\dagger(t') \} | \Psi_0 \rangle \equiv \begin{array}{c} a \\ \uparrow \uparrow \\ \downarrow \downarrow \\ b \end{array}$$

$$i G_{ab}^{21}(t, t') \equiv \langle \Psi_0 | T \{ \bar{a}_a^\dagger(t) a_b^\dagger(t') \} | \Psi_0 \rangle \equiv \begin{array}{c} \bar{a} \\ \downarrow \downarrow \\ \uparrow \uparrow \\ b \end{array}$$

$$i G_{ab}^{12}(t, t') \equiv \langle \Psi_0 | T \{ a_a(t) \bar{a}_b(t') \} | \Psi_0 \rangle \equiv \begin{array}{c} a \\ \uparrow \uparrow \\ \downarrow \downarrow \\ \bar{b} \end{array}$$

$$i G_{ab}^{22}(t, t') \equiv \langle \Psi_0 | T \{ \bar{a}_a^\dagger(t) \bar{a}_b(t') \} | \Psi_0 \rangle \equiv \begin{array}{c} \bar{a} \\ \downarrow \downarrow \\ \uparrow \uparrow \\ \bar{b} \end{array}$$

[Gorkov 1958]



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

Gorkov equations

$$\boldsymbol{\Sigma}_{ab}^*(\omega) \equiv \begin{pmatrix} \Sigma_{ab}^{*11}(\omega) & \Sigma_{ab}^{*12}(\omega) \\ \Sigma_{ab}^{*21}(\omega) & \Sigma_{ab}^{*22}(\omega) \end{pmatrix}$$

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

# Lehmann representation

✱ Set eigenstates of  $\Omega$   $\Omega|\Psi_k\rangle = \Omega_k|\Psi_k\rangle$

define

$$\begin{aligned} \mathcal{U}_a^{k*} &\equiv \langle \Psi_k | \bar{a}_a^\dagger | \Psi_0 \rangle \\ \mathcal{V}_a^{k*} &\equiv \langle \Psi_k | a_a | \Psi_0 \rangle \end{aligned}$$

$$\begin{aligned} \bar{\mathcal{U}}_a^{k*} &\equiv \langle \Psi_k | a_a^\dagger | \Psi_0 \rangle \\ \bar{\mathcal{V}}_a^{k*} &\equiv \langle \Psi_k | \bar{a}_a | \Psi_0 \rangle \end{aligned}$$

✱ Lehmann representation

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

$$G_{ab}^{21}(\omega) = \sum_k \left\{ \frac{\bar{\mathcal{V}}_a^k \bar{\mathcal{U}}_b^{k*}}{\omega - \omega_k + i\eta} + \frac{\mathcal{U}_a^{k*} \mathcal{V}_b^k}{\omega + \omega_k - i\eta} \right\}$$

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

$$G_{ab}^{22}(\omega) = \sum_k \left\{ \frac{\bar{\mathcal{V}}_a^k \bar{\mathcal{V}}_b^{k*}}{\omega - \omega_k + i\eta} + \frac{\mathcal{U}_a^{k*} \mathcal{U}_b^k}{\omega + \omega_k - i\eta} \right\}$$

where  $\omega_k \equiv \Omega_k - \Omega_0$  and

$$\begin{aligned} E_k^+ &\equiv +\omega_k + \mu \\ E_k^- &\equiv -\omega_k + \mu \end{aligned}$$

✱ Generalized spectroscopic factors

$$\mathcal{S}_k^+ \equiv \sum_a |\langle \psi_k | a_a^\dagger | \psi_0 \rangle|^2 = \sum_a |\mathcal{U}_a^k|^2$$

$$\mathcal{S}_k^- \equiv \sum_a |\langle \psi_k | a_a | \psi_0 \rangle|^2 = \sum_a |\mathcal{V}_a^k|^2$$

# Gorkov equations (2)

✱ Gorkov equations  $\xrightarrow{\text{Lehmann}}$  energy-dependent eigenvalue problem

$$\sum_b \begin{pmatrix} t_{ab} - \mu_{ab} + \Sigma_{ab}^{11}(\omega) & \Sigma_{ab}^{12}(\omega) \\ \Sigma_{ab}^{21}(\omega) & -t_{ab} + \mu_{ab} + \Sigma_{ab}^{22}(\omega) \end{pmatrix} \Big|_{\omega_k} \begin{pmatrix} \mathcal{U}_b^k \\ \mathcal{V}_b^k \end{pmatrix} = \omega_k \begin{pmatrix} \mathcal{U}_a^k \\ \mathcal{V}_a^k \end{pmatrix}$$

$\Sigma^{g_1 g_2}(\omega)$  play the role of energy-dependent potentials

Iterative problem: the number of poles  $\omega_k$  grows with iterations

Constraint: correct number of particles in average  $N = \sum_{a,k} |\mathcal{V}_a^k|^2$

Normalization condition  $\sum_a (\mathcal{V}_a^k \mathcal{U}_a^k) \begin{pmatrix} \mathcal{V}_a^{k*} \\ \mathcal{U}_a^{k*} \end{pmatrix} = 1 + \sum_{ab} (\mathcal{V}_a^k \mathcal{U}_a^k) \frac{\partial \Sigma_{ab}(\omega)}{\partial \omega} \Big|_{-\omega_k} \begin{pmatrix} \mathcal{V}_a^{k*} \\ \mathcal{U}_a^{k*} \end{pmatrix}$

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Objective  $\left\{ \begin{array}{l} \text{Short term} \quad \Rightarrow \text{Self-consistent second order} \\ \text{Longer term} \quad \Rightarrow \text{Self-consistent Faddeev-QRPA} \end{array} \right.$



# 1st order diagrams and HFB limit

✱ Energy-independent self-energy

$$\Sigma_{ab}^{11(1)} = \text{Diagram: } \begin{array}{c} a \\ \bullet \\ b \end{array} \text{---} \begin{array}{c} c \\ \bullet \\ d \end{array} \text{---} \text{Loop} \downarrow \omega'$$

$$\Sigma_{ab}^{11(1)} = \sum_{cd,k} \bar{V}_{acbd} \mathcal{V}_d^{k*} \mathcal{V}_c^k \equiv \Lambda_{ab} = -\Sigma_{ab}^{22(1)}$$

$$\Sigma_{ab}^{12(1)} = \text{Diagram: } \begin{array}{c} a \\ \bullet \\ c \end{array} \text{---} \begin{array}{c} \bar{b} \\ \bullet \\ \bar{d} \end{array} \text{---} \text{Loop} \leftarrow \omega'$$

$$\Sigma_{ab}^{12(1)} = \frac{1}{2} \sum_{cd,k} \bar{V}_{a\bar{b}c\bar{d}} \mathcal{V}_c^{k*} \mathcal{U}_d^k \equiv \tilde{h}_{ab} = \left[ \Sigma_{ba}^{21(1)} \right]^*$$

✱ HFB problem is recovered  $\longrightarrow$  energy-independent eigenvalue problem

$$\sum_b \begin{pmatrix} t_{ab} + \Lambda_{ab} - \mu \delta_{ab} & \tilde{h}_{ab} \\ \tilde{h}_{ab}^\dagger & -t_{ab} - \Lambda_{ab} + \mu \delta_{ab} \end{pmatrix} \begin{pmatrix} U_b^k \\ V_b^k \end{pmatrix} = \omega_k \begin{pmatrix} U_a^k \\ V_a^k \end{pmatrix}$$

with the normalization condition

$$\sum_a |U_a^k|^2 + \sum_a |V_a^k|^2 = 1$$

# 2nd order diagrams

## ✱ Energy-dependent self-energy

$$\Sigma_{ab}^{11(2)}(\omega) = \begin{array}{c} a \\ \vdots \\ c \\ \uparrow \omega' \\ \vdots \\ d \\ \vdots \\ b \end{array} \begin{array}{c} e \\ \vdots \\ f \\ \uparrow \omega'' \\ \vdots \\ g \\ \vdots \\ h \end{array} + \begin{array}{c} a \\ \vdots \\ c \\ \uparrow \omega' \\ \vdots \\ d \\ \vdots \\ b \end{array} \begin{array}{c} e \\ \vdots \\ f \\ \uparrow \omega'' \\ \vdots \\ \bar{h} \\ \vdots \\ \bar{g} \end{array} \downarrow \omega'''$$

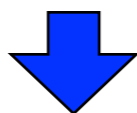
$$\Sigma_{ab}^{12(2)}(\omega) = \begin{array}{c} a \\ \vdots \\ c \\ \uparrow \omega' \\ \vdots \\ \bar{d} \\ \vdots \\ \bar{b} \end{array} \begin{array}{c} e \\ \vdots \\ f \\ \uparrow \omega'' \\ \vdots \\ g \end{array} \downarrow \omega''' + \begin{array}{c} a \\ \vdots \\ c \\ \uparrow \omega' \\ \vdots \\ \bar{d} \\ \vdots \\ \bar{b} \end{array} \begin{array}{c} e \\ \vdots \\ f \\ \uparrow \omega'' \\ \vdots \\ \bar{h} \end{array} \downarrow \omega'''$$

$$\Sigma_{ab}^{11(2)}(\omega) = \sum_{k_1 k_2 k_3} \left\{ \frac{\mathcal{C}_a^{k_1 k_2 k_3} \mathcal{C}_b^{k_1 k_2 k_3 \dagger}}{\omega - E_{k_1 k_2 k_3} + i\eta} + \frac{\mathcal{D}_a^{k_1 k_2 k_3 \dagger} \mathcal{D}_b^{k_1 k_2 k_3}}{\omega + E_{k_1 k_2 k_3} + i\eta} \right\}$$

$$\Sigma_{ab}^{12(2)}(\omega) = - \sum_{k_1 k_2 k_3} \left\{ \frac{\mathcal{C}_a^{k_1 k_2 k_3} \mathcal{D}_b^{k_1 k_2 k_3}}{\omega - E_{k_1 k_2 k_3} + i\eta} + \frac{\mathcal{D}_a^{k_1 k_2 k_3 \dagger} \mathcal{C}_b^{k_1 k_2 k_3 \dagger}}{\omega + E_{k_1 k_2 k_3} + i\eta} \right\}$$

$$\mathcal{C}_a^{k_1 k_2 k_3} \equiv \frac{1}{\sqrt{6}} \sum_{\{1,2,3\}} \sum_{ijk} \bar{V}_{akij} \bar{u}_i^{k_1} \bar{u}_j^{k_2} v_k^{k_3}$$

$$\mathcal{D}_a^{k_1 k_2 k_3} \equiv \frac{1}{\sqrt{6}} \sum_{\{1,2,3\}} \sum_{ijk} \bar{V}_{akij} v_i^{k_1} v_j^{k_2} \bar{u}_k^{k_3}$$



## ✱ Recast known energy dependence into new quantities

$$(\omega_k - E_{k_1 k_2 k_3}) \mathcal{W}_k^{k_1 k_2 k_3} \equiv \sum_a \left[ \mathcal{C}_a^{k_1 k_2 k_3 \dagger} \mathcal{U}_a^k - \mathcal{D}_a^{k_1 k_2 k_3} \mathcal{V}_a^k \right]$$

$$(\omega_k + E_{k_1 k_2 k_3}) \mathcal{Z}_k^{k_1 k_2 k_3} \equiv \sum_a \left[ -\mathcal{D}_a^{k_1 k_2 k_3} \mathcal{U}_a^k + \mathcal{C}_a^{k_1 k_2 k_3 \dagger} \mathcal{V}_a^k \right]$$

# Gorkov equations (3)

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$$\sum_b \begin{pmatrix} t_{ab} - \mu_{ab} + \Sigma_{ab}^{11}(\omega) & \Sigma_{ab}^{12}(\omega) \\ \Sigma_{ab}^{21}(\omega) & -t_{ab} + \mu_{ab} + \Sigma_{ab}^{22}(\omega) \end{pmatrix} \Big|_{\omega_k} \begin{pmatrix} \mathcal{U}_b^k \\ \mathcal{V}_b^k \end{pmatrix} = \omega_k \begin{pmatrix} \mathcal{U}_a^k \\ \mathcal{V}_a^k \end{pmatrix}$$

Expand in terms  of  $W$  and  $Z$

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

Energy *independent* eigenvalue problem

with the normalization condition

$$\sum_a \left[ |\mathcal{U}_a^k|^2 + |\mathcal{V}_a^k|^2 \right] + \sum_{k_1 k_2 k_3} \left[ |\mathcal{W}_k^{k_1 k_2 k_3}|^2 + |\mathcal{Z}_k^{k_1 k_2 k_3}|^2 \right] = 1$$

# Results

# Results

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- ✱ Calculations of  $^{40-48}\text{Ca}$  isotopes

- ➡ Spherical harmonic oscillator basis

- ➡  $V_{\text{low-k}}$  from Ch-EFT potential with cutoff  $\Lambda = 2.1$  &  $2.5 \text{ fm}^{-1}$

- ➡ NN interaction only

- ✱ CEA-CCRT massively-parallel high-performance cluster

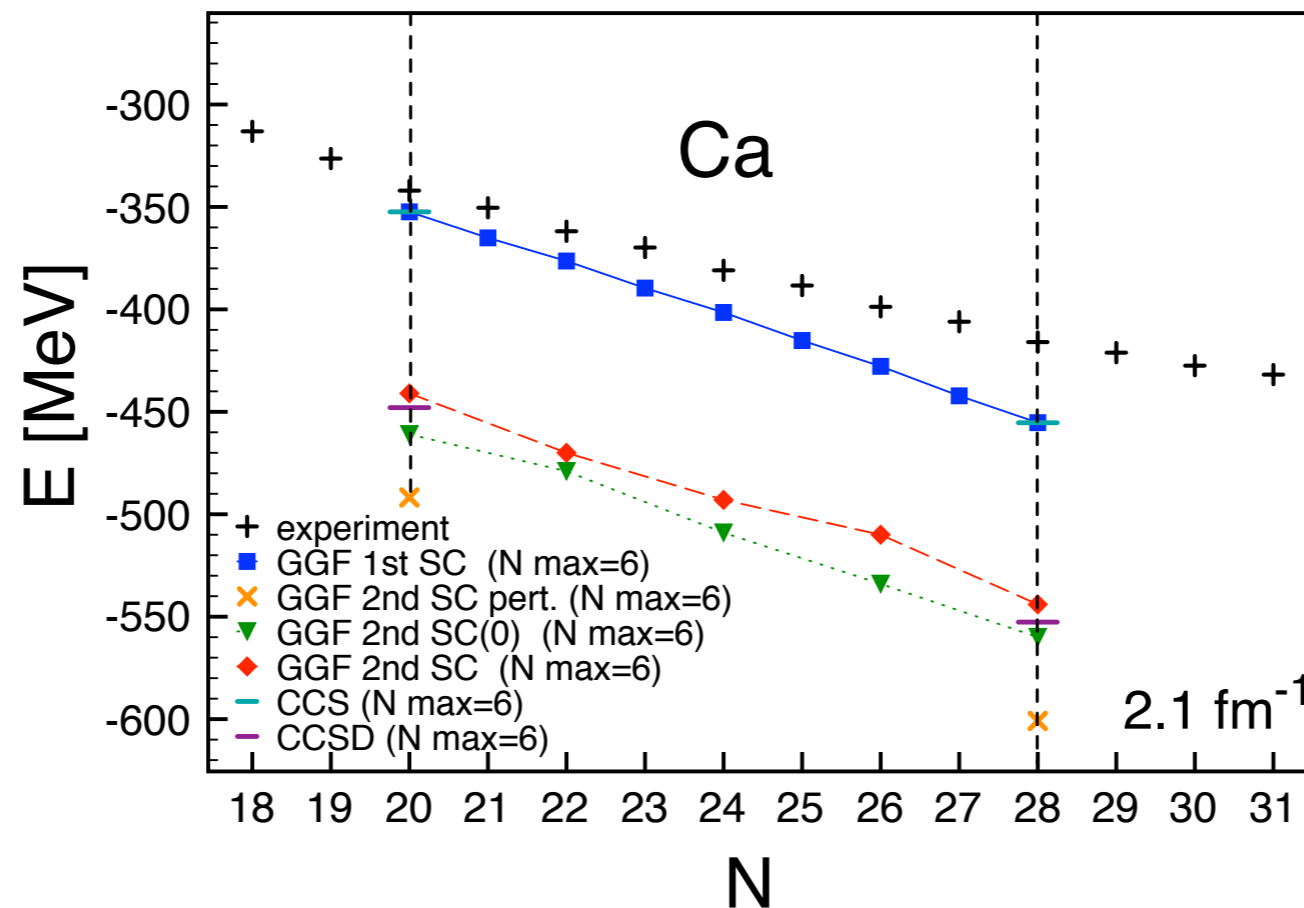
- ➡ ~ 58 000 cores, ~ 300 Tflops total

- ➡ Parallelized code

➡ Essential for self-consistent second-order calculations

# Binding energies

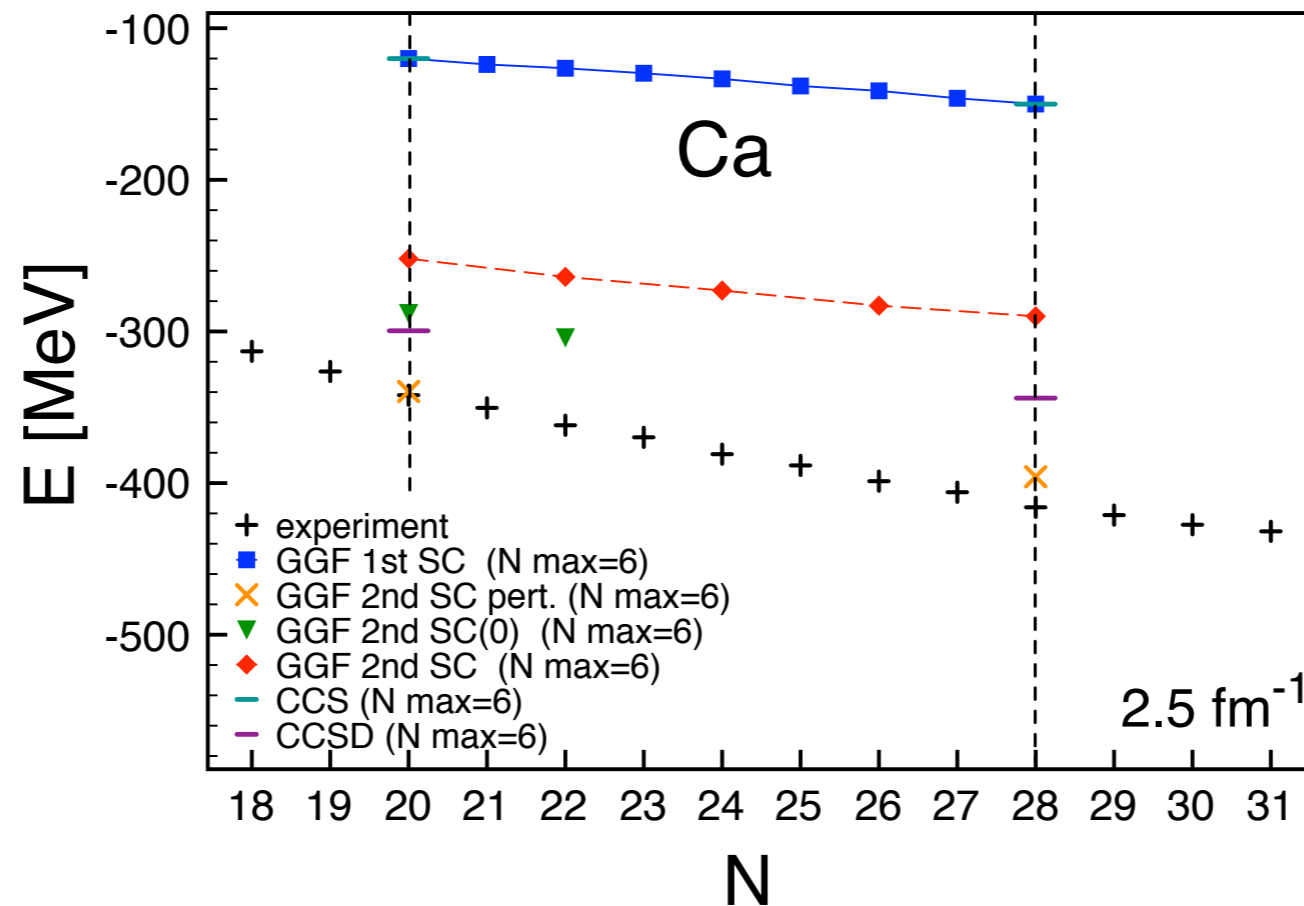
✱ Systematic along isotopic/isotonic chains become available



- ⇒ Correlation energy “consistent” with CCSD (quantitative analysis in progress)
- ⇒ Overbinding with A: traces need for (at least) NNN forces
- ⇒ Second-order SCGF qualitatively different from second-order MBPT

# Binding energies

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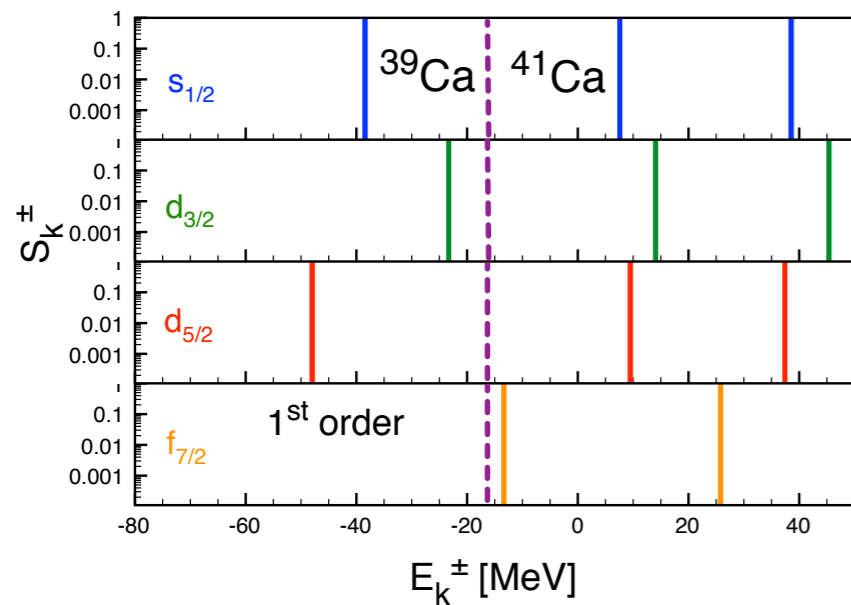
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# Spectral function

Dyson 1<sup>st</sup> order (HF)

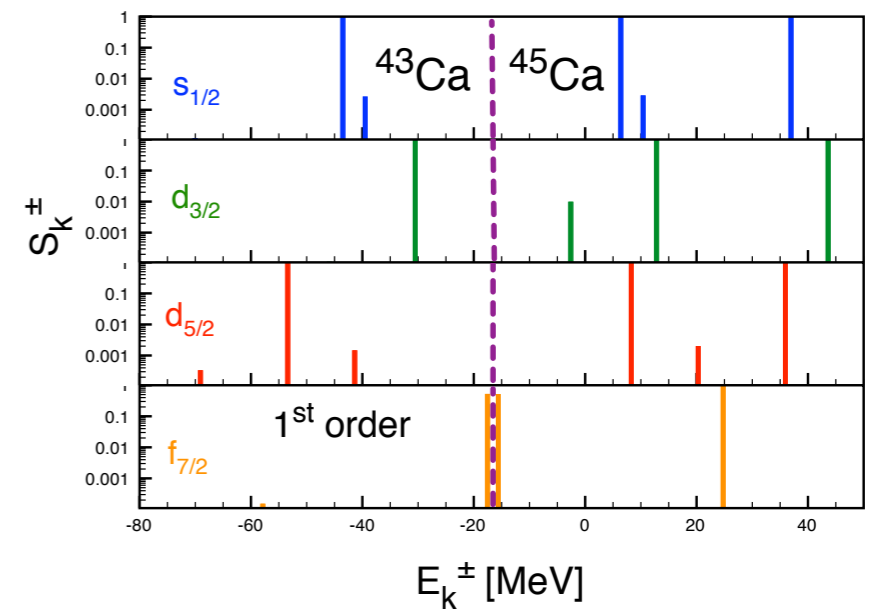


Fragmentation

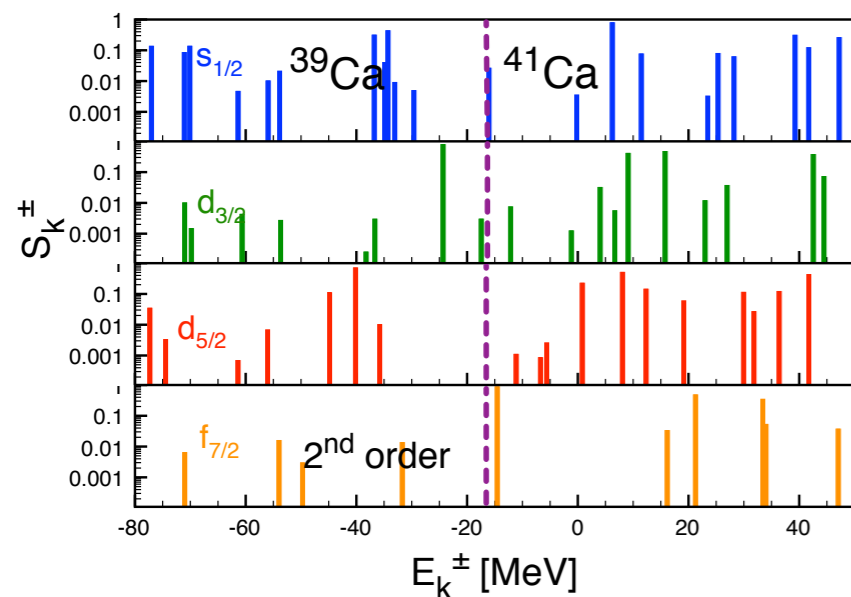
Static pairing



Gorkov 1<sup>st</sup> order (HFB)



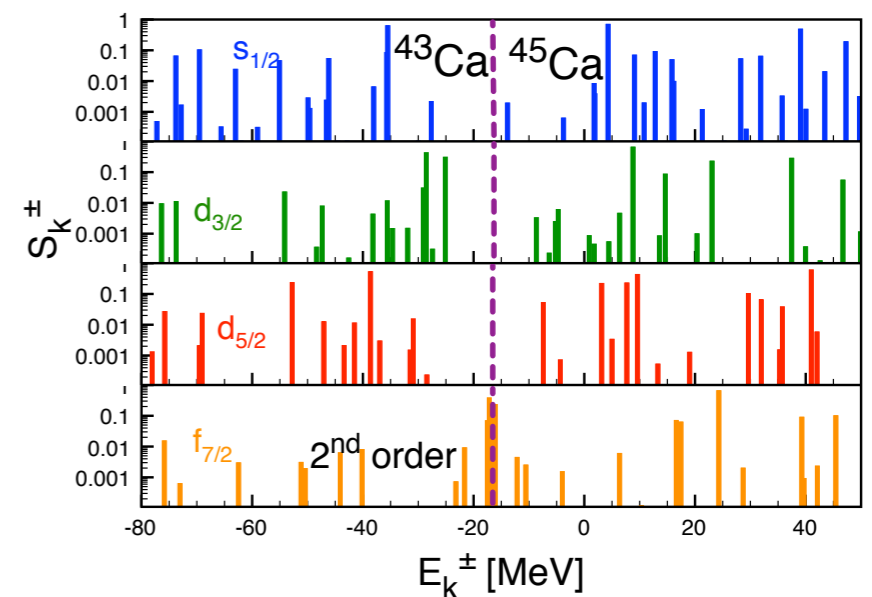
Dyson 2<sup>nd</sup> order



Dynamical fluctuations



Gorkov 2<sup>nd</sup> order



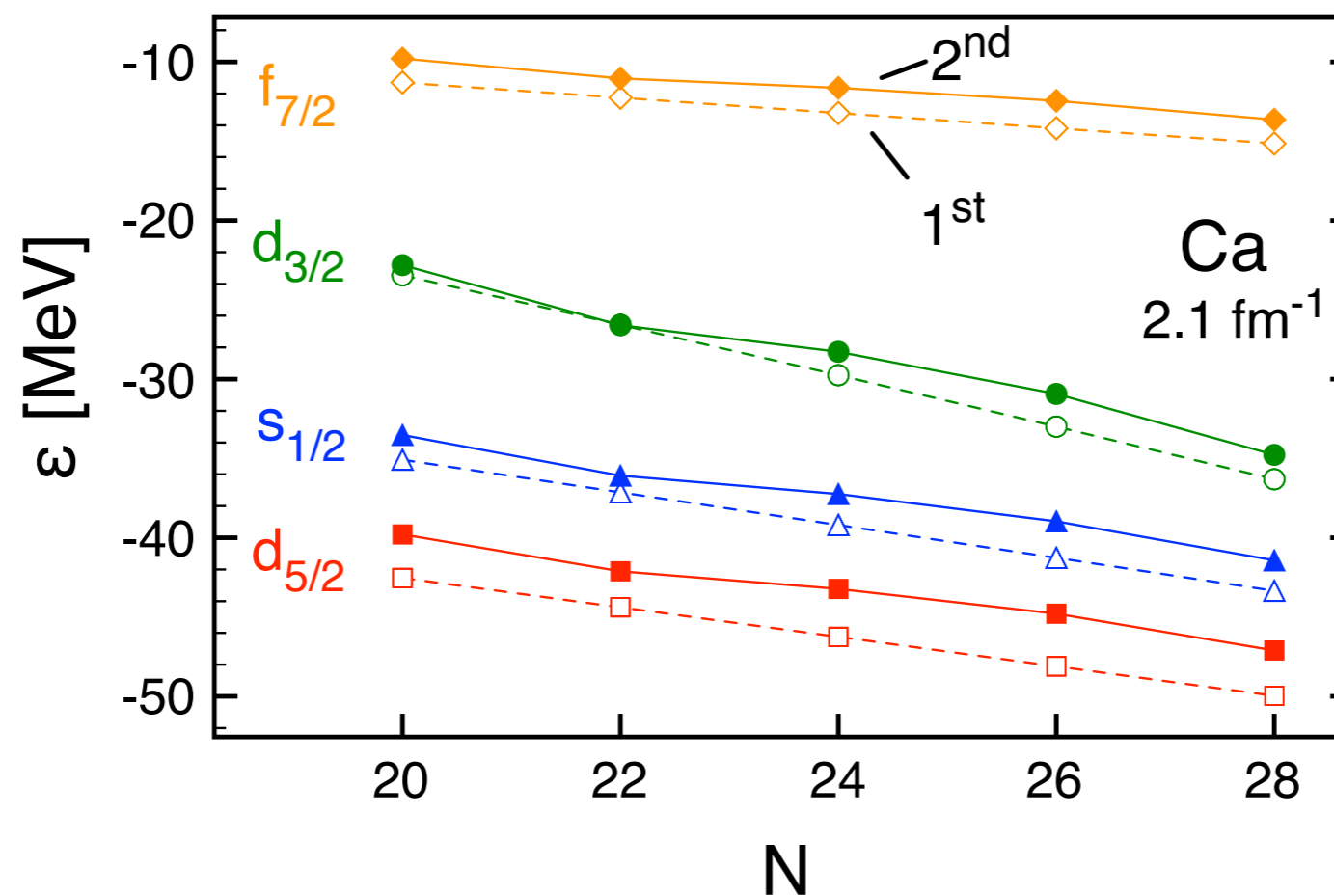


# Shell structure evolution

✱ ESPE collect fragmentation of “single-particle” strengths from both  $N \pm 1$

$$\epsilon_a = \sum_k S_k^{+a} E_k^+ + \sum_k S_k^{-a} E_k^- = t_{aa} + \sum_{cd} \bar{V}_{acad} \rho_{dc}$$

[Baranger 1970]



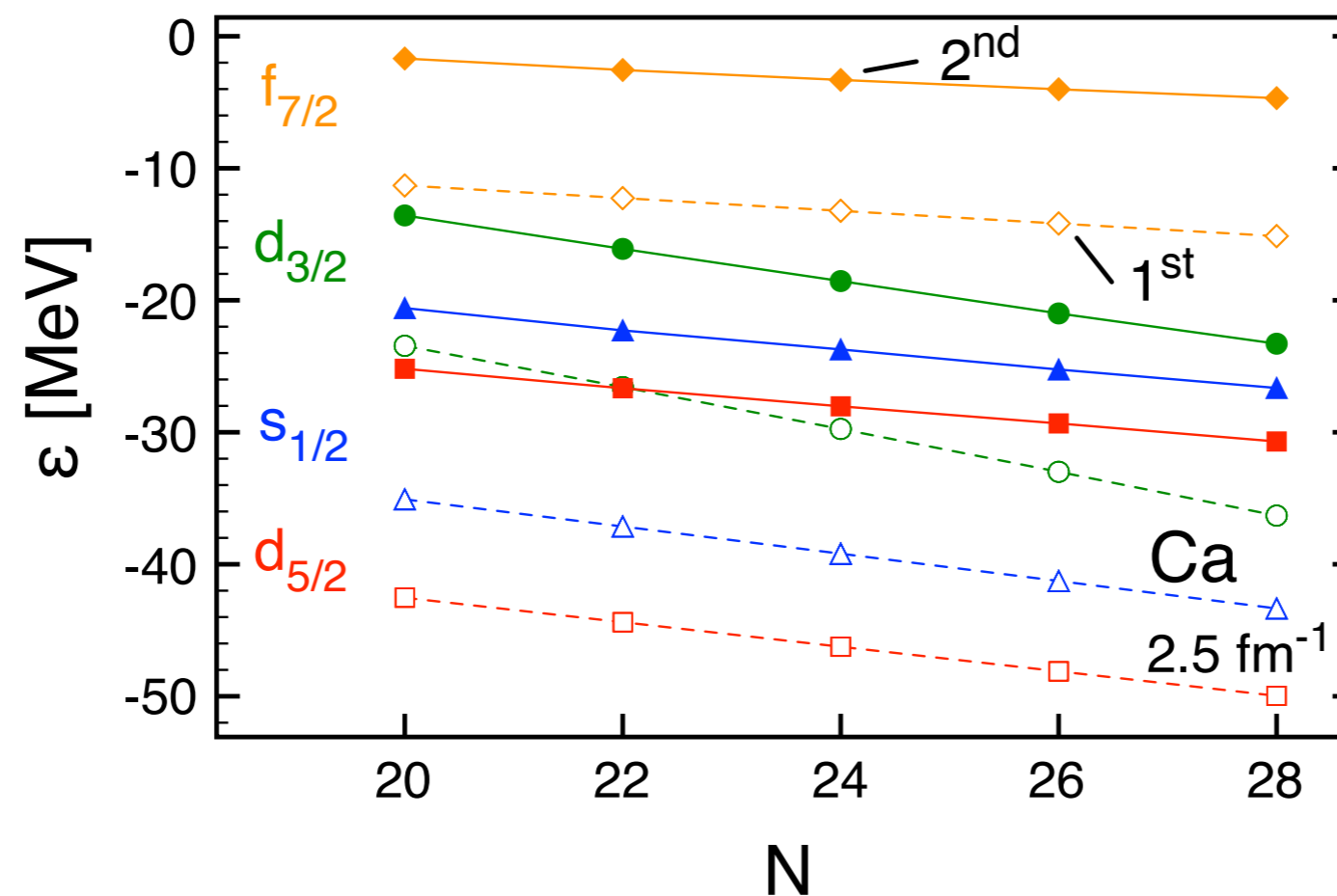
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[Baranger 1970]



➡ Correlations shift ESPE up in a non-uniform manner

# Next

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- ✱ Systematic comparison with CC in doubly magic  $\pm 1$  and  $\pm 2$  nuclei  
[in collaboration with G. Hagen]
- ✱ Implementation of **NNN** forces
- ✱ Formulation of **particle-number restored** Gorkov theory