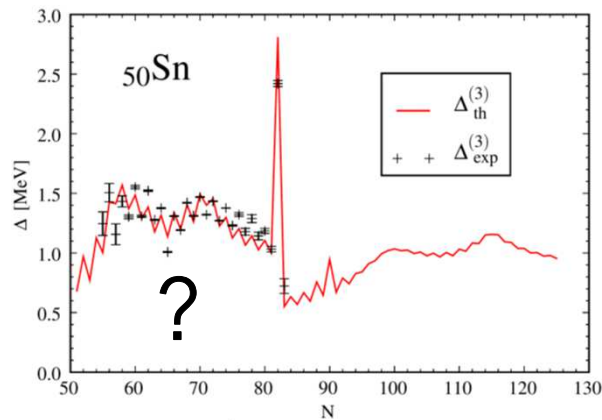


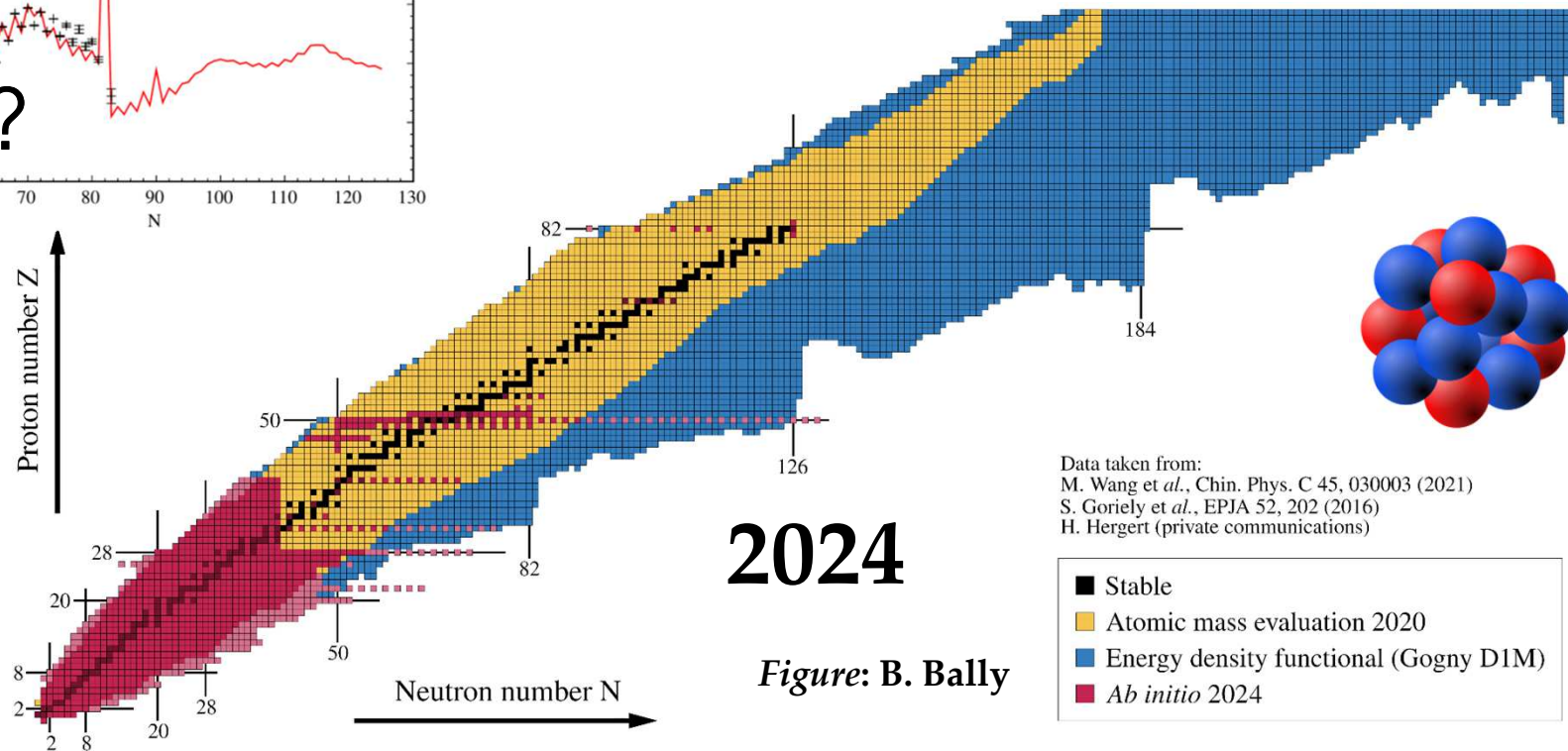
Ab initio description of neutron-neutron and proton-proton pairing in finite nuclei

Introductory Lecture



Infinite matter background: Lectures by G. Palkanoglou, M. Urban

Neutron-proton pairing counterpart: Lecture by S. Frauendorf



Data taken from:
M. Wang et al., Chin. Phys. C 45, 030003 (2021)
S. Goriely et al., EPJA 52, 202 (2016)
H. Hergert (private communications)

■ Stable
■ Atomic mass evaluation 2020
■ Energy density functional (Gogny D1M)
■ Ab initio 2024

2024

Figure: B. Bally

Ab initio many-body calculations: where has the nuclear pairing gone?

ESNT workshop, Saclay, 13-21 May 2025

Collaborators on ab initio many-body methods/calculations

PAN@CEA



B. Bally
G. Blanchon
S. Bofos
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T. Demartini
M. Dupuis
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L. González-Miret Zaragoza
L. Heitz
S. Sainato
V. Somà
G. Stellin
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KU LEUVEN



P. Demol
M. Aytekin

A. Scalesi



G. Hagen
T. Papenbrock



H. Hergert



P. Navratil



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R. Roth
A. Tichai
U. Vernik



T. R. Rodriguez



J. M. Yao

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- Introduction
 - The ab initio nuclear many-body problem
 - Phenomenology of isospin-triplet pairing in finite nuclei
 - Ab initio many-body expansion methods
- Ab initio description of isospin-triplet pairing in finite nuclei
 - Gorkov self-consistent Green's function theory in a nutshell
 - Lessons from empirical and semi-empirical HFB calculations
 - Ab initio GSCGF(1,2) calculations
 - Phenomenology of the induced pairing interaction
- Getting back the increased numerical cost of breaking $U(1)$ symmetry
 - Tensor factorization of triaxially deformed BMBPT(2) calculations

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The atomic nucleus as a 4-components quantum mesoscopic system

An extremely rich and diverse phenomenology

Nucleus: bound (or resonant) state of Z protons and N neutrons

“Ab initio” (= In medias res) long-term endeavor

Can nuclear systems be convincingly described

- 1) From nucleons and their interactions: right balance between reductionism/emergence?
- 2) Rooted into QCD in a systematically improvable way: sound connection via EFT(s)?
- 3) Systematically: complete phenomenology up to (super) heavy nuclei?
- 4) Accurately enough: relevant to experimental investigations/applications?

Practical benefit...



...yet to be proven

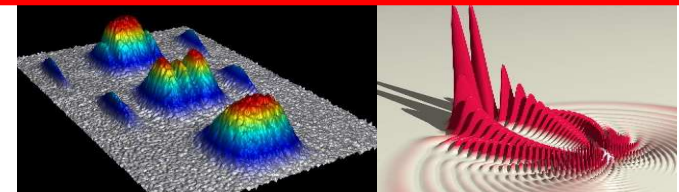
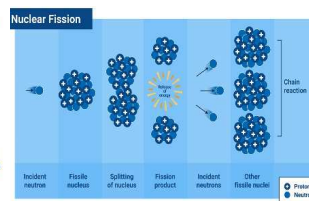
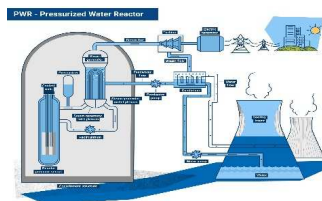
Nuclear observables can be

- 1) Described consistently
- 2) With (small enough) uncertainties
- 3) Extrapolated in a controlled fashion

What about nuclear superfluidity?

Great challenge as Δ is exponentially sensitive to

- a. “Effective” pairing interaction
- b. Density of “single-particle states”



Ab initio theoretical scheme

In this talk “Ab initio” scheme = Chiral effective field theory (χ EFT) in A-body sector

- 1) Structure-less nucleons
- 2) Inter-nucleon interactions at low-energy rooted into QCD = mediated by pions and contacts

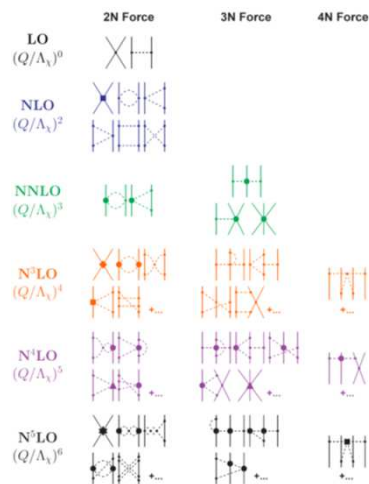
Weinberg Power Counting

$$H|\Psi_k^\sigma\rangle = E_k^{\tilde{\sigma}}|\Psi_k^\sigma\rangle \quad \text{with } \sigma \equiv JM\Pi NZ \equiv \tilde{\sigma}M$$



Systematic expansion of H

$$H = T + V_{\text{LO}} + V_{\text{NLO}} + V_{\text{N}^2\text{LO}} + \dots$$



Exponential curse with A

Full solution / $|\Psi_k\rangle$

$|\Psi_k^A\rangle$

Limited to $A \sim 16$

Talk A. Ekström

Ab initio theoretical scheme

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Systematic expansion of H

$$H = T + V_{\text{LO}} + V_{\text{NLO}} + V_{\text{N}^2\text{LO}} + \dots$$

Exponential \rightarrow Polynomial cost

Systematic expansion of $|\Psi_k\rangle$

$$|\Psi_k^A\rangle = \Omega|\Theta_k^{(0)}\rangle = |\Theta_k^{(0)}\rangle + |\Theta_k^{(1)}\rangle + |\Theta_k^{(2)}\rangle + \dots$$

Global philosophy

Double expansion **systematically improvable** towards **well-defined limit**

+

Uncertainties evaluation

H

Chiral EFT truncation
LECs adjustment
Rank reduction of V^{3N}

$|\Psi_k\rangle$

Basis truncation
Expansion truncation

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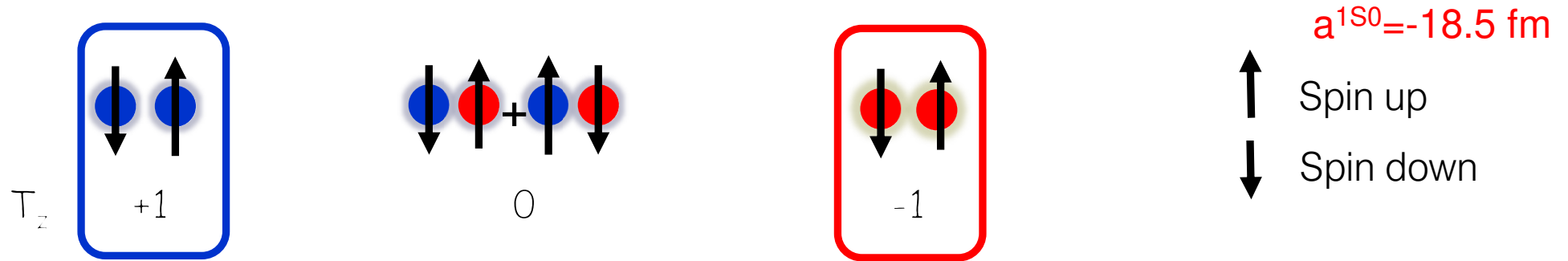
- ⊙ Phenomenology of the induced pairing interaction

- ⊙ Getting back the increased numerical cost of breaking $U(1)$ symmetry

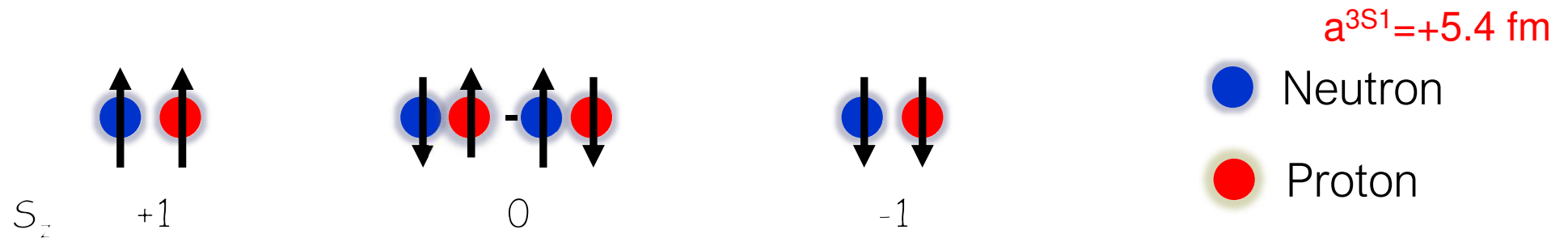
- ⊙ Tensor factorization of triaxially deformed BMBPT(2) calculations

Two isospin pairing channels = Cooper pairs

Isovector pairs ($T=1$) dominated by spin-singlet S -wave interaction (1S_0 channel)



Isoscalar pairs ($T=0$) dominated by spin-triplet S -wave interaction (3S_1 channel)



Focus on neutron-neutron/proton-proton pairing in finite nuclei in this lecture

Phenomenology = main signatures of (T=1,S=0) superfluidity

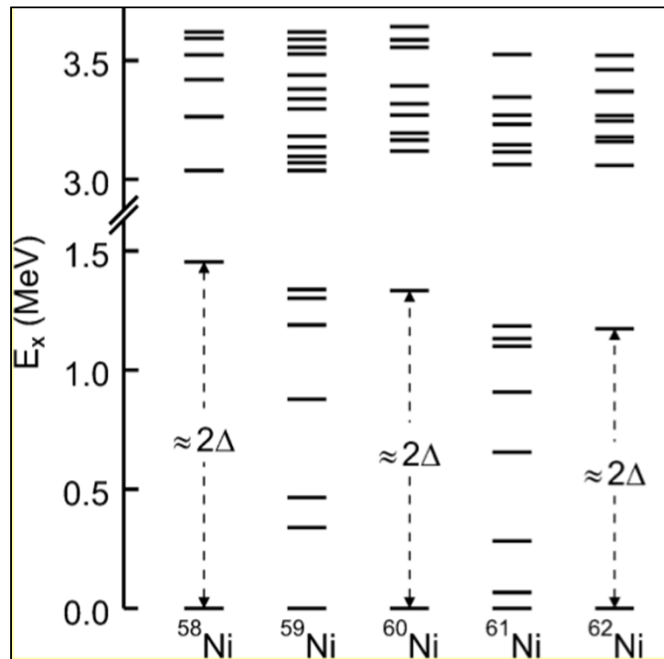
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Phenomenology = main signatures of ($T=1, S=0$) superfluidity

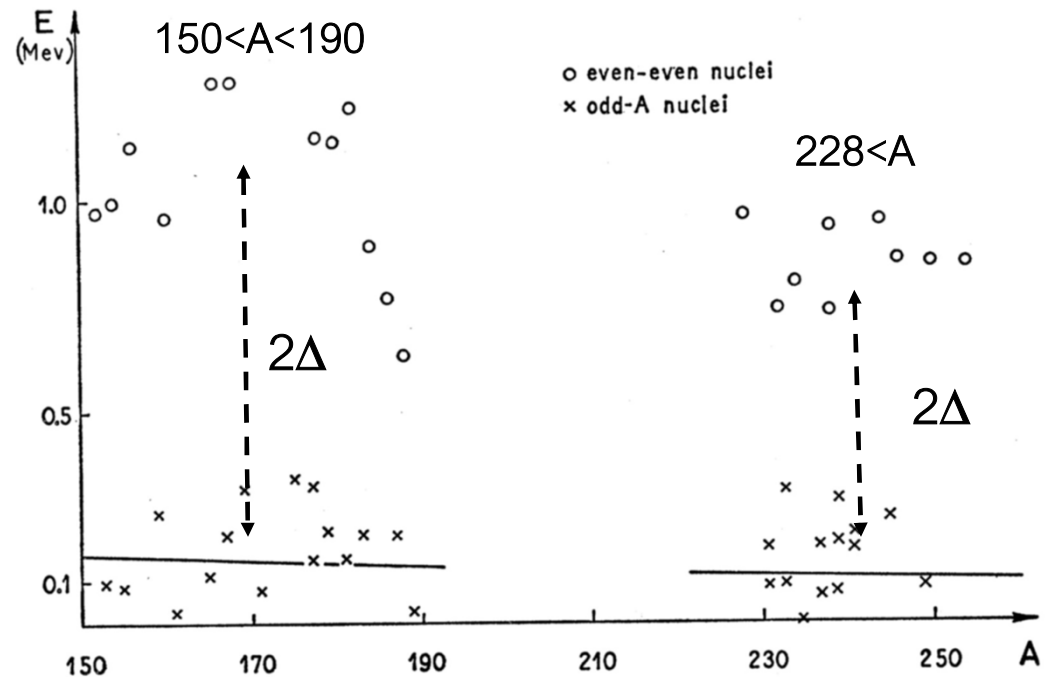
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First excited state: even-even vs even-odd open-shell nuclei

Singly open-shell (« spherical »)



Doubly open-shell (« deformed »)



Typical scale in even-even nuclei: $E_x \sim 1\text{-}2 \text{ MeV} = 2\Delta$

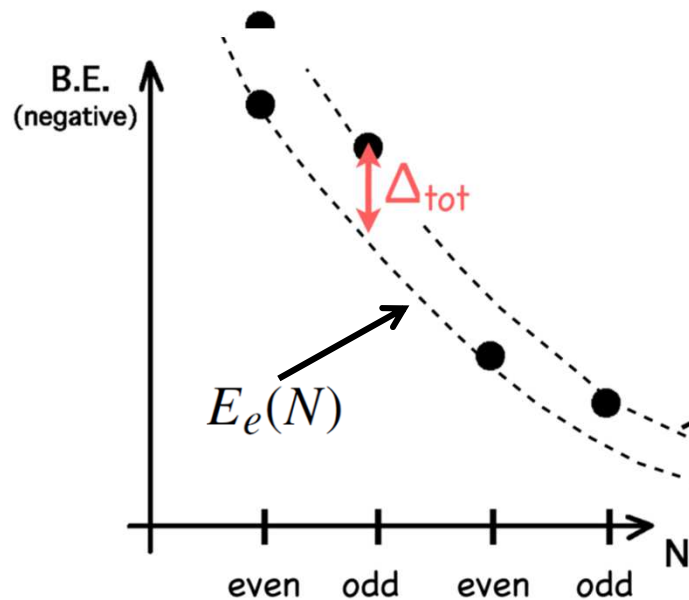
→ Observed to decrease with A

No such gap in even-odd nuclei: $E_x \sim 100\text{-}300 \text{ keV} = d$

Phenomenology = main signatures of ($T=1, S=0$) superfluidity

- 1) Energy of first excited state in even-even versus even-odd open-shell nuclei
- 2) Odd-even mass staggering Talks P. Demol, H. Hergert, V. Somà
- 3) Ground-state band moment of inertia
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Odd-even mass staggering



If odd and even isotopes had a similar structure

Real life: deficit of binding of odd isotopes

→ Two parabolas with odd one shifted up by Δ due to unpaired nucleon

→ Binding deficit Δ to be extracted via finite difference formulae

Three-point mass difference

$$\Delta^{(3)}(N) \equiv \frac{(-1)^N}{2} [E(N+1) - 2E(N) + E(N-1)]$$

Duguet et al., PRC (2002)

Oscillating around Δ Positive & constant curvature

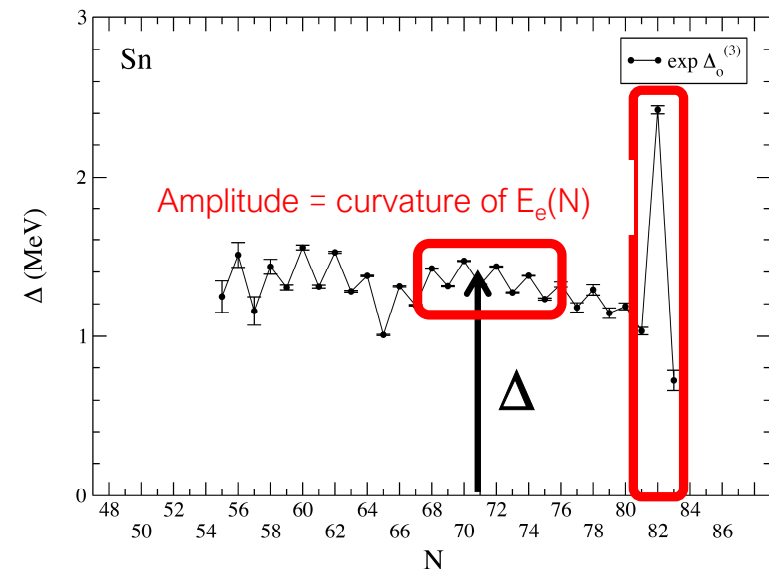
$$\begin{aligned} E_e(N) &\equiv E_e(N) \\ E_o(N) &\equiv E_e(N) + \Delta \end{aligned} \Rightarrow \Delta^{(3)}(N) = \frac{(-1)^N}{2} \frac{\partial^2 E_e(N)}{\partial N^2} + \Delta$$

Smooth/quadratic/convex part of the energy



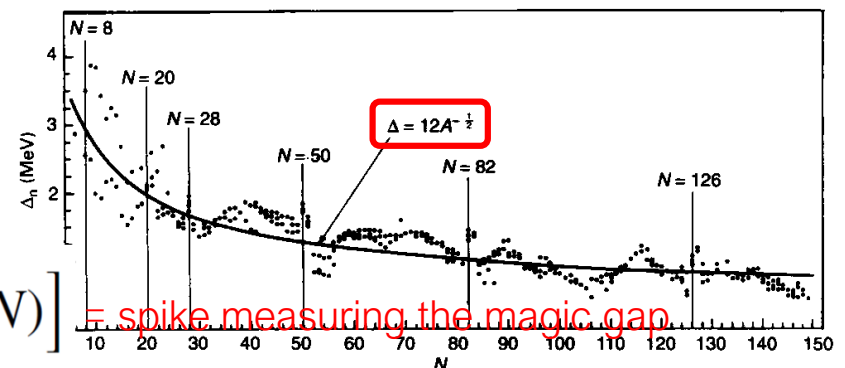
Except at closed shell

$$\equiv \frac{1}{2} [S_n(N+1) - S_n(N)]$$



Amplitude = curvature of $E_e(N)$

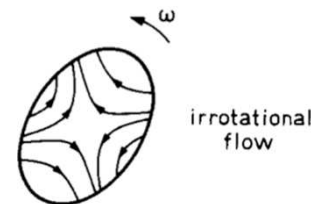
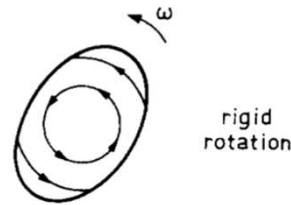
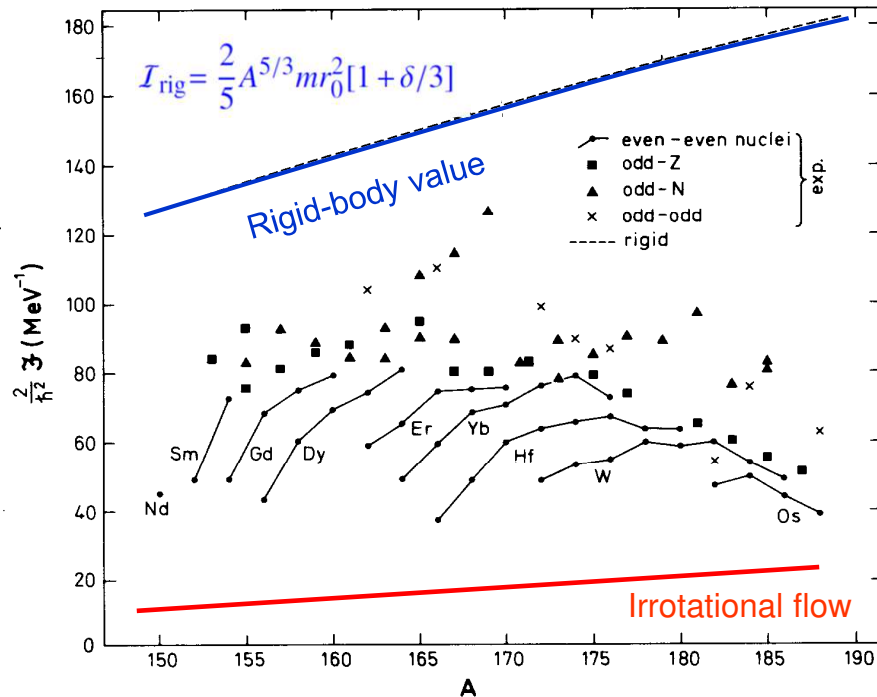
Evolution with A



Phenomenology = main signatures of ($T=1, S=0$) superfluidity

- 1) Energy of first excited state in even-even versus even-odd open-shell nuclei
- 2) Odd-even mass staggering
- 3) Ground-state band moment of inertia Talk G. Hagen
- 4) Energy of first 2^+ excitation in even-even semi-magic open-shell nuclei
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Ground-state band moment of inertia



Rotational band

$$E^J - E^0 \equiv \frac{\hbar^2 J(J+1)}{2\mathcal{I}(J)}$$



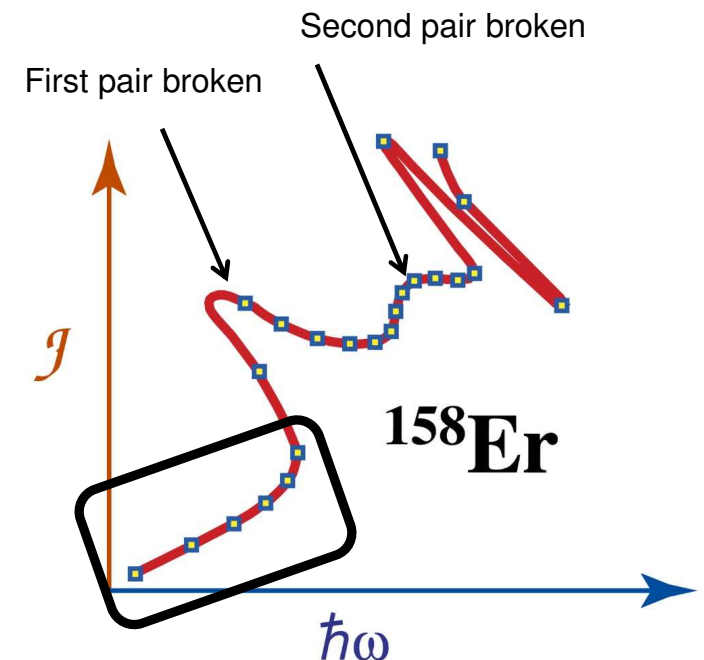
Static moment of inertia $\equiv \mathcal{I}(2)$

About half the rigid-body value
Larger in odd-Z and odd-N

Dynamical moment of inertia versus rotation

$$\mathcal{I}_{\text{dyn}}(J) \equiv \hbar^2 \left[\frac{d^2 E^J}{dJ^2} \right]^{-1}$$

Pairing weakening \leftrightarrow Meissner effect \rightarrow Gradual increase of \mathcal{I}_{dyn}
Sudden pair breaking \rightarrow Backbending of \mathcal{I}_{dyn}

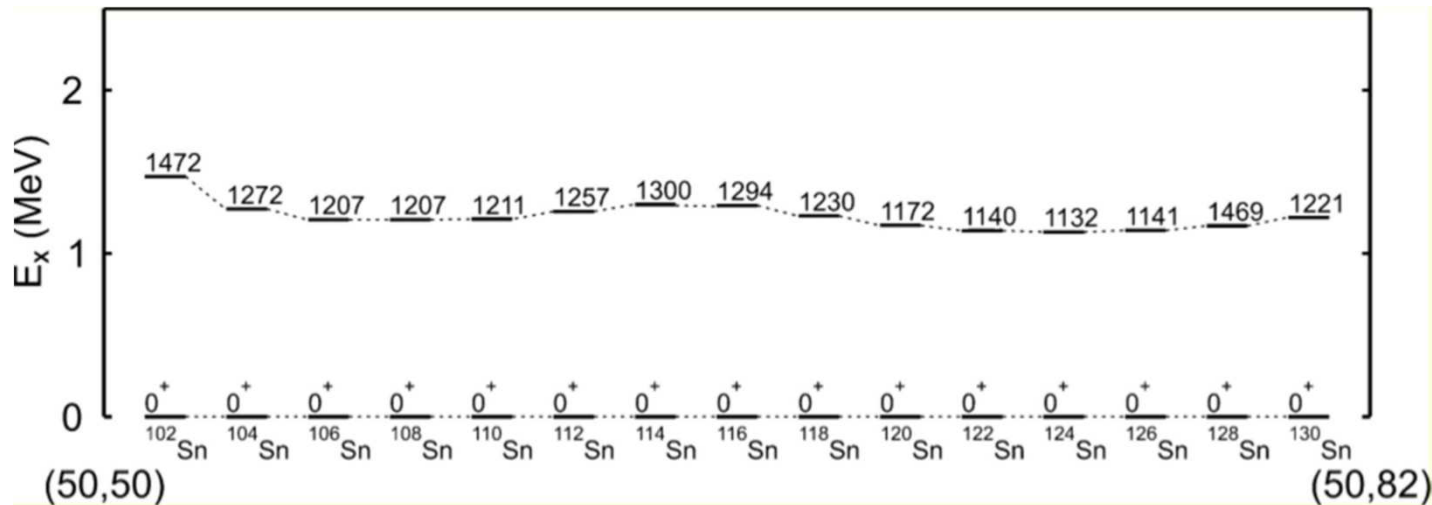


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First 2^+ excitation in even-even semi-magic open-shell nuclei

Lowest 2^+ excitations energy between ^{102}Sn and ^{130}Sn



$J=0$ pair creation operator

$$P_j^\dagger \equiv \sum_{m>0} a_{jm}^\dagger a_{j\bar{m}}^\dagger$$

Pure pairing Hamiltonian

$$H \equiv -GP_j^\dagger P_j$$

$E^{2^+} \sim \text{constant}$ between $N=50$ and $N=82$ shell closures

→ Interpreted (in “0th order”) as seniority excitation: E^{2^+} does not depend on n_{val}

Ground-state $\boxed{\leftrightarrow}$ $J=0$ seniority 0 pair condensate

First excited states $\boxed{\leftrightarrow}$ $J>0$ seniority 2 pair broken states

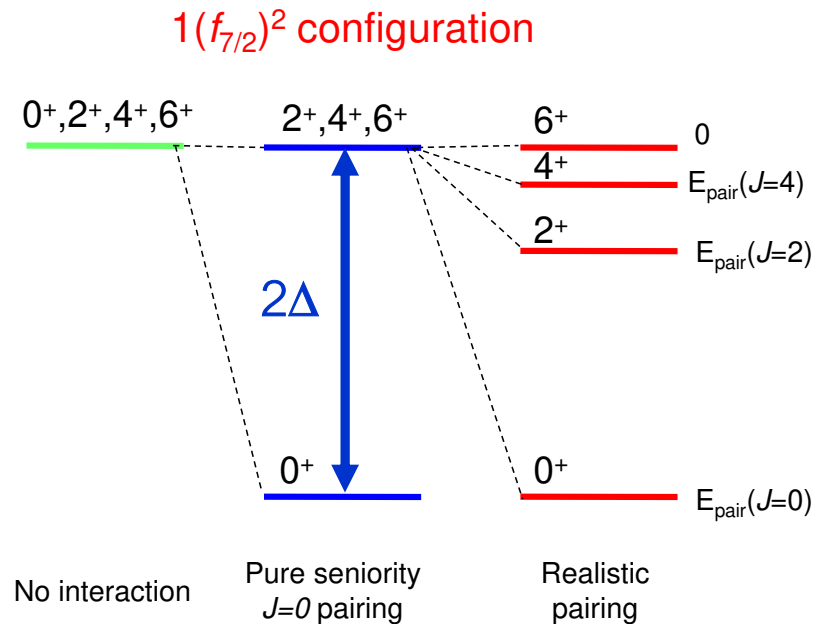
$$|\Phi_{\nu=0}^{JM=00}(n_{\text{val}})\rangle \equiv (P_j^\dagger)^{n_{\text{val}}/2} |\Phi_{\nu=0}^{JM=00}(0)\rangle \quad \Rightarrow \quad |\Phi_{\nu=2}^{JM}(n_{\text{val}})\rangle \equiv (P_j^\dagger)^{(n_{\text{val}}-2)/2} A^\dagger(j^2 JM) |\Phi_{\nu=0}^{JM=00}(n_{\text{val}})\rangle$$

$$\Rightarrow E_{\nu=2}^{JM}(n_{\text{val}}) - E_{\nu=0}^{JM=00}(n_{\text{val}}) = -\frac{G}{2}(2j+1) \quad \left| \begin{array}{l} \text{Independent on } n_{\text{val}} \\ \text{Equal to } 2\Delta \\ \text{Independent on } J \end{array} \right.$$

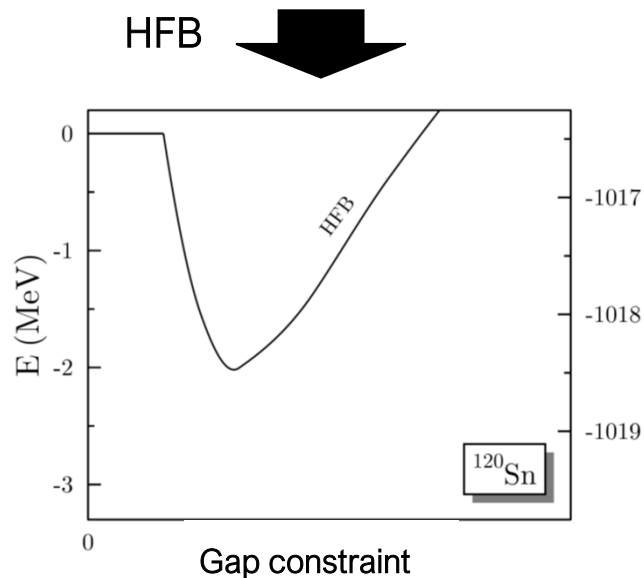
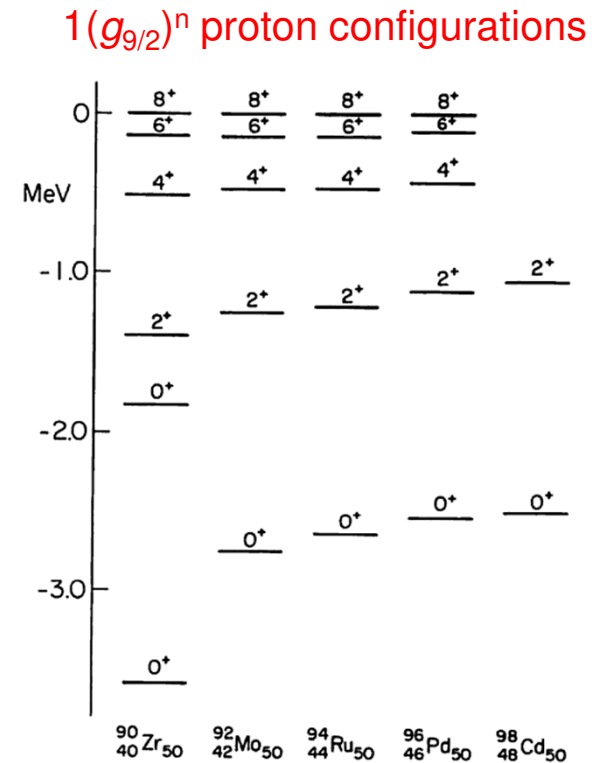
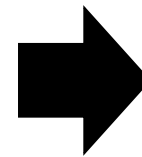
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Correlation energy and anisotropic ($J>0$) pairing



Varying n_{val}



Up to 2-3 MeV when matching experimental gap

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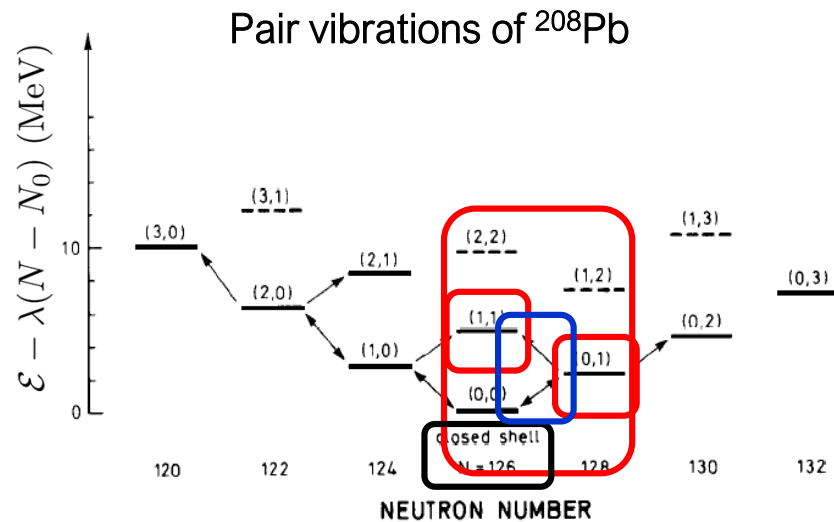
Pairing vibrations and rotations

On top of closed-shell nucleus (e.g. ^{208}Pb)

→ No static deformation of pairing field

Vibrational-like excitation spectrum

Enhanced pair-transfer (t,p)/(p,t) reactions



Mottelson, Nobel Lecture (1975)

First phonon = ground state for $n_{\text{val}}=2$

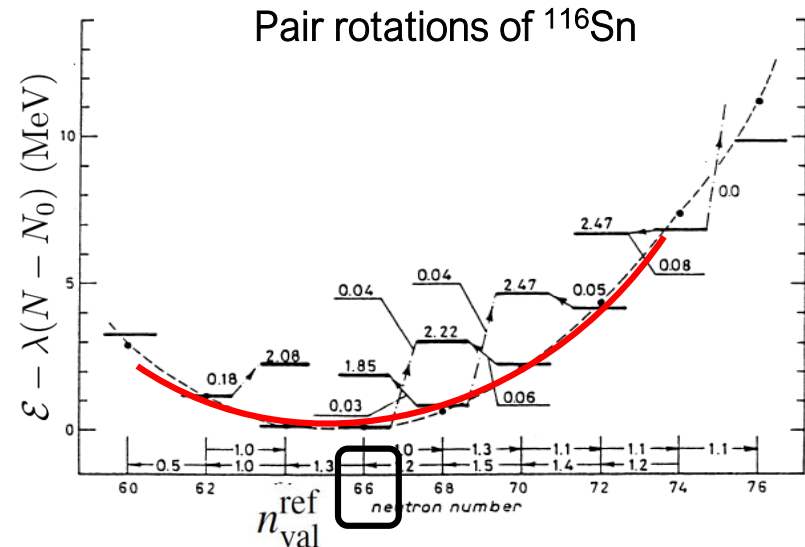
$$|\Phi_{\nu=0}^{JM=00}(2)\rangle \equiv P_j^\dagger |\Phi_{\nu=0}^{JM=00}(0)\rangle$$

Second phonon = 0^+ excited state of closed-shell

On top of well-paired mid-shell nucleus (e.g. ^{116}Sn)

→ Static deformation of the pairing field

Rotational-like spectrum of even ground-states



Broglia, Terasaki, Giovanardi, PR (2000)

Rotational excitations = open-shell ground-states

$$|\Phi_{\nu=0}^{JM=00}(n_{\text{val}})\rangle \equiv e^{cP_j^\dagger} |\Phi_{\nu=0}^{JM=00}(n_{\text{val}}^{\text{ref}})\rangle$$

$$E_{\nu=0}^{JM=00}(n_{\text{val}}) - E_{\nu=0}^{JM=00}(n_{\text{val}}^{\text{ref}}) = \frac{(n_{\text{val}} - n_{\text{val}}^{\text{ref}})^2}{2\mathcal{I}_{\text{pair}}} \quad \text{Pair MOI}$$

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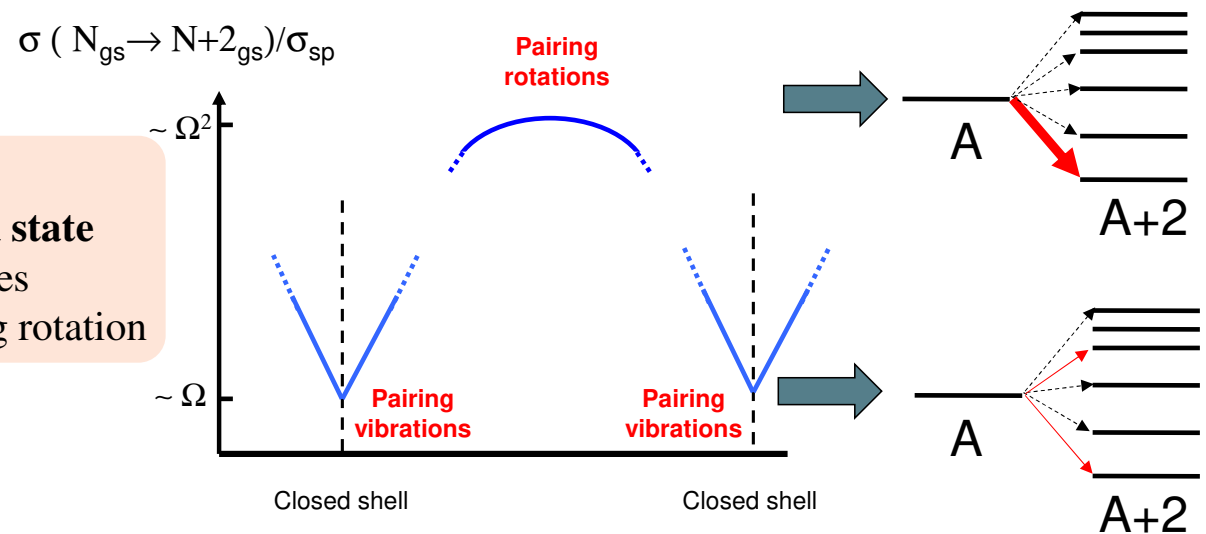
Two-particle transfer reactions

Specific tool to probe pairing correlations

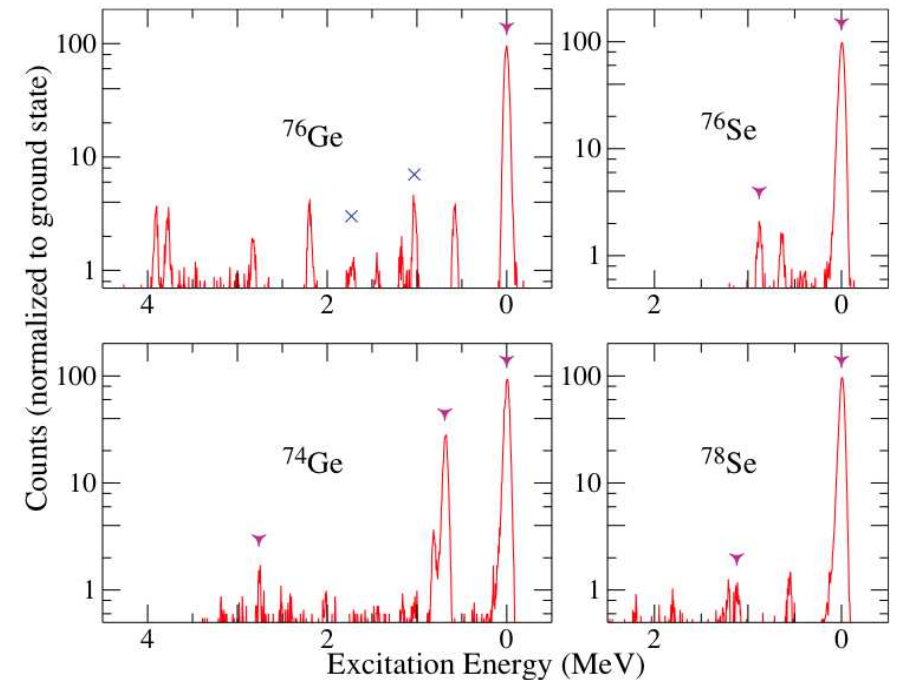
Enhanced two-nucleon transfer for superfluid state

→ Constructive interference of reaction amplitudes

→ Stronger and mostly to ground state for pairing rotation



Modern example from (p,d) reactions



Freeman et al. PRC (2007)

Strength predominantly to ground state in ^{76}Ge and $^{76,78}\text{Se}$

→ Pair rotational states

Less true for ^{74}Ge

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- 9) Giant monopole resonances Talks E. Khan, A. Porro, D. Thisse
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Expansion many-body methods

$$H|\Psi_k^\sigma\rangle = E_k^{\tilde{\sigma}}|\Psi_k^\sigma\rangle \text{ with } \sigma \equiv JM\Pi NZ \equiv \tilde{\sigma}M$$

$$[H, R(\theta)] = 0 \text{ with } G_H \equiv \{R(\theta), \theta \in \mathcal{D}_{G_H}\}$$

$$U(1)_N \times U_Z(1) \times SU(2)_J \times I_\Pi$$

One-body Hilbert space

$$\mathcal{H}(1)$$

$$\dim \mathcal{H}(1) \equiv n_{\text{dim}}$$

One-body basis size

A-body Hilbert space

$$\mathcal{H}_A = \mathcal{H}(1) \otimes \dots \otimes \mathcal{H}(A)$$

$$\dim \mathcal{H}(A) \equiv n_{\text{dim}}^A$$

Curse of dimensionality

Expansion many-body methods to achieve polynomial scaling with n_{dim}

Hamiltonian partitioning

$$H = \boxed{H_0} + H_1$$

« Easy »
to solve

$$\text{Mean-field-like} = O(n_{\text{dim}}^4)$$

Symmetry

Symmetry conserving?
Symmetry breaking (and restoration)?

Unperturbed state

$$H_0|\Theta_k^{(0)}\rangle = E_k^{(0)}\boxed{|\Theta_k^{(0)}\rangle}$$

Nature of the state

Single product state?
Mixing of product states?

Expansion
series

Fully correlated state

$$|\Psi_k^\sigma\rangle = \boxed{\Omega_k}\Theta_k^{(0)}\rangle$$

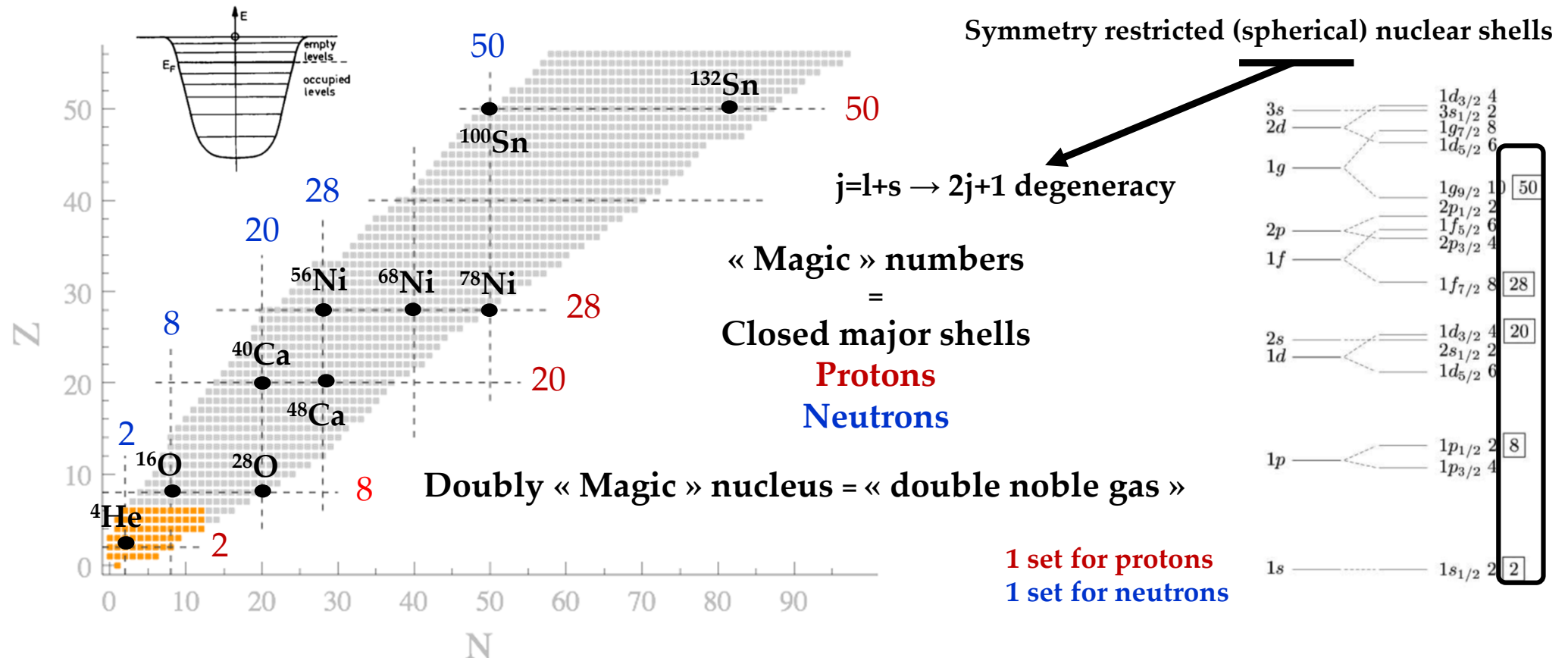
Wave operator

Nature of the expansion

Perturbative?
Non perturbative?

How to consistently capture static and dynamical correlations?
Can we describe nuclear superfluidity at « low » polynomial cost?

Background to set up expansion methods in nuclei



Spherical Slater determinant unperturbed state

Spherical nuclear orbitals: $\alpha = nlm$

Spherical HO 1-body basis

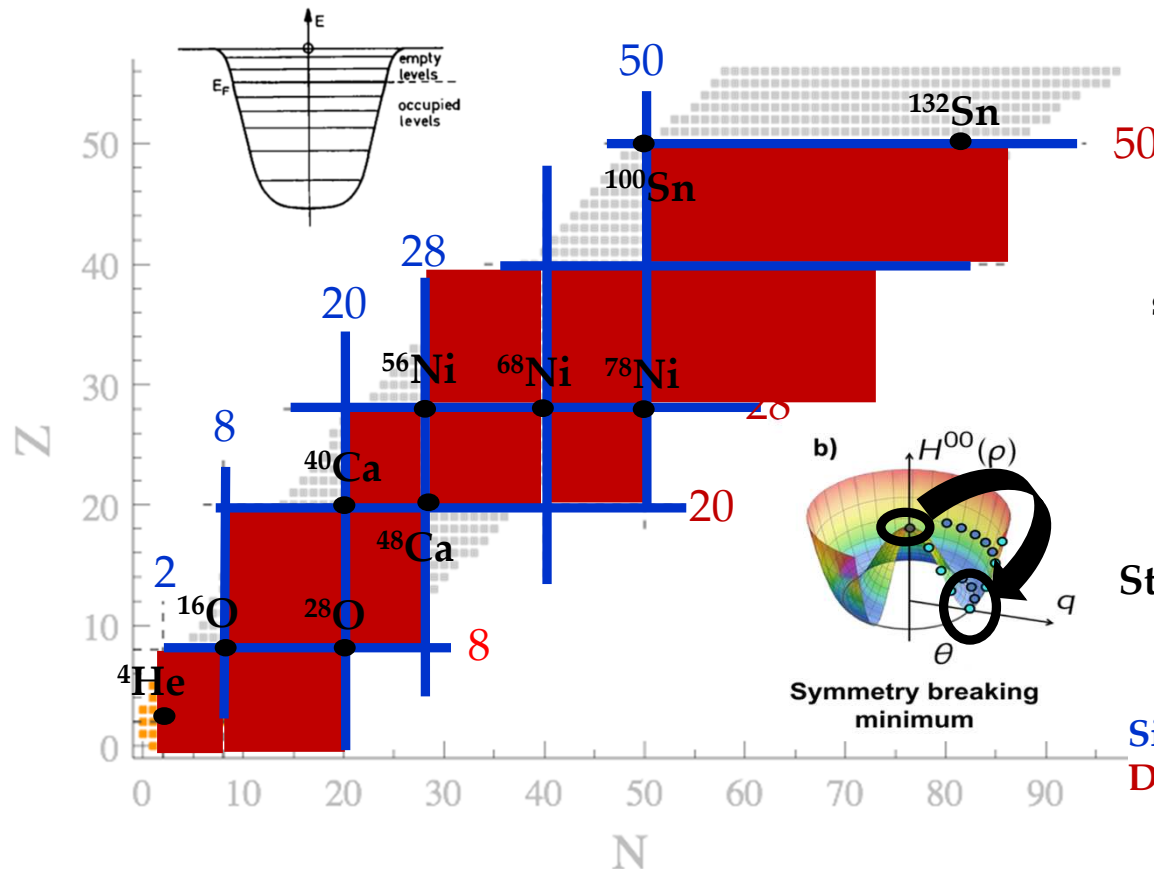
$$|\Theta_0^{(0)}\rangle = \prod_{i=1}^A a_i^\dagger |0\rangle$$

$$\begin{aligned} a_\alpha^\dagger &= \sum_p U_{p\alpha} c_p^\dagger \\ a_\alpha &= \sum_p U_{p\alpha}^* c_p \end{aligned}$$

Variational optimal = Spherical Hartree-Fock

$$\delta \langle \Theta_0^{(0)} | H | \Theta_0^{(0)} \rangle = 0$$

Background to set up expansion methods in nuclei



Singly/doubly open shell

90% of nuclear ground states

sHF state degenerate w/t spherical p-h excitations
Precursor of strong static correlations

Let symmetries break!

Static correlations included and degeneracy lifted
...at mean-field cost!

Singly : break U(1) = def in gauge space = superfluidity
Doubly: + break SU(2) = def in real space = deformation

Spherical Slater determinant unperturbed state

Spherical nuclear orbitals: $\alpha = nlm$

Spherical HO 1-body basis

$$|\Theta_0^{(0)}\rangle = \prod_{i=1}^A a_i^\dagger |0\rangle$$

$$\begin{aligned} \textcircled{a_\alpha^\dagger} &= \sum_p U_{pa} \textcircled{c_p^\dagger} \\ a_\alpha &= \sum_p U_{p\alpha}^* c_p \end{aligned}$$

Variational optimal = Spherical Hartree-Fock

Deformed Bogoliubov unperturbed state

Deformed quasi-particles: $\alpha = n\pi m / n\pi / n$

$$\begin{aligned} |\Theta_0^{(0)}\rangle &= \prod_k \beta_k |0\rangle & \textcircled{\beta_\alpha^\dagger} &= \sum_p U_{p\alpha} \textcircled{c_p^\dagger} + V_{p\alpha} \textcircled{c_p} \\ & & \beta_\alpha &= \sum_p U_{p\alpha}^* c_p + V_{p\alpha}^* c_p^\dagger \end{aligned}$$

= Deformed Hartree-Fock-Bogoliubov

$$\delta \langle \Theta_0^{(0)} | H | \Theta_0^{(0)} \rangle = 0$$

Expansion many-body methods

$$H|\Psi_k^\sigma\rangle = E_k^{\tilde{\sigma}}|\Psi_k^\sigma\rangle \text{ with } \sigma \equiv JM\Pi NZ \equiv \tilde{\sigma}M$$

$$[H, R(\theta)] = 0 \text{ with } G_H \equiv \{R(\theta), \theta \in \mathcal{D}_{G_H}\}$$

One-body Hilbert space

$$\mathcal{H}(1)$$

$$\dim \mathcal{H}(1) \equiv n_{\text{dim}}$$



A-body Hilbert space

$$\mathcal{H}_A = \mathcal{H}(1) \otimes \dots \otimes \mathcal{H}(A)$$

$$\dim \mathcal{H}(A) \equiv n_{\text{dim}}^A$$

Expansion many-body methods to achieve polynomial scaling with n_{dim}

Hamiltonian partitioning

$$H = \boxed{H_0} + H_1$$

« Easy »
to solve

Mean-field-like $= O(n_{\text{dim}}^4)$

Broken symmetries

U(1) and SU(2)

Unperturbed state

$$H_0|\Theta_k^{(0)}\rangle = E_k^{(0)}\boxed{|\Theta_k^{(0)}\rangle}$$

Nature of the state

Deformed HFB state

Expansion
series

Fully correlated state

$$|\Psi_k^\sigma\rangle = \boxed{\Omega_k}\Theta_k^{(0)}\rangle$$

Wave operator

Nature of the expansion

(Non) perturbative

Is pairing phenomenology described by non-polynomial methods, i.e. is there an issue with the Hamiltonian?

Is breaking U(1) doing the expected job to achieve it at « low » polynomial cost?

→ How far from the full answer is the lowest order based on a Bogoliubov unperturbed state?

→ Do needed dynamical correlations beyond lowest order require non-perturbative methods at « high » orders?

If so, does using a multi-reference (i.e. « rich » PGCM) unperturbed state bypasses the problem?

Can we rather describe pairing phenomenology by only breaking SU(2), at least in doubly open-shell nuclei?

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Gorkov self-consistent Green's function: basics

Normal
Anomalous

Somà, Duguet, Barbieri, PRC (2011,2022)

Talk V. Somà

One-body Gorkov Green's functions

$$G_{\alpha\beta}^{11}(t-t') \equiv -i\langle\Psi_0| T[c_\alpha(t)c_\beta^\dagger(t')] |\Psi_0\rangle$$

$$G_{\alpha\beta}^{12}(t-t') \equiv -i\langle\Psi_0| T[c_\alpha(t)\bar{c}_\beta(t')] |\Psi_0\rangle$$

$$G_{\alpha\beta}^{21}(t-t') \equiv -i\langle\Psi_0| T[\bar{c}_\alpha^\dagger(t)c_\beta^\dagger(t')] |\Psi_0\rangle$$

$$G_{\alpha\beta}^{22}(t-t') \equiv -i\langle\Psi_0| T[\bar{c}_\alpha^\dagger(t)\bar{c}_\beta(t')] |\Psi_0\rangle$$

Fourier



$$G_{\alpha\beta}^{g_1 g_2}(\omega) = \int_{-\infty}^{\infty} e^{i\omega\tau} G_{\alpha\beta}^{g_1 g_2}(\tau) d\tau$$

One-body Gorkov irreducible self-energies

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

Decomposition



Dynamical self energy

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

Static self energy

Gorkov's equation: dynamical equation for $\mathbf{G}_{\alpha\beta}(\omega)$

Unperturbed propagator

Irreducible self energy

$$\mathbf{G}_{\alpha\beta}(\omega) = \mathbf{G}_{\alpha\beta}^{(0)}(\omega) + \sum_{\gamma\delta} \mathbf{G}_{\alpha\gamma}^{(0)}(\omega) \Sigma_{\gamma\delta}^{\star}(\omega) \mathbf{G}_{\delta\beta}(\omega)$$

Self-consistent equation

Gorkov self-consistent Green's function: basics

Lehmann representation

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

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

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

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

One-nucleon addition/removal spectroscopic factors & energies

$$S_k^+ \equiv \sum_{\alpha} \mathcal{U}_{\alpha}^k \mathcal{U}_{\alpha}^{k*}$$

$$E_k^+ \equiv E_k^{N+1} - E_0^N = \mu + \omega_k$$

$$S_k^- \equiv \sum_{\alpha} \bar{\mathcal{V}}_{\alpha}^k \bar{\mathcal{V}}_{\alpha}^{k*}$$

$$E_k^- \equiv E_0^N - E_k^{N-1} = \mu - \omega_k$$

Three point mass difference $\Delta^{(3)}(N) \equiv \frac{(-1)^N}{2} [E_0^+ - E_0^-]$

Binding energy from Galitskii-Koltun sum rule

$$E(N) \equiv \sum_{\alpha\beta} \frac{1}{4\pi i} \int_{C\uparrow} d\omega [t_{\alpha\beta} + \omega \delta_{\alpha\beta}] G_{\beta\alpha}^{11}(\omega)$$

$$= \frac{1}{2} \left[\sum_{\alpha\beta} t_{\alpha\beta} \rho_{\beta\alpha} + \sum_k S_k^- E_k^- \right]$$

Rewriting Gorkov's equation as generalized HFB eigenvalue problem

Generalized Hartree-Fock-like potential

Generalized Bogoliubov-like pairing field

Generalized Bogoliubov Matrices

Quasi-particle energies

$$\sum_{\beta} \begin{pmatrix} t_{\alpha\beta} - \mu \delta_{\alpha\beta} + \boxed{\Sigma_{\alpha\beta}^{(\infty)11} + \widetilde{\Sigma}_{\alpha\beta}^{11}(\omega)} \\ \boxed{\Sigma_{\alpha\beta}^{(\infty)21} + \widetilde{\Sigma}_{\alpha\beta}^{21}(\omega)} \end{pmatrix} \begin{pmatrix} \mathcal{U}_{\beta}^k \\ \mathcal{V}_{\beta}^k \end{pmatrix} = \omega_k \begin{pmatrix} \mathcal{U}_{\alpha}^k \\ \mathcal{V}_{\alpha}^k \end{pmatrix}$$

$$\begin{pmatrix} \boxed{\Sigma_{\alpha\beta}^{(\infty)12} + \widetilde{\Sigma}_{\alpha\beta}^{12}(\omega)} \\ -t_{\alpha\beta} + \mu \delta_{\alpha\beta} + \boxed{\Sigma_{\alpha\beta}^{(\infty)22} + \widetilde{\Sigma}_{\alpha\beta}^{22}(\omega)} \end{pmatrix} \begin{pmatrix} \mathcal{U}_{\beta}^k \\ \mathcal{V}_{\beta}^k \end{pmatrix} = \omega_k \begin{pmatrix} \mathcal{U}_{\alpha}^k \\ \mathcal{V}_{\alpha}^k \end{pmatrix}$$

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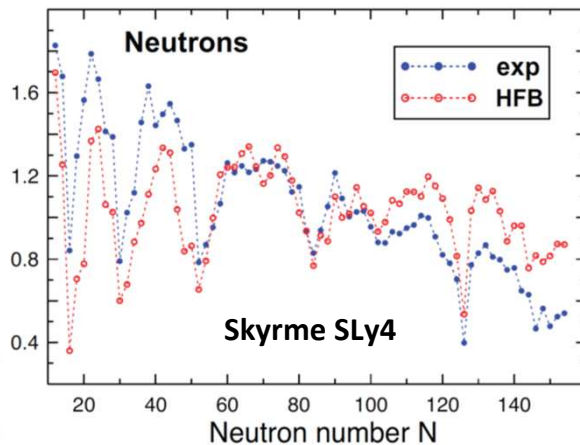
Single-reference energy density functional

Effective mean field from, e.g., Skyrme EDF with $m^* \sim 0.7$

Effective pairing field from, e.g., DDDI with duly fitted strength

$$\sum_{\beta} \begin{pmatrix} t_{\alpha\beta} - \mu\delta_{\alpha\beta} + \Sigma_{\alpha\beta}^{(\infty)11} + \widetilde{\Sigma}_{\alpha\beta}^{11}(\omega) & \Sigma_{\alpha\beta}^{(\infty)12} + \widetilde{\Sigma}_{\alpha\beta}^{12}(\omega) \\ \Sigma_{\alpha\beta}^{(\infty)21} + \widetilde{\Sigma}_{\alpha\beta}^{21}(\omega) & -t_{\alpha\beta} + \mu\delta_{\alpha\beta} + \Sigma_{\alpha\beta}^{(\infty)22} + \widetilde{\Sigma}_{\alpha\beta}^{22}(\omega) \end{pmatrix} \begin{pmatrix} \mathcal{U}_{\beta}^k \\ \mathcal{V}_{\beta}^k \end{pmatrix} = \omega_k \begin{pmatrix} \mathcal{U}_{\alpha}^k \\ \mathcal{V}_{\alpha}^k \end{pmatrix}$$

Systematics of pairing gaps

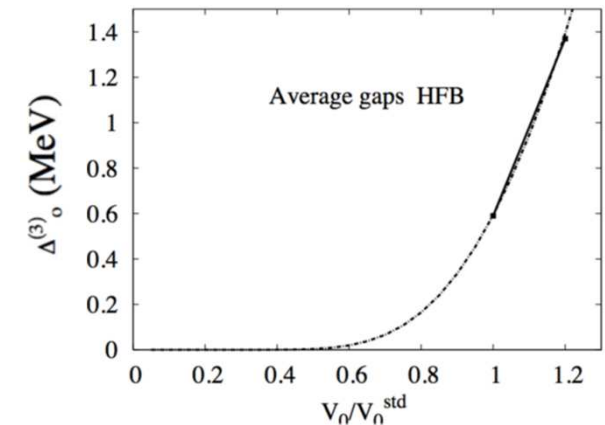


Bertsch *et al.*, PRC (2009)

Theory	pairing	residual neutrons	residual protons
HFB	mixed	0.27	0.33

908 data points for neutrons

864 data points for protons



Good global account of experimental $\Delta^{(3)}$ can be achieved

The trend with A is not exactly right

Rem: 25% of HFB states collapse to HF ones (notably in deformed nuclei)

Exponential dependence on m^* & effective pairing interaction

$$\Delta_{\alpha\beta} = \frac{1}{2} \sum_{\gamma\delta} v_{\alpha\beta\gamma\delta} \kappa_{\gamma\delta} \xrightarrow[g(\varepsilon) \text{ on } [a, b]]{v_{\alpha\beta\gamma\delta} = G} \Delta = \frac{G}{2} \int_a^b d\varepsilon \frac{\Delta g(\varepsilon)}{\sqrt{\varepsilon^2 + \Delta^2}} \xrightarrow[\bar{g}G \ll 1]{g(\varepsilon) \approx \bar{g}} \boxed{\Delta \propto e^{-2/\bar{g}G}}$$

Conclusion: average pairing properties ok at *effective/empirical* HFB level...

...but requires (i) fine tuning (ii) *by hand*

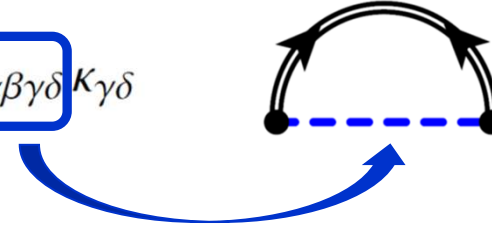
Semi-empirical HFB calculations

Effective mean field from, e.g. Skyrme EDF with $m^* \sim 0.7$

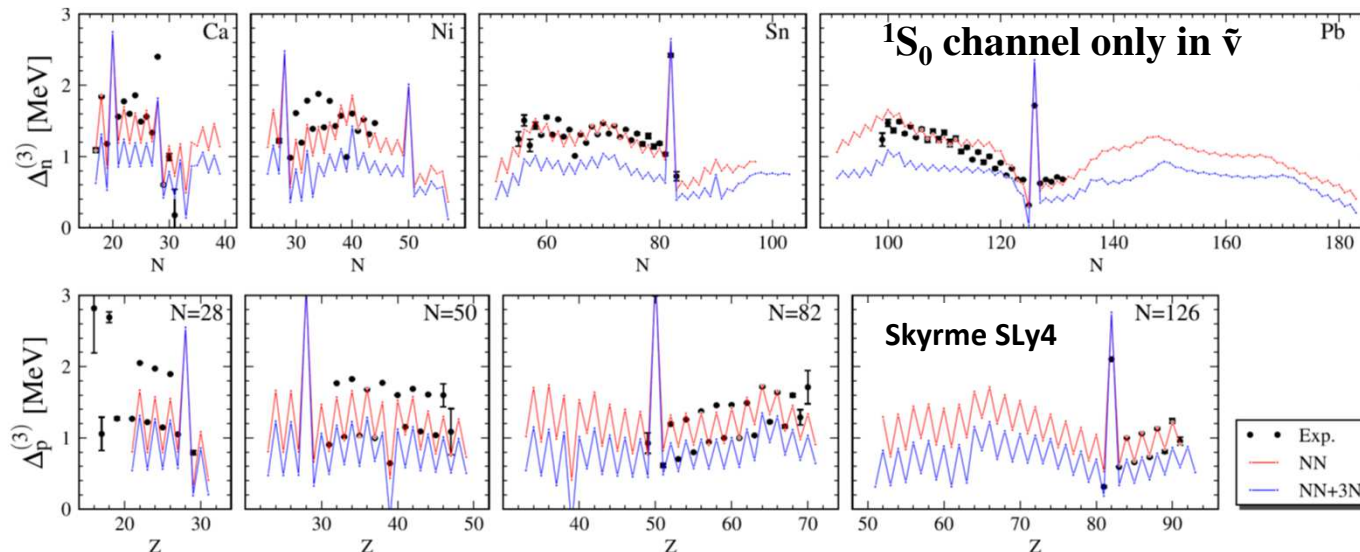
Bogoliubov field from realistic (low-k) 2N+3N interactions

$$\sum_{\beta} \begin{pmatrix} t_{\alpha\beta} - \mu\delta_{\alpha\beta} + \boxed{\Sigma_{\alpha\beta}^{(\infty)11}} + \cancel{\widetilde{\Sigma}_{\alpha\beta}^{11}(\omega)} \\ \Sigma_{\alpha\beta}^{(\infty)21} + \widetilde{\Sigma}_{\alpha\beta}^{21}(\omega) \end{pmatrix} \begin{pmatrix} \mathcal{U}_{\beta}^k \\ \mathcal{V}_{\beta}^k \end{pmatrix} = \omega_k \begin{pmatrix} \mathcal{U}_{\alpha}^k \\ \mathcal{V}_{\alpha}^k \end{pmatrix}$$

Static *semi-effective* HFB problem

$$\xrightarrow{\text{red arrow}} \Sigma_{\alpha\beta}^{(\infty)12} = \frac{1}{2} \sum_{\gamma\delta} v_{\alpha\beta\gamma\delta} K_{\gamma\delta} + \frac{1}{2} \sum_{\gamma\delta\zeta\epsilon} w_{\alpha\beta\gamma\delta\zeta\epsilon} K_{\delta\zeta} \rho_{\epsilon\gamma} \equiv \frac{1}{2} \sum_{\gamma\delta} \boxed{\tilde{v}_{\alpha\beta\gamma\delta}} K_{\gamma\delta}$$


Pairing gaps in semi-magic spherical nuclei



$\Delta^{(3)}$ from $\tilde{v} = v^{2N}(1S_0)$ nearly perfect
 → Anti-pairing from Coulomb (-40%)
Gaps with $\tilde{v} = v^{2N+3N}(1S_0)$ 30% too low
Oscillations of $\Delta^{(3)}$ (curvature of $E_c(N)$)
 → Match data = tailored mean-field
 → Larger amplitude for protons (Coulomb)


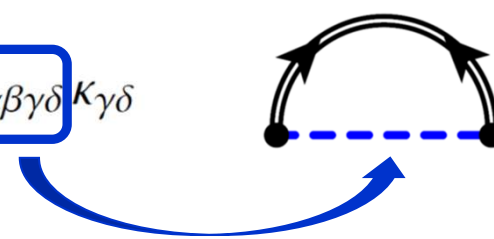
Semi-empirical HFB calculations

Effective mean field from, e.g. Skyrme EDF with $m^* \sim 0.7$

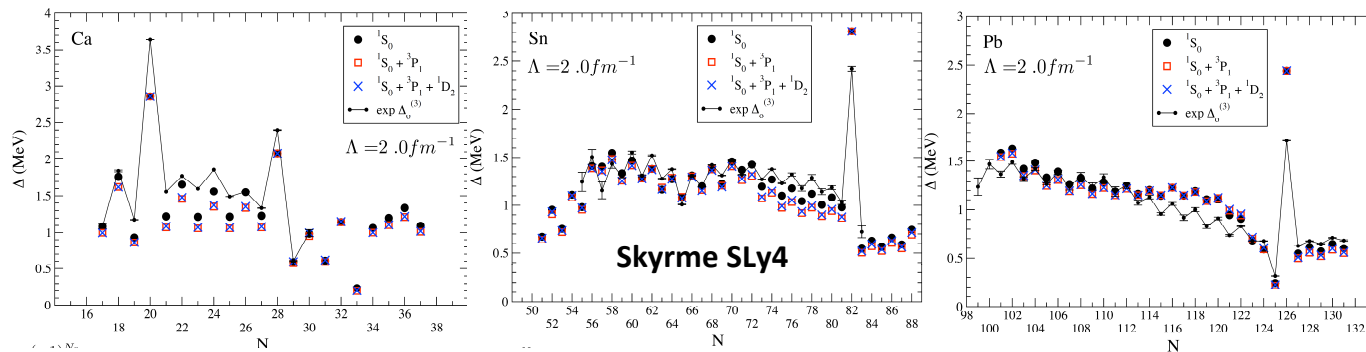
Bogoliubov pairing field from chiral (SRG-evolved) 2N+3N

$$\sum_{\beta} \begin{pmatrix} t_{\alpha\beta} - \mu\delta_{\alpha\beta} + \boxed{\Sigma_{\alpha\beta}^{(\infty)11}} + \cancel{\widetilde{\Sigma}_{\alpha\beta}^{11}(\omega)} \\ \Sigma_{\alpha\beta}^{(\infty)21} + \widetilde{\Sigma}_{\alpha\beta}^{21}(\omega) \end{pmatrix} \begin{pmatrix} \mathcal{U}_{\beta}^k \\ \mathcal{V}_{\beta}^k \end{pmatrix} = \omega_k \begin{pmatrix} \mathcal{U}_{\alpha}^k \\ \mathcal{V}_{\alpha}^k \end{pmatrix}$$

$$\begin{pmatrix} \boxed{\Sigma_{\alpha\beta}^{(\infty)12}} + \cancel{\widetilde{\Sigma}_{\alpha\beta}^{12}(\omega)} \\ -t_{\alpha\beta} + \mu\delta_{\alpha\beta} + \Sigma_{\alpha\beta}^{(\infty)22} + \widetilde{\Sigma}_{\alpha\beta}^{22}(\omega) \end{pmatrix} \begin{pmatrix} \mathcal{U}_{\beta}^k \\ \mathcal{V}_{\beta}^k \end{pmatrix} = \omega_k \begin{pmatrix} \mathcal{U}_{\alpha}^k \\ \mathcal{V}_{\alpha}^k \end{pmatrix}$$


 $\Sigma_{\alpha\beta}^{(\infty)12} = \frac{1}{2} \sum_{\gamma\delta} v_{\alpha\beta\gamma\delta} K_{\gamma\delta} + \frac{1}{2} \sum_{\gamma\delta\zeta\epsilon} w_{\alpha\beta\gamma\delta\zeta\epsilon} K_{\delta\zeta} \rho_{\epsilon\gamma} \equiv \frac{1}{2} \sum_{\gamma\delta} \boxed{\tilde{v}_{\alpha\beta\gamma\delta}} K_{\gamma\delta}$


Effect from partial waves beyond 1S_0



Anti-pairing from 3P_1 partial wave
 \rightarrow -10% in Ca but negligible in Sn
 No effect from higher partial waves

Baroni, Macchiavelli, Schwenk, PRC (2010)

Lesson: behavior of $\Delta^{(3)}$ from HFB with (i) $\tilde{v} = v^{2N+3N}$ and (ii) tailored mean-field ok but too low by about 30-40%

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Ab initio GSCGF calculations

Consistent static and dynamic self energies from from chiral (SRG-evolved) 2N+3N

Talk V. Somà

$$\sum_{\beta} \begin{pmatrix} t_{\alpha\beta} - \mu\delta_{\alpha\beta} + \boxed{\Sigma_{\alpha\beta}^{(\infty)11} + \widetilde{\Sigma}_{\alpha\beta}^{11}(\omega)} & \boxed{\Sigma_{\alpha\beta}^{(\infty)12} + \widetilde{\Sigma}_{\alpha\beta}^{12}(\omega)} \\ \Sigma_{\alpha\beta}^{(\infty)21} + \widetilde{\Sigma}_{\alpha\beta}^{21}(\omega) & -t_{\alpha\beta} + \mu\delta_{\alpha\beta} + \Sigma_{\alpha\beta}^{(\infty)22} + \widetilde{\Sigma}_{\alpha\beta}^{22}(\omega) \end{pmatrix} \begin{pmatrix} \mathcal{U}_{\beta}^k \\ \mathcal{V}_{\beta}^k \end{pmatrix} = \omega_k \begin{pmatrix} \mathcal{U}_{\alpha}^k \\ \mathcal{V}_{\alpha}^k \end{pmatrix}$$

First order

$$\Sigma_{\alpha\beta}^{(\infty)11} = \text{diagram: incoming dashed line, loop, outgoing dashed line}$$

$$\Sigma_{\alpha\beta}^{(\infty)12} = \text{diagram: incoming dashed line, loop, outgoing solid line}$$

Second order

$$\Sigma_{\alpha\beta}^{11(2)}(\omega) = \text{diagram: incoming dashed line, loop, loop, outgoing dashed line}$$

$$\Sigma_{\alpha\beta}^{12(2)}(\omega) = \text{diagram: incoming dashed line, loop, loop, outgoing solid line}$$

Changing one external line orientation

Third order

$$\Sigma_{\alpha\beta}^{11(3)}(\omega) = \text{diagram: incoming dashed line, loop, loop, loop, outgoing dashed line}$$

+ 4 with hh intermediate states
+ 9 with ph intermediate states

$$\Sigma_{\alpha\beta}^{12(3)}(\omega) = \text{17 diagrams obtained by permuting direction of line as illustrated above}$$

Numerical applications

Hamiltonian



Empirically optimal for ground-state energies [Stroberg et al., PRL \(2021\)](#)

- Chiral-based Hamiltonian EM 1.8/2.0 [Hebeler et al., PRC \(2011\)](#)
- Three-nucleon interaction rank-reduced to effective two-body interaction [Frosini et al., EPJA \(2021\)](#)

Systems

- Ca (Z=20) **singly open-shell** isotopes

Model-space parameters

- Spherical harmonic oscillator basis ($\hbar\omega = 12$)
- $e_{\max} \equiv \max(2n + 1) = 12$ and $e_{3\max} = 16-24$

Low-order polynomial many-body methods

- sBMBPT(2) [Tichai et al., PLB \(2018\)](#)
- sGSCGF(2) [Somà et al., PRC \(2013\)](#)
- sBCCSD[T] [Tichai et al., PLB \(2024\)](#)
- dBMBPT(2) [Frosini et al., EPJA \(2021\)](#)
- dDSCGF[2] [Scalesi et al., unpublished](#)

Non-polynomial many-body method

- VS-IMSRG(2) [Stroberg et al., PRL \(2021\)](#)

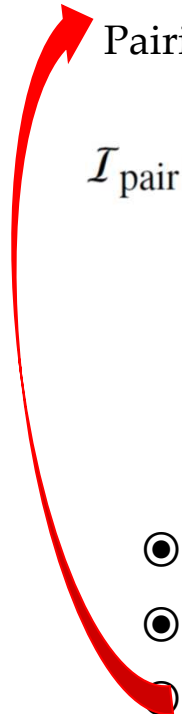
Standard gap at closed shells

Pairing rotation momentum of inertia in open shell

$$\mathcal{I}_{\text{pair}}(N) \equiv \left[\frac{E(N-2, Z) - 2E(N, Z) + E(N+2, Z)}{4} \right]^{-1} \\ = 4/\Delta_{2n}(N, Z)$$

Observables

- Absolute binding energy $E(N, Z)$
- Two-neutron separation energy $S_{2n}(N, Z)$
- Two-neutron shell gap $\Delta_{2n}(N, Z)$
- Neutron three-point mass difference $\Delta_n^{(3)}(N, Z)$

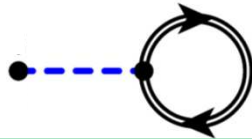


Ab initio GSCGF calculations

$$\sum_{\beta} \begin{pmatrix} t_{\alpha\beta} - \mu\delta_{\alpha\beta} + \Sigma_{\alpha\beta}^{(\infty)11} + \widetilde{\Sigma}_{\alpha\beta}^{11}(\omega) & \Sigma_{\alpha\beta}^{(\infty)12} + \widetilde{\Sigma}_{\alpha\beta}^{12}(\omega) \\ \Sigma_{\alpha\beta}^{(\infty)21} + \widetilde{\Sigma}_{\alpha\beta}^{21}(\omega) & -t_{\alpha\beta} + \mu\delta_{\alpha\beta} + \Sigma_{\alpha\beta}^{(\infty)22} + \widetilde{\Sigma}_{\alpha\beta}^{22}(\omega) \end{pmatrix} \begin{pmatrix} \mathcal{U}_{\beta}^k \\ \mathcal{V}_{\beta}^k \end{pmatrix} = \omega_k \begin{pmatrix} \mathcal{U}_{\alpha}^k \\ \mathcal{V}_{\alpha}^k \end{pmatrix}$$

First order

$$\Sigma_{\alpha\beta}^{(\infty)11} =$$



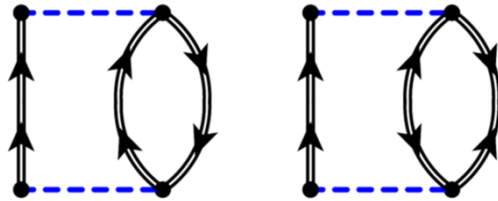
$$\Sigma_{\alpha\beta}^{(\infty)12} =$$



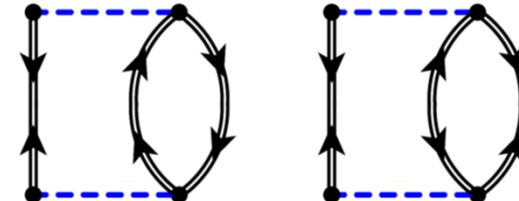
Static HFB equation
 → Ab initio mean-field
Consistent potentials
 → Density of states « m^* »
 → Pairing interaction « \tilde{v} »

Second order

$$\Sigma_{\alpha\beta}^{11(2)}(\omega) =$$

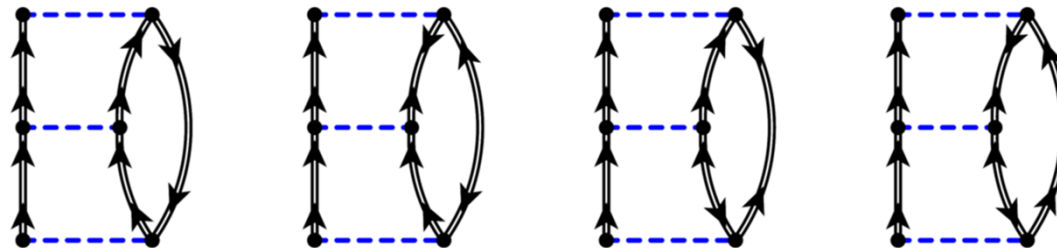


$$\Sigma_{\alpha\beta}^{12(2)}(\omega) =$$



Third order

$$\Sigma_{\alpha\beta}^{11(3)}(\omega) =$$

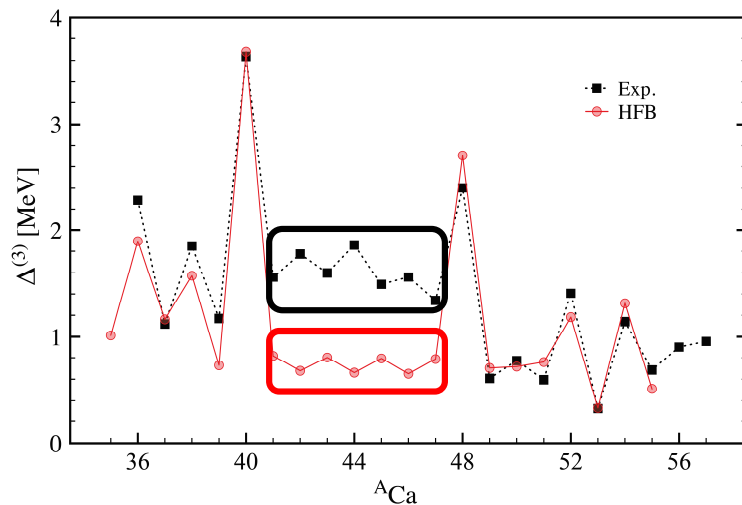


+ 4 with hh intermediate states
 + 9 with ph intermediate states

$$\Sigma_{\alpha\beta}^{12(3)}(\omega) =$$

17 diagrams obtained by permuting direction of line as illustrated above

Ab initio sHFB calculations in Ca isotopes



Only 45% of experimental $\Delta^{(3)}$ in $f_{7/2}$ shell

→ Consistent with semi empirical HFB with Skyrme mean-field...
...but even slightly lower (exponential sensitivity to “ m^* ”)

→ Even smaller % in Sn isotopes *Talk by P. Demol*

Despite $a^{1S_0} = -18.5$ fm and large BCS gap in INM

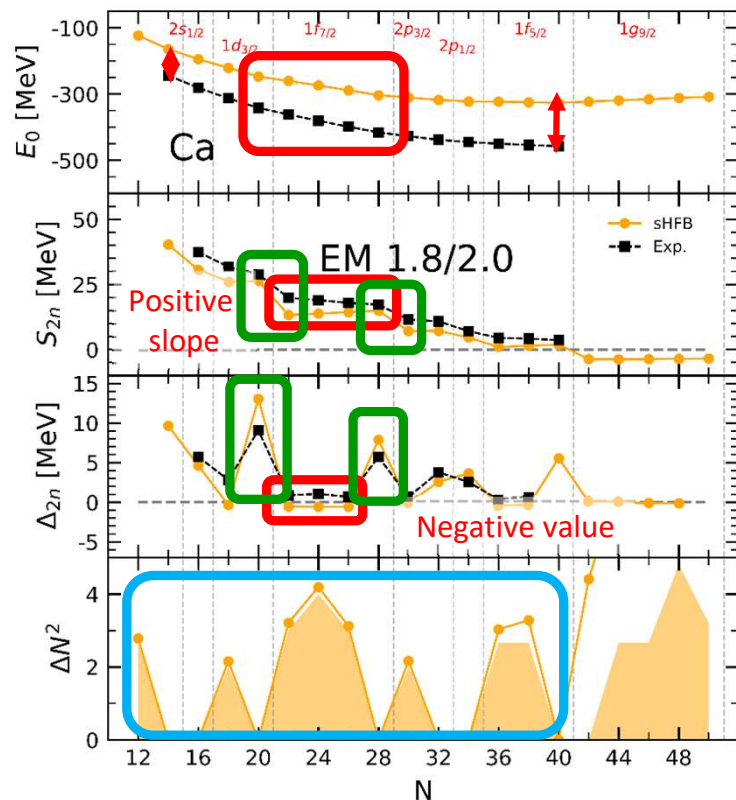
→ Too low density of states from the ab initio HF field?

→ Anti-pairing from spin-orbit in finite nuclei *Bertsch, Baroni, PRC (2009)*

Similar results for other χ -EFT (based) interactions

→ See *Talk by A. Ekström* for proper sensitivity analysis

Oscillation inverted... wrong curvature of the energy!



Scalese et al., EPJA (2024)

sHFB unbound by [80,130] MeV (account for ~70% of BE)

- Expected due to missing dynamical correlations
- Would be more pronounced with a “harder” Hamiltonian
- Deficit increases with neutron excess

sHFB $E(N,Z)$ wrongly concave throughout open-shells

- Pairing rotational moment of inertia $\mathcal{I}_{\text{pair}}$ has wrong sign!
- Systematic with (soften) χ EFT Hamiltonians

sHFB $S_{2n}(N,Z)$

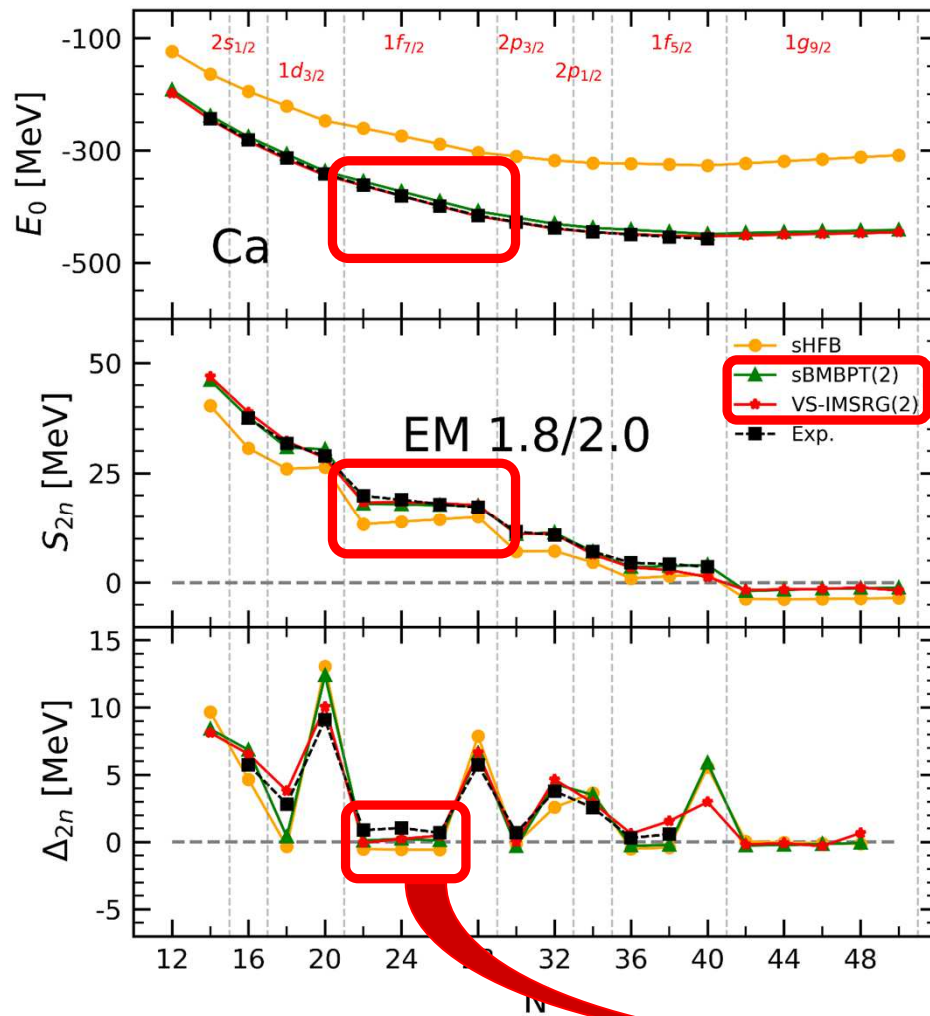
- Too low at the beginning of the shells
- Exaggerated jumps/magicity at $N=20,28$ (too low m^*)

Close to zero-pairing limit of sHFB *Duguet, Bally, Tichai, PRC (2020)*

- Variance close to formal zero-pairing limit
- Pairing typically zero in doubly open-shell mid-mass nuclei

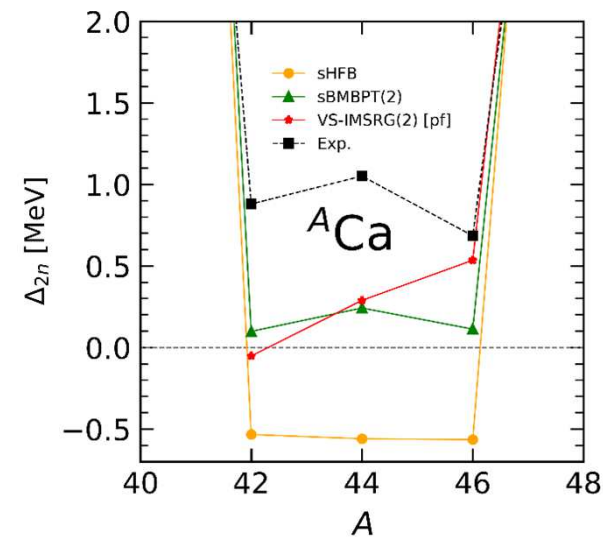
Effect of dynamical correlations in Ca isotopes

Scalesi *et al.*, EPJA (2024)



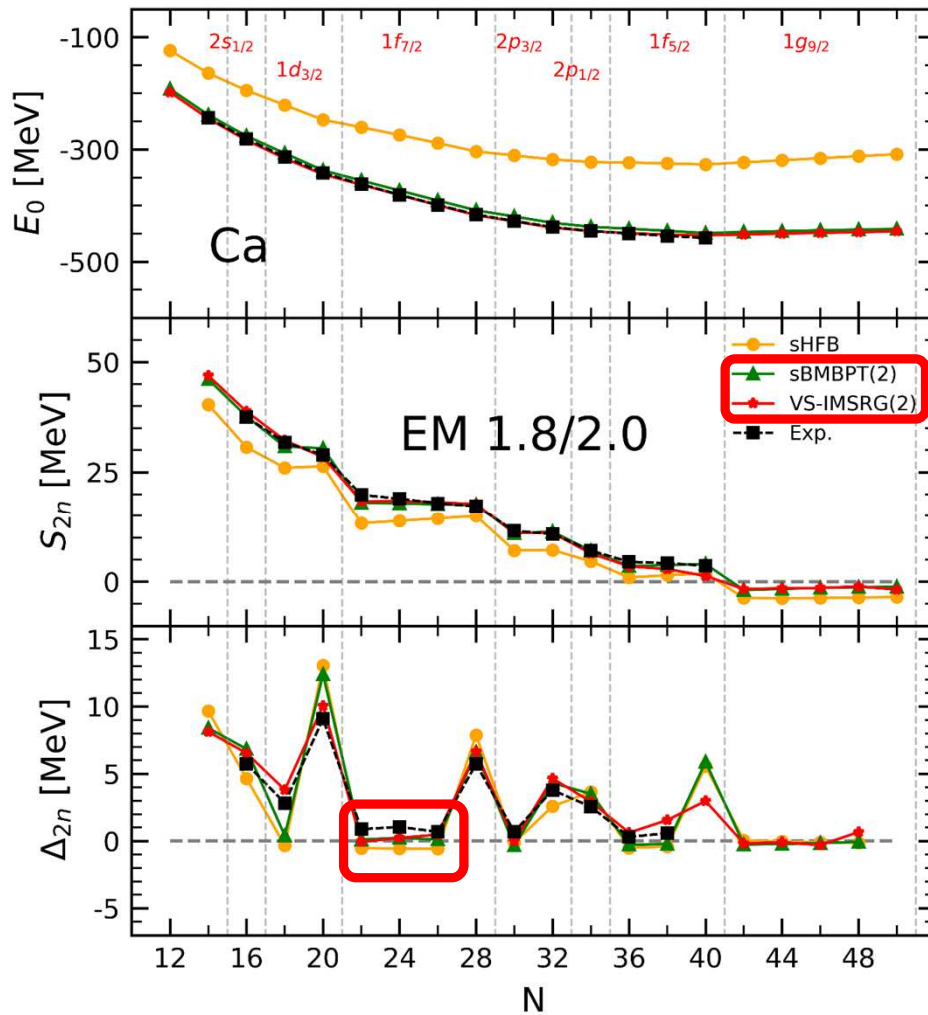
sBMBPT(2) adds [80,130] MeV correlation energy
 → Compensates deficit with neutron excess (a_{sym})
 → rms error to sVS-IMSRG(2) (exp) = 6.9 (7.3) MeV

sBMBPT(2) $E(N,Z)$ correctly convex in open-shells
 → Curvature has correct sign but too small
 → Similar for sVS-IMSRG(2) with ^{40}Ca core



Effect of dynamical correlations in Ca isotopes

Scalesi *et al.*, EPJA (2024)



sBMBPT(2) adds [80,130] MeV correlation energy
 → Compensates deficit with neutron excess (a_{sym})
 → rms error to sVS-IMSRG(2) (exp) = 6.9 (7.3) MeV

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 → Curvature has correct sign but too small
 → Similar for sVS-IMSRG(2) with ^{40}Ca core

Understanding the curvature of $E(N,Z)$

Open shell	$\beta_{\tilde{v}}$ (MeV)
$1f_{7/2}$	-0.290
$1g_{9/2}$	-0.270

Concave

sHFB (EFA)

$$\beta_{\tilde{v}} = \frac{1}{d_v} \sum_{m_v, m_{v'}} \bar{v}_{vv'vv'} + \bar{v}_{vv'hvv'h} < 0$$

Monopole valence-shell 2-body matrix element

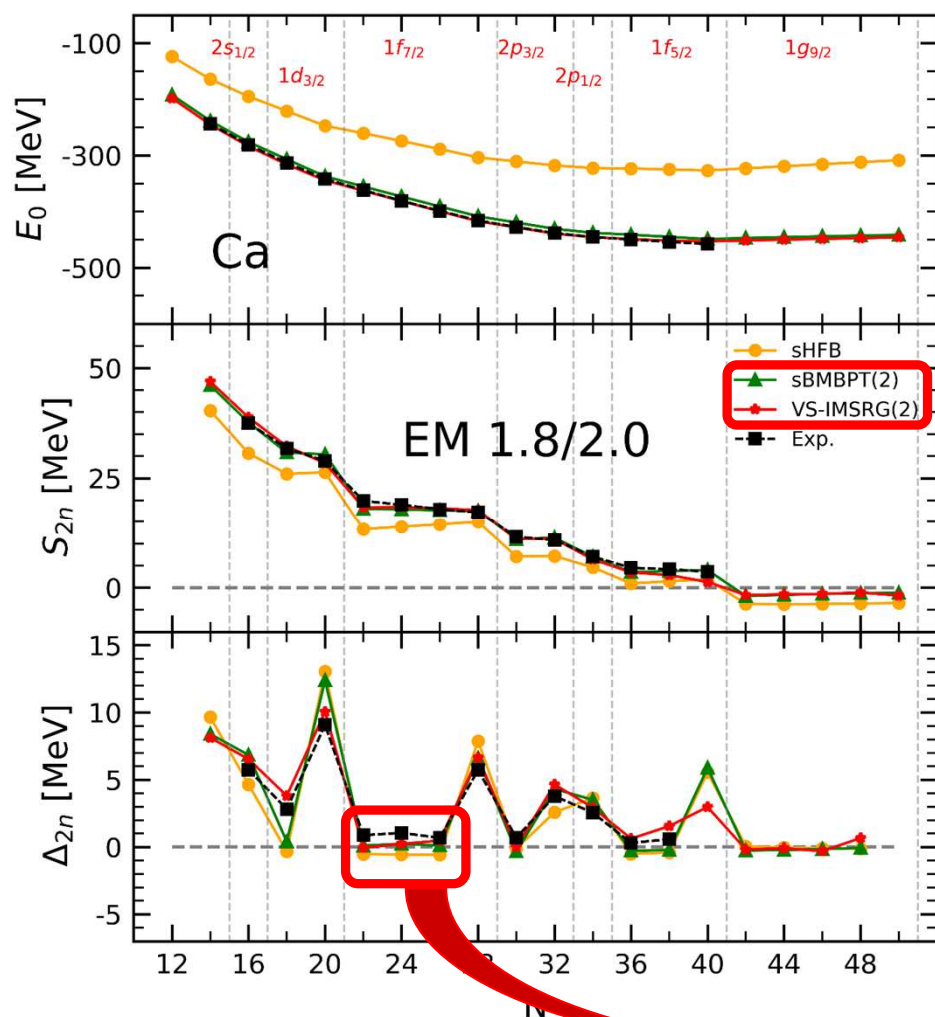
sBMBPT(2) (EFA)

$$\beta_{\tilde{v}}^{(2)} \equiv \frac{1}{d_v} \sum_{m_v, m_{v'}} h \bar{v}_{vv'hh'} + p \bar{v}_{pp'vv'} > 0$$

2nd order effective valence-shell monopole 2-body matrix element due to 2p and 2h excitations

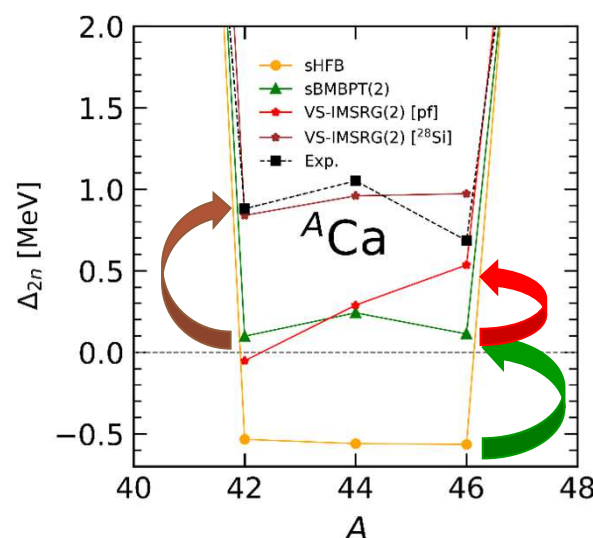
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Diago via sVS-IMSRG(2) only better at ^{46}Ca

Miyagi, Priv. Comm.

- sVS-IMSRG(2) with ^{28}Si core gets it right
 → Collective fluctuations of ^{40}Ca core key
- Infamous charge radius problem not solved
 → At variance with Caurier *et al.*, PLB (2001)

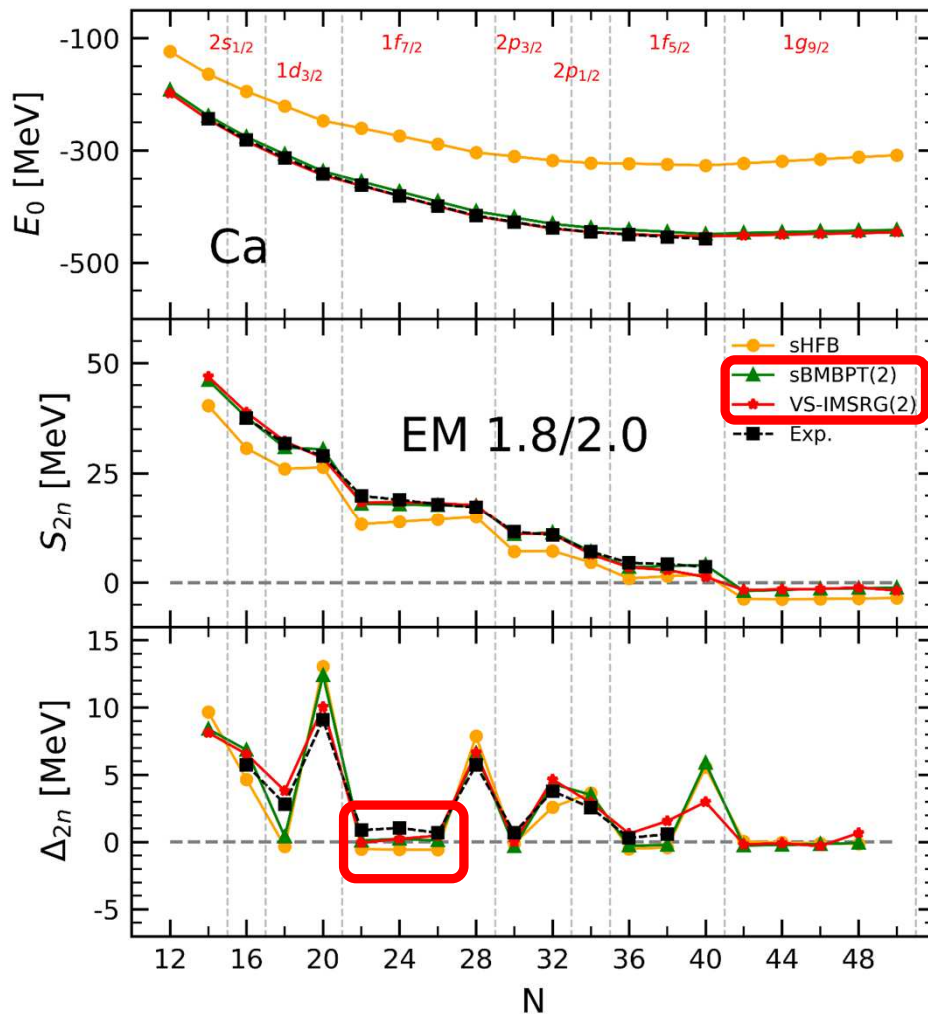
Curvature improved by low-order dynamical correlations

Collective fluctuations are needed to be quantitative

► At least third order in non-perturbative expansion methods...

Effect of dynamical correlations in Ca isotopes

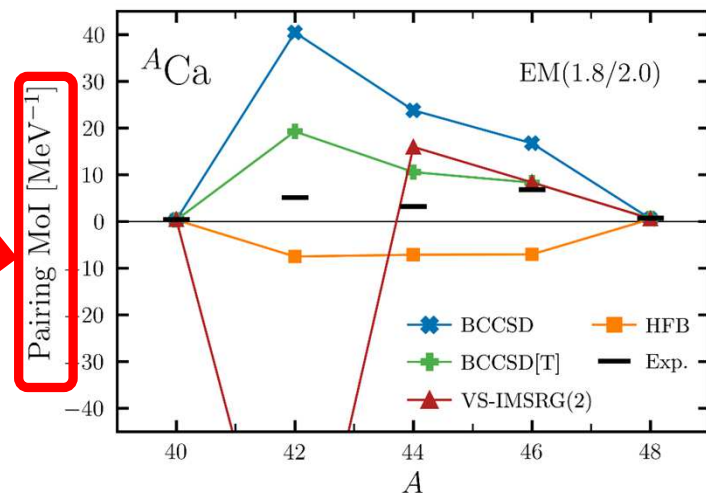
Scalesi *et al.*, EPJA (2024)



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Demol *et al.*, unpublished (2025)



Pair MOI ($4/\Delta_{2n}$) via sBCCSD[T]

→ Significantly improves over sBCCSD (sBMBPT(2))
 → Better than VS-IMSRG(2)[^{40}Ca] throughout $f_{7/2}$ shell
 → Not quite as good as VS-IMSRG(2)[^{28}Si] (not shown)

Insentive to access $\Delta^{(3)}$ via EOM-BCCSD[T]...

... under development Aytekin *et al.*, unpublished (2025)

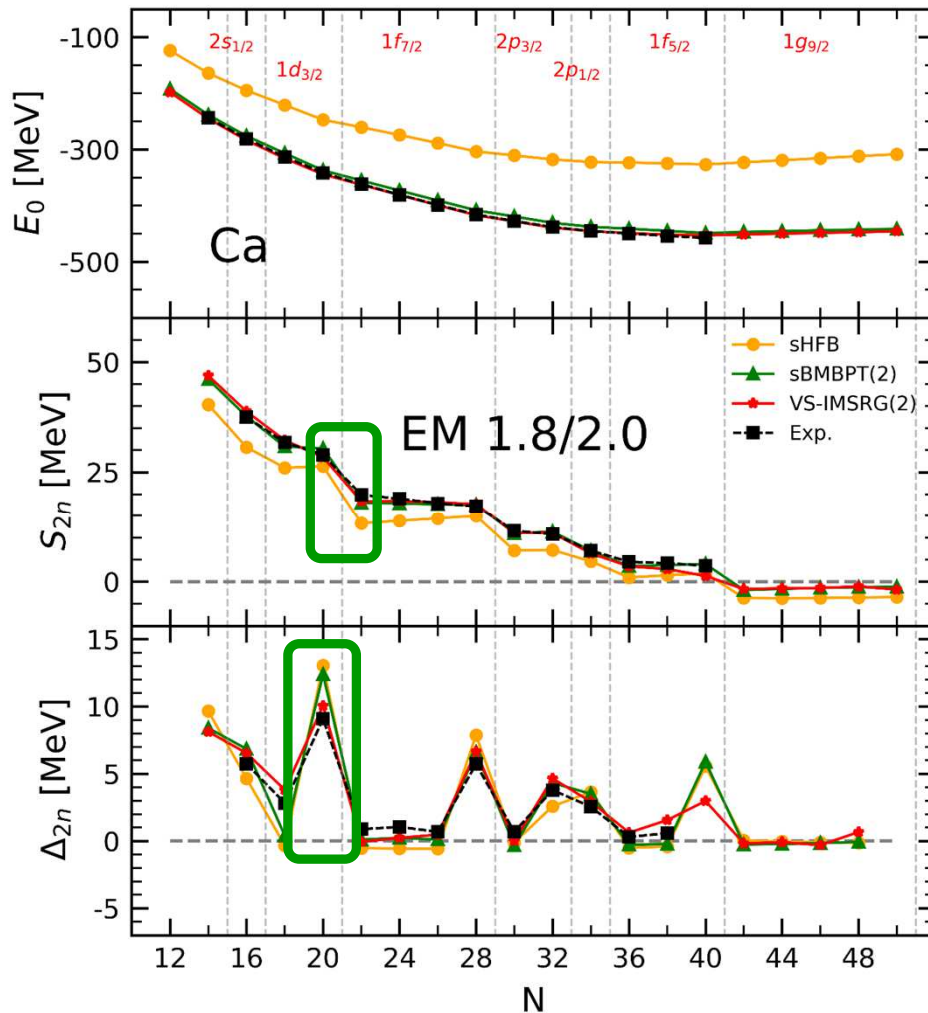
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Effect of dynamical correlations in Ca isotopes

Scalesi *et al.*, EPJA (2024)



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sBMBPT(2) $S_{2n}(N,Z)$
 → Increases at the beginning of the open shells
 → Exaggerated jump/magicity at $N=20$ remains (too low m^*)

Understand S_{2n} at starting open shell $S_{2n}^{(2)} = -2\epsilon_v^{\text{CS}(2)}$

HF-EFA

Mean-field valence shell single-particle energy

$$\epsilon_v^{\text{CS}} \equiv t_{vv} + \text{diagram 1} + \text{diagram 2} \quad \text{[Too small]}$$

Diagram 1: A vertex v connected to a vertex h via a dashed line labeled \bar{v}_{vvh} , with a loop on h .
 Diagram 2: A vertex v connected to a vertex h via a dashed line labeled $\bar{w}_{vhh'vhh'}$, with a loop on h and a vertex h' connected to h .

2nd order self-energy correction due to 2h-1p and 1h-2p excitations

MBPT(2)-EFA

$$\Sigma_v^{(2)}(\epsilon_v^{\text{CS}}) = \text{diagram 3} + \text{diagram 4} < 0$$

Diagram 3: A vertex v connected to a vertex h via a dashed line labeled $\bar{v}_{vphh'}$, with a loop on h and a vertex h' connected to h .
 Diagram 4: A vertex v connected to a vertex h via a dashed line labeled $\bar{v}_{pp'vh}$, with a loop on h and a vertex p' connected to h .
 Additional labels: $\bar{v}_{hh'vp}$ and $\bar{v}_{vhpp'}$ are shown near the vertices.

Starting S_{2n} ok with low-order dynamical correlations
 Not sufficient for Δ_{2n} at $N=20$ (" m^* " not sufficiently increased)
 What about superfluidity?

$$\Sigma_{f7/2}^{(2)} = -5 \text{ MeV}$$

Ab initio GSCGF calculations

$$\sum_{\beta} \begin{pmatrix} t_{\alpha\beta} - \mu\delta_{\alpha\beta} + \Sigma_{\alpha\beta}^{(\infty)11} + \widetilde{\Sigma}_{\alpha\beta}^{11}(\omega) & \Sigma_{\alpha\beta}^{(\infty)12} + \widetilde{\Sigma}_{\alpha\beta}^{12}(\omega) \\ \Sigma_{\alpha\beta}^{(\infty)21} + \widetilde{\Sigma}_{\alpha\beta}^{21}(\omega) & -t_{\alpha\beta} + \mu\delta_{\alpha\beta} + \Sigma_{\alpha\beta}^{(\infty)22} + \widetilde{\Sigma}_{\alpha\beta}^{22}(\omega) \end{pmatrix} \begin{pmatrix} \mathcal{U}_{\beta}^k \\ \mathcal{V}_{\beta}^k \end{pmatrix} = \omega_k \begin{pmatrix} \mathcal{U}_{\alpha}^k \\ \mathcal{V}_{\alpha}^k \end{pmatrix}$$

First order

$$\Sigma_{\alpha\beta}^{(\infty)11} = \text{diagram: a dashed line from left to a loop on the right}$$

$$\Sigma_{\alpha\beta}^{(\infty)12} = \text{diagram: a dashed line from left to a bubble on the right}$$

ω -dependent self-energies
 → Impact « m^* » as just seen
 → Also fragment qp strength
 → Correct « \tilde{v} » as well... how?

Second order

$$\Sigma_{\alpha\beta}^{11(2)}(\omega) = \text{diagram 1} + \text{diagram 2}$$

$$\Sigma_{\alpha\beta}^{12(2)}(\omega) = \text{diagram 1} + \text{diagram 2}$$

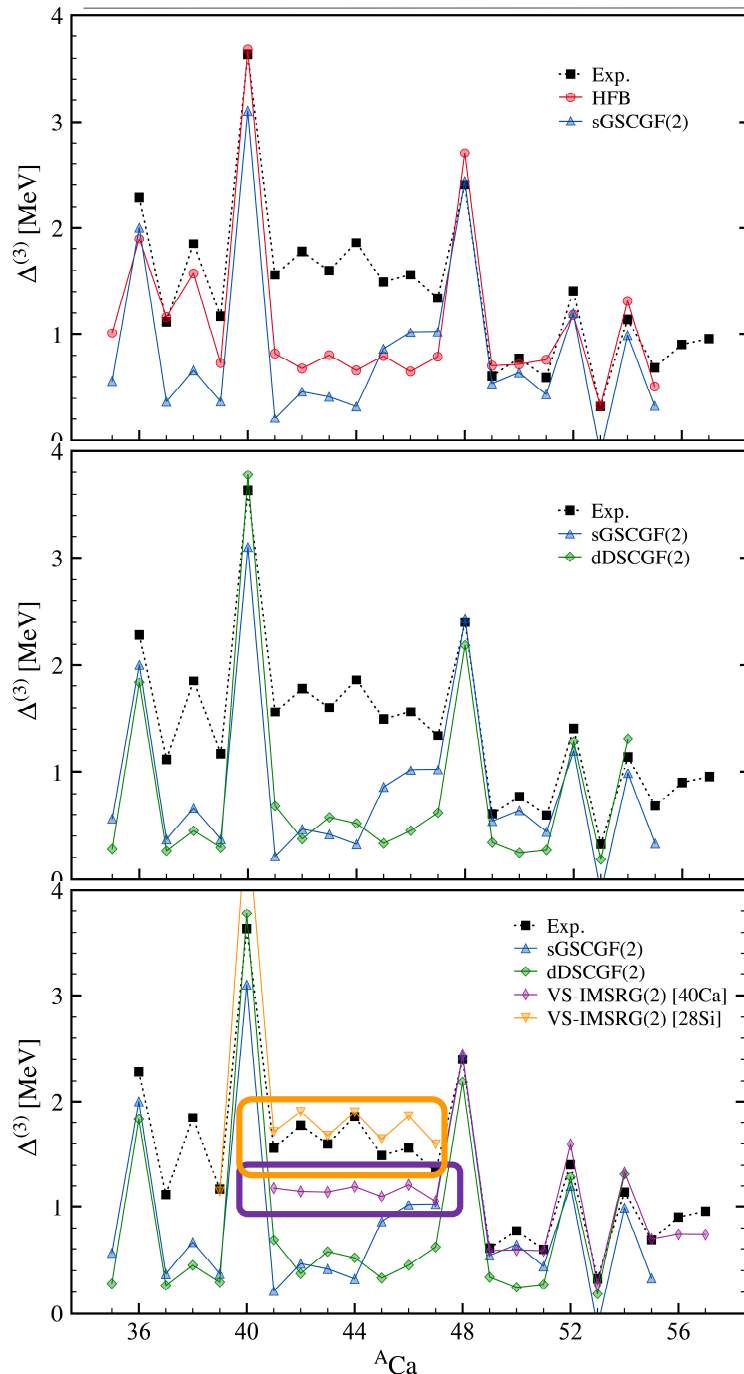
Third order

$$\Sigma_{\alpha\beta}^{11(3)}(\omega) = \text{diagram 1} + \text{diagram 2} + \text{diagram 3} + \text{diagram 4}$$

+ 4 with hh intermediate states
 + 9 with ph intermediate states

$$\Sigma_{\alpha\beta}^{12(3)}(\omega) = \text{17 diagrams obtained by permuting direction of line as illustrated above}$$

Ab initio sGSCGF(2) gaps in Ca isotopes



Somà et al., EPJA (2021)

Scalese et al., unpublished

Scalese et al., unpublished

Gaps are even often reduced compared to HFB

- Anti-pairing effect of fragmentation of strength wins
 - Insufficient m^* increase (as seen before)
 - Attractive (?) induced contribution to \tilde{v} not large enough
- More detailed analysis of the above components needed**

Solutions remain close to zero-pairing limit

- sGSCGF(2) close to dDSCGF(2) (no U(1) but SU(2) breaking)
- Does not benefit from U(1) breaking of reference state**
- $\Delta_{\alpha\beta}$ (or ΔN^2) constrained HFB unperturbed state to be explored

Pairing is in fact not gone anywhere!

- VS-IMSRG(2)[^{40}Ca] improves to 70% of exp. $\Delta^{(3)}$
- VS-IMSRG(2)[^{28}Si] reach 100%: fluctuation of ^{40}Ca core key
- Curvature and $\mathcal{I}_{\text{pair}}$ restored in VS-IMSRG(2)[^{28}Si]
- $\mathcal{I}_{\text{pair}}$, i.e. the oscillation of Δ , scales with Δ [Ruiké et al. arXiv:2504.11908](#)
- Not the Hamiltonian to be blamed (it seems*)
- Collective fluctuations required in *polynomial* methods
- GSCGF[3] = ADC(3) = Tamm Dancoff (i.e. beyond 3rd order)**
- Derived formally [Barbieri, Duguet, Somà, PRC \(2022\)](#)
- To be implemented numerically

Contents

- Introduction

- The ab initio nuclear many-body problem
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- Ab initio many-body expansion methods

- Ab initio description of isospin-triplet pairing in finite nuclei

- Gorkov self-consistent Green's function theory in a nutshell
- Lessons from empirical and semi-empirical HFB calculations
- Ab initio GSCGF(1,2) calculations

- Phenomenology of the induced pairing interaction

- Getting back the increased numerical cost of breaking $U(1)$ symmetry

- Tensor factorization of triaxially deformed BMBPT(2) calculations

Phenomenology of the induced pairing interaction

For infinite matter counterpart see [Lecture by G. Palkanoglou](#)

Talks E. Vigezzi, F. Barranco

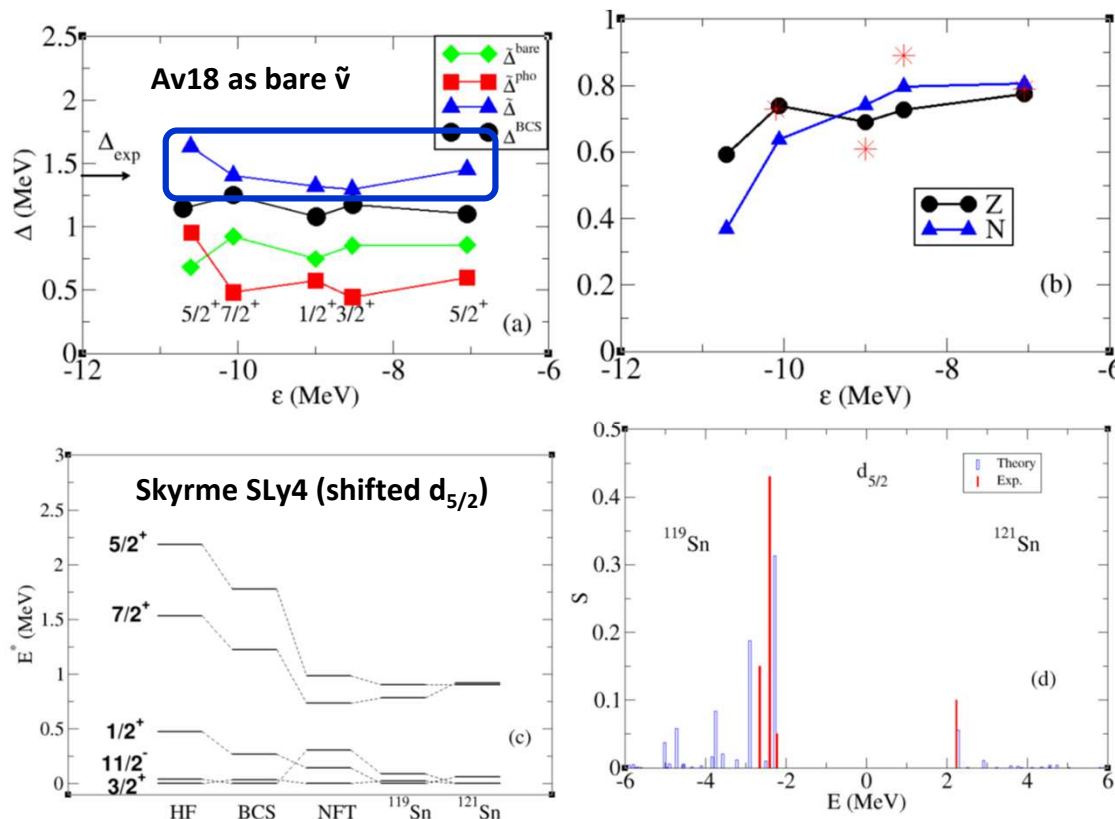
Exchange of low-lying *collective vibrations* among pairs of nucleons in time-reversal states

- Density (natural parity) modes attractive while spin (unnatural parity) modes repulsive
- Balance depends on isospin asymmetry

Consistent renormalization of single particle motion

- Pro-pairing effective mass increase (" ω -mass m_ω ")
- Anti-pairing fragmentation of one-nucleon addition and removal strength (" Z_ω ")

Barranco *et al.*, EPJA (2004); PRC (2005); Gori *et al.*, PRC (2005); Idini *et al.*, PRC (2012)



Empirically consistent picture

- Effect of coupling to vibrations essential
- Attractive induced $\tilde{v} + m_\omega$ win over Z_ω

Challenge

- Achieve the same ab initio
- GSCGF[3] = ADC(3) to be done (n_{dim}^7)
- Sufficient?

Collective fluctuations into unperturbed state

- Advanced PGCM unperturbed state
- Add correlations via PT [Frosini et al., EPJA \(2022\)](#)
- Leverage with MR-IMSRG [Frosini et al., EPJA \(2022\)](#)

Talks H. Hergert

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Expansion many-body methods

$$H|\Psi_k^\sigma\rangle = E_k^{\tilde{\sigma}}|\Psi_k^\sigma\rangle \text{ with } \sigma \equiv JM\Pi NZ \equiv \tilde{\sigma}M$$

$$[H, R(\theta)] = 0 \text{ with } G_H \equiv \{R(\theta), \theta \in \mathcal{D}_{G_H}\}$$

One-body Hilbert space

$$\mathcal{H}(1)$$

$$\dim \mathcal{H}(1) \equiv n_{\text{dim}}$$



A-body Hilbert space

$$\mathcal{H}_A = \mathcal{H}(1) \otimes \dots \otimes \mathcal{H}(A)$$

$$\dim \mathcal{H}(A) \equiv n_{\text{dim}}^A$$

Expansion many-body methods

Hamiltonian partitioning

Unperturbed state

Fully correlated state

$$H = H_0 + H_1 \xrightarrow{\text{« Easy » to solve}} H_0|\Theta_k^{(0)}\rangle = E_k^{(0)}|\Theta_k^{(0)}\rangle \xrightarrow{\text{Expansion series}} |\Psi_k^\sigma\rangle = \Omega_k|\Theta_k^{(0)}\rangle$$

q_{max}	(B)MBPT	(B)CC	(B)IMSRG	PGCM-PT
1	$O(n_{\text{dim}}^4)$	$O(n_{\text{dim}}^4)$	$O(n_{\text{dim}}^4)$	$O(n_{\text{proj}} n_{\text{gcm}}^2 n_{\text{dim}}^4)$
2	$O(n_{\text{dim}}^5)$	$O(n_{\text{dim}}^6)$	$O(n_{\text{dim}}^6)$	$O(n_{\text{proj}} n_{\text{gcm}}^2 n_{\text{dim}}^8)$
3	$O(n_{\text{dim}}^6)$	$O(n_{\text{dim}}^8)$	$O(n_{\text{dim}}^9)$	Heinz <i>et al.</i> , PRC (2021)

Large prefactor

Frosini *et al.*, EPJA (2022)

Tichai *et al.*, PLB (2016)

Binder *et al.*, PRC (2013)

Demol *et al.*, EPJA. (2025)

(Demol *et al.*, unp. (2024))

Mean-field cost = few 10% errors

Work-horse = few % error

State-of-the-art = sub% error \blacktriangleright (B)CC and (B)IMSRG based on manageable approximation ($\sim n_{\text{dim}}^7$)

Question: what is the difference between HF- and HFB-based methods?

Example: BMBPT(2)

⊙ Expansion many-body methods formulated in terms of **tensors** and **tensor networks**

1) Input tensors: the Hamiltonian

$$\begin{aligned}
 H &\approx h^{00}[\rho] \\
 &+ \frac{1}{(1!)^2} \sum_{\alpha\beta} \boxed{h_{\alpha\beta}^{11}[\rho]} c_{\alpha}^{\dagger} c_{\beta} \\
 &+ \frac{1}{(2!)^2} \sum_{\alpha\beta\gamma\delta} \boxed{h_{\alpha\beta\gamma\delta}^{22}[\rho]} c_{\alpha}^{\dagger} c_{\beta}^{\dagger} c_{\delta} c_{\gamma}
 \end{aligned}
 \xrightarrow[\text{Wick theorem}]{\text{HFB } |\Phi\rangle}
 \begin{aligned}
 H &= H^{00} + \frac{1}{1!} \sum_{k_1 k_2} H_{k_1 k_2}^{11} \beta_{k_1}^{\dagger} \beta_{k_2} + \frac{1}{(2!)^2} \sum_{k_1 k_2 k_3 k_4} H_{k_1 k_2 k_3 k_4}^{22} \beta_{k_1}^{\dagger} \beta_{k_2}^{\dagger} \beta_{k_4} \beta_{k_3} \\
 &+ \frac{1}{3!} \sum_{k_1 k_2 k_3 k_4} \{ H_{k_1 k_2 k_3 k_4}^{31} \beta_{k_1}^{\dagger} \beta_{k_2}^{\dagger} \beta_{k_3}^{\dagger} \beta_{k_4} + H_{k_1 k_2 k_3 k_4}^{13} \beta_{k_1}^{\dagger} \beta_{k_4} \beta_{k_3} \beta_{k_2} \} \\
 &+ \frac{1}{4!} \sum_{k_1 k_2 k_3 k_4} \boxed{H_{k_1 k_2 k_3 k_4}^{40}} \beta_{k_1}^{\dagger} \beta_{k_2}^{\dagger} \beta_{k_3}^{\dagger} \beta_{k_4} + H_{k_1 k_2 k_3 k_4}^{04} \beta_{k_4} \beta_{k_3} \beta_{k_2} \beta_{k_1} \}
 \end{aligned}$$

$\mathbf{n_{dim}^5}$ cost

2) Output tensors: the wave function

$$|\Psi_0^{\sigma}\rangle = \boxed{\Omega_0^{\text{BMBPT}}} |\Phi\rangle$$

$$|\Psi_0^{(2)}\rangle = |\Phi\rangle + \frac{1}{(4)!} \sum_{k_1 k_2 k_3 k_4} \boxed{C_{k_1 k_2 k_3 k_4}^{40}(2)} |\Phi^{k_1 k_2 k_3 k_4}\rangle \quad \text{Unknown mode-4 tensor}$$

BMBPT(2)

$$C_{k_1 k_2 k_3 k_4}^{40}(2) = - \frac{\boxed{H_{k_1 k_2 k_3 k_4}^{40}}}{E_{k_1} + E_{k_2} + E_{k_3} + E_{k_4}}$$

Storage $\mathbf{n_{dim}^4}$ cost

$$E_0^{(2)} = H^{00} + \frac{1}{4!} \sum_{k_1 k_2 k_3 k_4} H_{k_1 k_2 k_3 k_4}^{04} C_{k_1 k_2 k_3 k_4}^{40}(2) \quad \text{Tensor network of } \mathbf{n_{dim}^4} \text{ cost}$$

e_{\max}	n_{dim}	\tilde{n}_{dim}
2	40	12
4	140	30
6	336	56
8	660	90
10	1144	132
12	1820	182
14	2720	240
16	3876	306

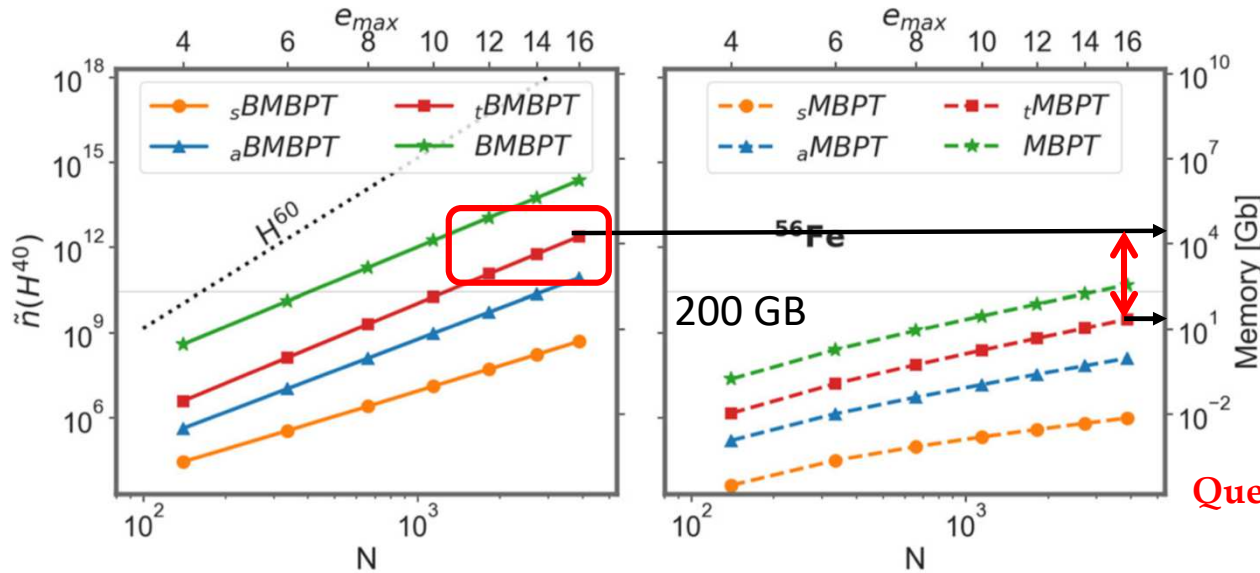
J-scheme for sBMBPT up to A~200 ► OK

M-scheme for dBMBPT ► too expensive to compute and store

Example: what about performing $_t\text{dMBPT}(2)$?

Frosini, Duguet, Tamagno, EPJA (2024)

⊙ The explicit U(1) breaking strongly impact numerical scaling, e.g. n_{dim}^4 memory cost



$_t\text{dMBPT}(2)$ vs $_t\text{dMBPT}(2)$ at $e_{\text{max}}=16$
 → 3 orders of magnitude for $A=56$
 → $_t\text{dMBPT}(2)$ undoable beyond $e_{\text{max}}=10$
 → Breaking U(1) better be useful!

Question: can we gain some of the difference back?

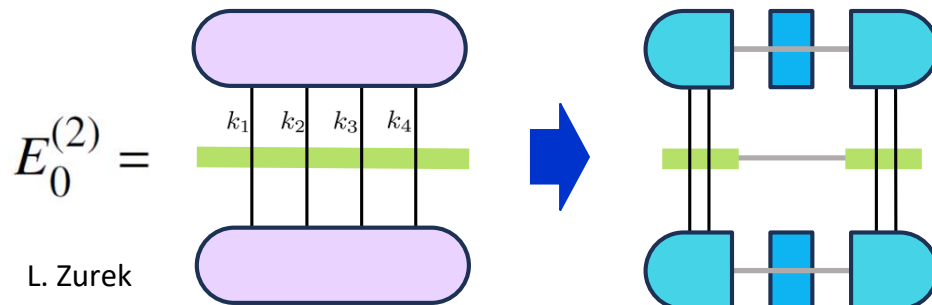
Tensor factorize $C_{k_1 k_2 k_3 k_4}^{40}(2)$ via randomize (truncated) SVD *without* ever constructing $C_{k_1 k_2 k_3 k_4}^{40}(2)$

$$\mathcal{C} \frac{1}{(E_{k_1} + E_{k_2}) + (E_{k_3} + E_{k_4})} = \sum_{i=1}^{\sim 10} d_{k_1 k_2}^i d_{k_3 k_4}^i$$

Laplace transform

$$H_{k_1 k_2 k_3 k_4}^{40} \approx \sum_{\mu=1}^r F_{k_1 k_2}^{\mu} S_{\mu} G_{k_3 k_4}^{\mu}$$

Matrix-less rSVD



Evaluation cost $n_d r^2 N^2 \gtrsim N^4$

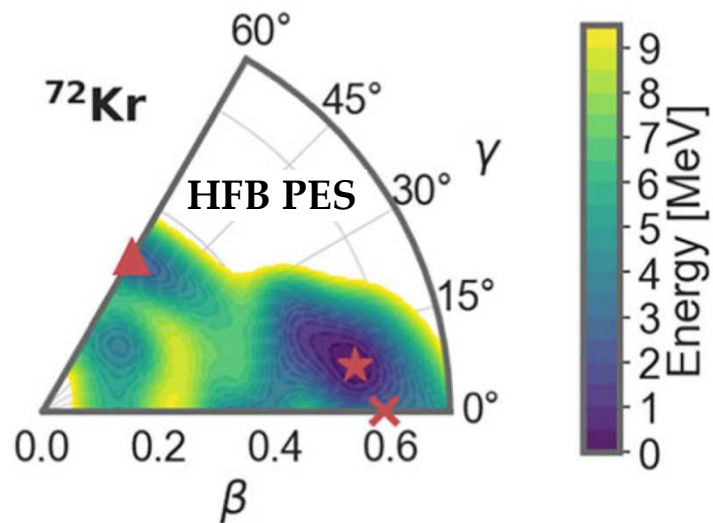
Memory usage $r N^2 \ll N^4$

Tensor factorization of many-body tensor in $_t\text{dMBPT}(2)$

Frosini, Duguet, Tamagno, EPJA (2024)

◎ Triaxial $\text{dMBPT}(2)$ in ^{72}Kr in large bases

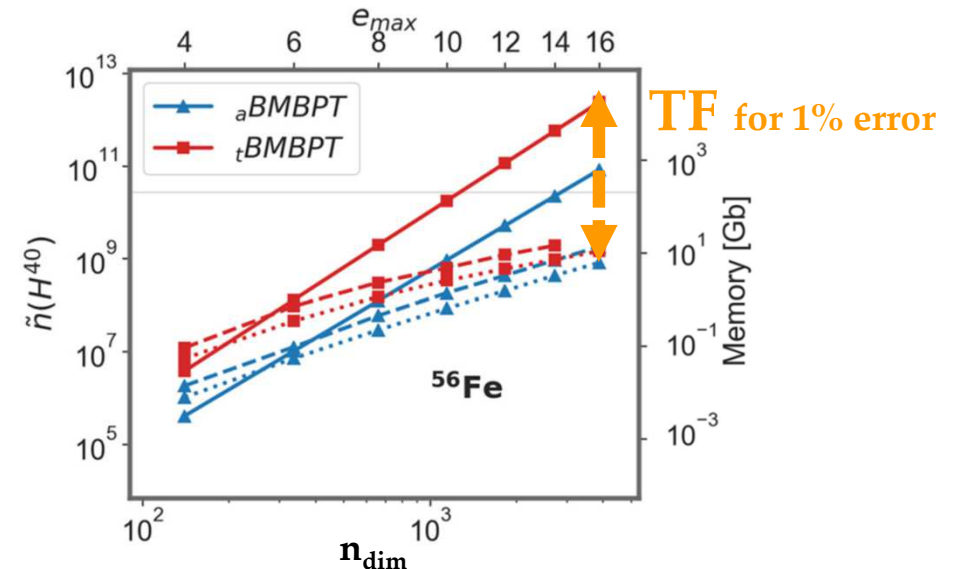
► Undoable full fledged



$_{a,t}\text{BMBPT}(2)$



rSVD



Gain becomes very significant for large e_{max} (heavy nuclei)

→ Compression by 10^4 for 1% error on $\Delta E^{(2)}_0$ at $e_{\text{max}}=16$ ($n_{\text{dim}}=4000$)

→ Effective $e_{\text{max}} = 7$ calculations

→ Just inferior to the cost of $e_{\text{max}}=16$ $_t\text{dMBPT}$ calculations

Much greater gain expected for initially much costlier approaches

→ $_{a,t}\text{dMBPT}(3)$ for greater accuracy [Zurek et al., in preparation \(2025\)](#)

→ Non-perturbative methods such as (B)CC

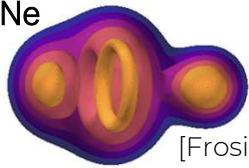
Backup slides

Ab initio frontiers

SPECTROSCOPY

- Single-particle excitations
- Collective excitations
- Clustering

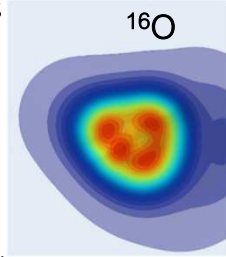
^{20}Ne



[Frosini et al., 2023]

$1^-/3^-$ vibration ($^{16}\text{O} + \alpha \leftrightarrow ^{12}\text{C} + 2\alpha$) at 7.2 MeV

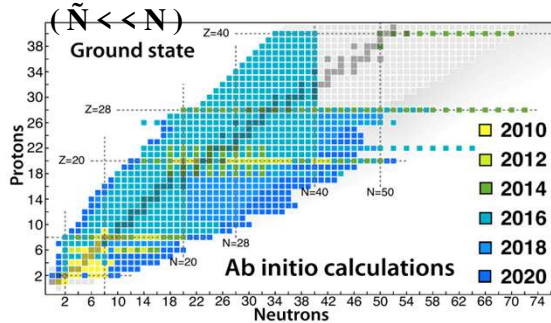
Tetrahedral
ground state
intrinsic density



[Bally et al., 2023]

OPEN-SHELL

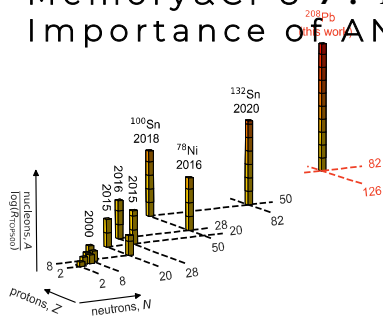
- Novel many-body methods
- Memory&CPU \nearrow : $\tilde{N}^p \rightarrow N^q$



[Hergert, 2020]

MASS

- Memory&CPU \nearrow : N^p with $N \nearrow$
- Importance of AN forces?



[Hu et al., 2022]

HAMILTONIAN

- $S=0/S \neq 0$ interactions
- Power counting
- Currents
- Fit

UNCERTAINTIES

- Systematic

Hamiltonian

$$H = T + V_{\text{LO}} + V_{\text{NLO}} + V_{\text{N}^2\text{LO}} + \dots$$

A-body solution

$$|\Psi_k^A\rangle = \Omega |\Theta_k^{(0)}\rangle = |\Theta_k^{(0)}\rangle + |\Theta_k^{(1)}\rangle + |\Theta_k^{(2)}\rangle + \dots$$

Basis representation

$$|\Theta_k^{(n)}\rangle = \sum_{p=0}^{\infty} A_{pk}^{(n)} |\Phi_p\rangle$$

- Statistical

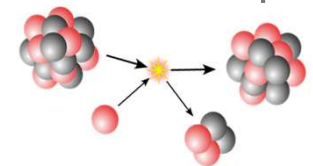
$$H \equiv H(\{\lambda_i\}) \xrightarrow{\text{fit}} \lambda_i = \bar{\lambda}_i + \Delta \bar{\lambda}_i$$

ACCURACY

- Algebra cost \nearrow
Difficult manually
- Numerical cost \nearrow
Memory&CPU: $N^p \rightarrow N^q$ ($q > p$)

REACTIONS

- Light nuclei
- Optical potential
- Transition densities



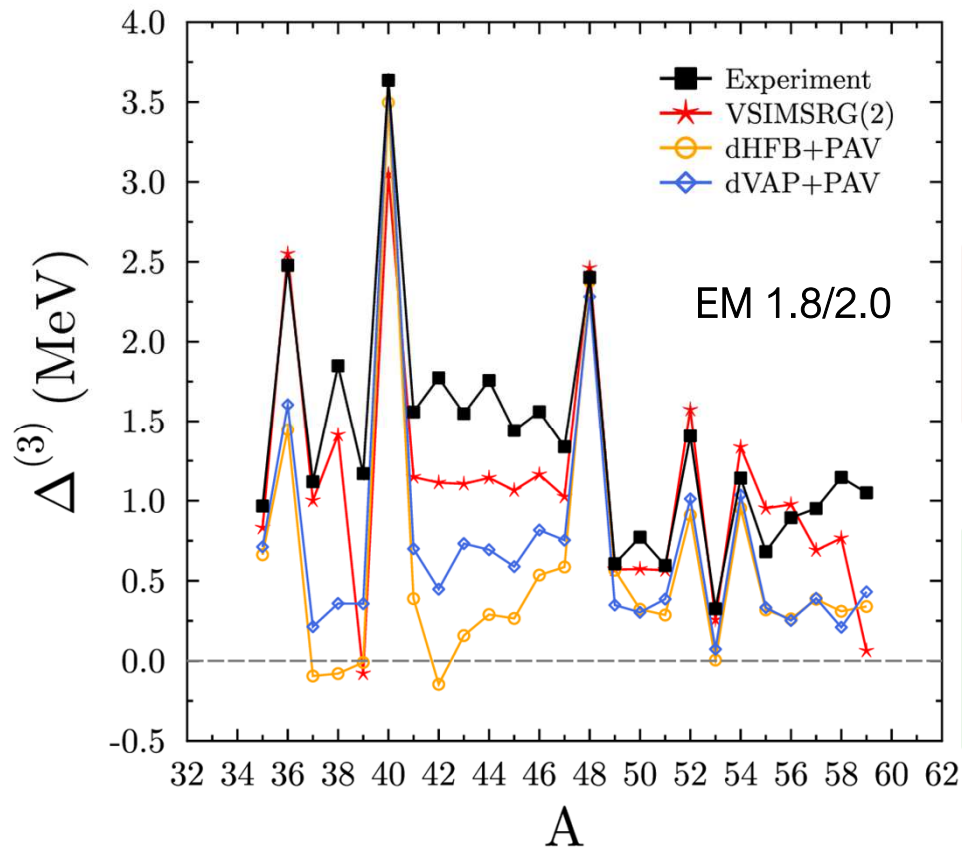
$$H|\Psi_k^A\rangle = E_k^A |\Psi_k^A\rangle$$



MANY-BODY
METHODS

Where is the pairing gone? © G. Hagen, T. Duguet

Bally *et al.*, unpublished



sHFB displays little pairing

- HF-EFA gives close results
- Give ~20% of exp $\Delta^{(3)}$

Dynamical correlations

- Low-order via sDSCGF(2) \approx 30% of exp $\Delta^{(3)}$
- sVS-IMSRG(2) with ^{40}Ca core \approx 70% of exp $\Delta^{(3)}$
- Higher-order collective process = exchange of vibrations

Use a mean-field “on steroid” as unperturbed state Deformed Bogoliubov with full blocking in odd isotopes

1. VAP on N&Z
2. PAV on J^π

- 40% of exp $\Delta^{(3)}$ but not enough as expected

Shape fluctuations of ^{40}Ca « core » adding GCM
Dynamical correlations on top via PGCM-PT

Frosini *et al.*, EPJA (2022)

Superfluidity “fine-tuned” from a many-body standpoint

► A quantitative ab initio description at polynomial cost is a challenge for the future

Uncertainty from order-by-order χEFT interactions should be propagated to $\Delta^{(3)}$ (but will be sub-leading)