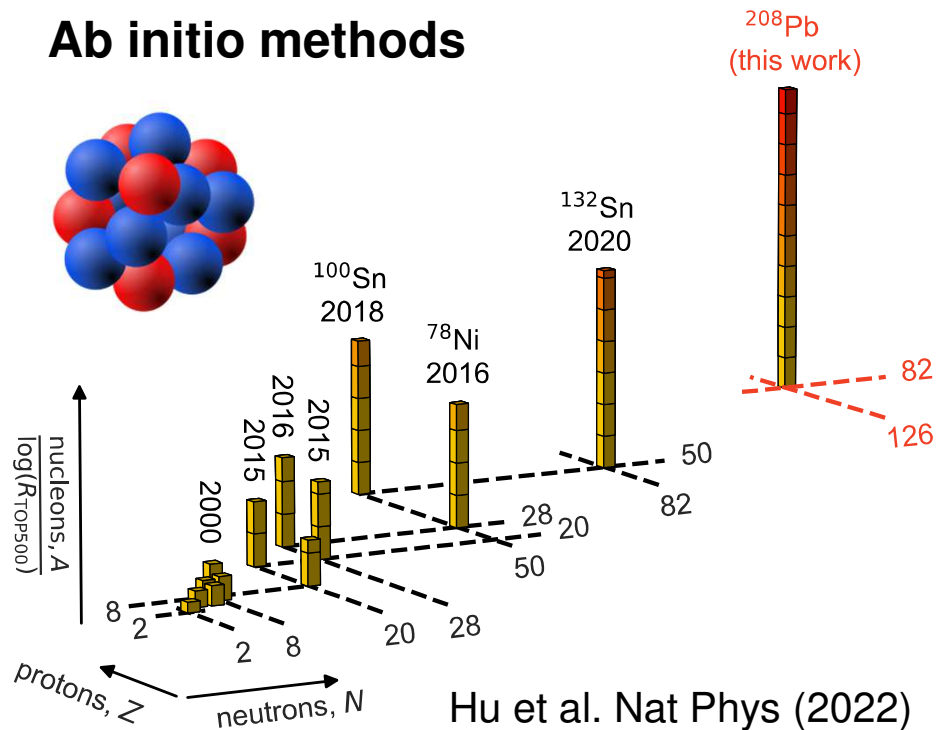


Effective theories of QCD for nuclei at low energy

Ab initio methods



Thomas DUGUET

DPhN, CEA-Saclay, France
IKS, KU Leuven, Belgium

Workshop on *Deciphering nuclear phenomenology across energy scales*

September 20-23 2022, ESNT, Saclay, France



Contents

- Introduction to low-energy nuclear physics
 - Phenomenology
 - Rationale from the theoretical viewpoint
- Strong inter-nucleon forces
 - Basic phenomenology and modelling
- The ab initio nuclear many-body problem
 - Pre-processing short-range correlations
 - Expansion methods handling both « weak/strong » dynamical/static correlations
 - Nuclear deformation from ab initio calculations
- Conclusions

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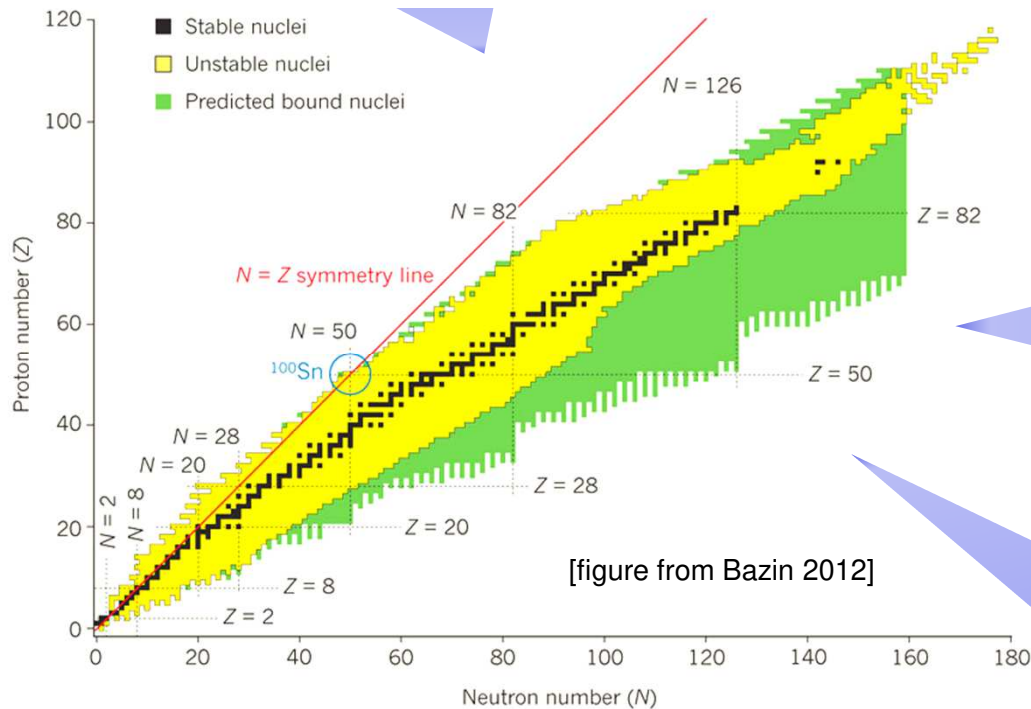
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⦿ Conclusions

Elementary facts and « big » questions about nuclei

- 252 **stable** isotopes, ~3100 synthesized in the lab
- **How many** bound (w.r.t strong force) nuclei exist; 9000?

Less than 50% known ($>10^{-22}$ s) → Discovery of ~15 per year in the years 2010s
 → Several 100s from next generation facilities



Oganesson ${}_{118}\text{Og}$ added to Mendeleïev table in 2016

- **Heaviest** synthesized element $Z=118$
- **Heaviest possible** element?
- Enhanced stability near $Z=120?126?$

2p decay beyond the proton drip line in ${}^{45}\text{Fe}$ in 2002

- Modes of **instability** (α , p , β , γ decays, fission)
- Are there more exotic/rare decay modes?
 Ex: ν -less 2β decay = test of standard model?

Gravitational wave + kilonova from neutron stars merger in 2017

- Elements **up to Fe** produced in stellar fusion
- How have heavier elements been produced?
- Exotic r-process nucleosynthesis ; but where?

Updated in 2019 to $Z=9$ (22 neutrons) and $Z=10$ (24 neutrons)

- Neutron **drip-line** known up to ~~$Z=8$ (16 neutrons)~~
- Where is the neutron drip-line beyond $Z=10$?

Shown to disappear away from stability in 1975/1993

- Over-stable "magic" nuclei (2, 8, ~~20, 28~~, 50, 82, ...)
- How **other magic numbers** evolve with N-Z?

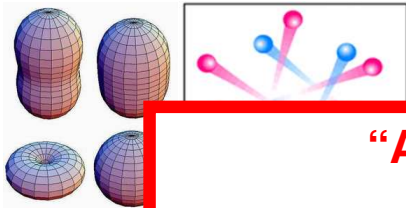
The atomic nucleus as a 4-components quantum mesoscopic system

An extremely rich and diverse phenomenology

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

Ground state

Mass, size, superfluidity, e.m. moments...



Several scales at play:

p & n momenta $\sim 10^8$ eV

Separation energies $\sim 10^7$ eV

Vibrational excitations $\sim 10^6$ eV

10^4 eV

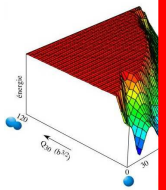
“Ab initio”, i.e. Chiral-EFT in A-body sector, long-term endeavor

Can nuclear systems be described

- 1) Consistently (from a single theoretical rationale?)
- 2) Systematically (complete phenomenology?)
- 3) Accurately enough (relevant to experimental uncertainty?)
- 4) From inter-nucleon interactions (right balance between reductionism/emergence?)
- 5) Rooted in QCD (sound connection to underlying EFT?)

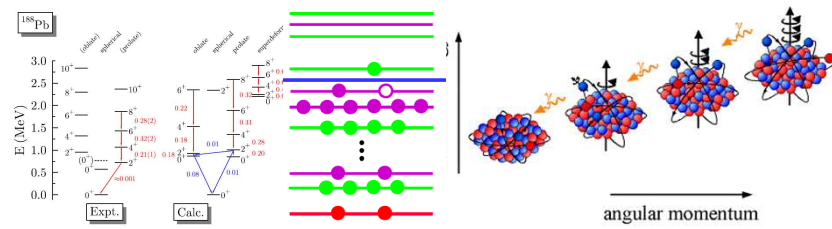
Radiation

β , 2β , ...



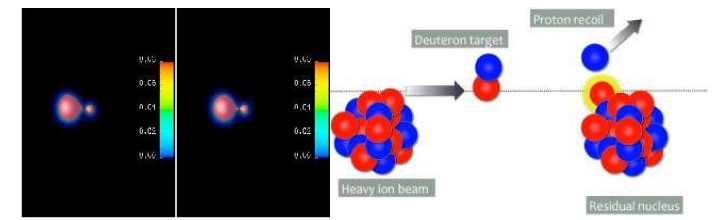
Spectroscopy

Excitation modes



Reaction processes

Fusion, transfer, knockout, ...



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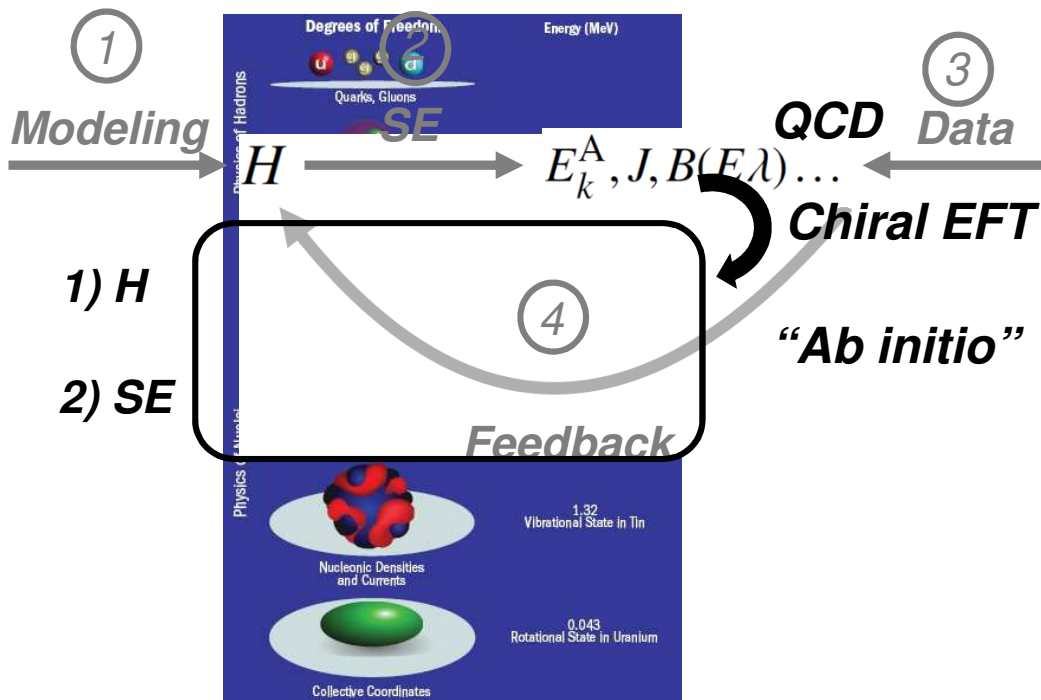
Ab initio (i.e. In medias res) quantum many-body problem

Ab initio nuclear many-body theory = Chiral Effective Field Theory (χ EFT) in A-nucleon sector

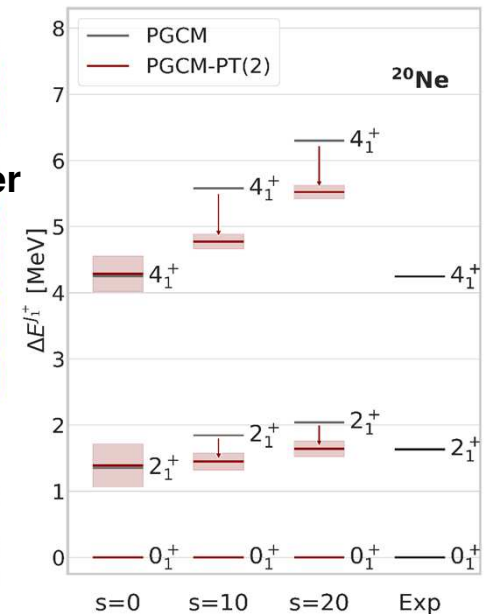
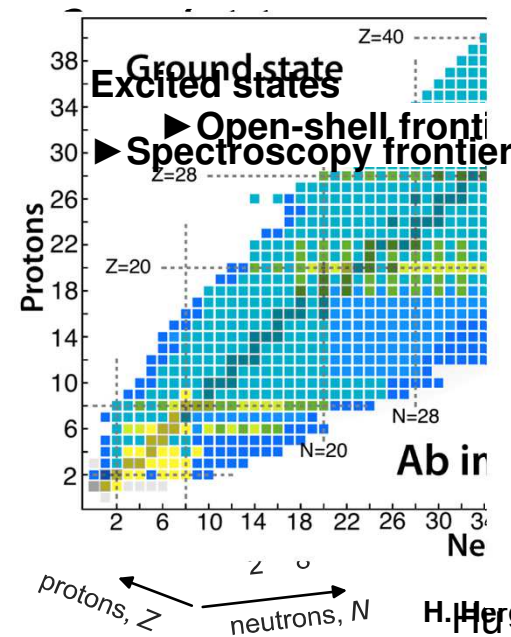
- 1) A structure-less nucleons as degrees of freedom at low energy
- 2) Interactions mediated by pions and contact operators based on, e.g., Weinberg, power counting
- 3) **Solve A-body Schrödinger equation to relevant accuracy**

A-body Schrödinger Equation

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



Rapidly evolving field in the last 15 years



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The nuclear Hamiltonian

Build H (and other operators) with χ EFT at various orders

- ⊙ Non-trivial formal task whose difficulty increases with order (e.g. **3N at N²LO, 4N at N³LO...**)
- ⊙ Fit LECs of mode-2k tensors to experimental data (or lattice QCD) in $A = k$ -body systems

Organization = power counting
Importance of interaction terms

A-body Schrödinger Equation

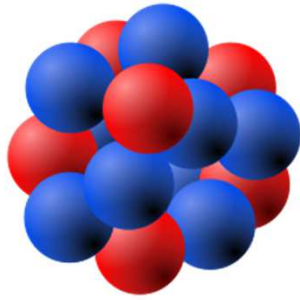
$$H|\Psi_k^A\rangle = E_k^A|\Psi_k^A\rangle$$

Effective description = A-body operator in principle

$$H = T + \boxed{V^{2N} + V^{3N}} + V^{4N} + \dots + V^{AN}$$

At least 3N necessary = major difficulty to solve SE next

Symmetries of the nuclear Hamiltonian



$$\vec{P} = \sum_{i=1}^A \vec{p}_i$$

Total center-of-mass momentum

$$\vec{J} = \vec{L} + \vec{S} = \sum_{i=1}^A \vec{l}_i + \sum_{i=1}^A \vec{s}_i$$

Total (internal) angular momentum

Nuclear systems are

❶ Translationally invariant: **T(1)**

$$[H, P_i] = 0 \Rightarrow | \Phi_{\text{cm}}^P \rangle | \Psi_{\text{im}} \rangle$$

❷ Rotationally invariant: **SU(2)**

$$[H, J^2] = [H, J_z] = 0 \Rightarrow | \Psi^{JM} \rangle$$

❸ Carry fixed neutrons/protons numbers: **U(1)**

$$[H, N] = [H, Z] = 0 \Rightarrow | \Psi^{JMNZ} \rangle$$

❹ + additional symmetries (time reversal, parity, ~isospin)

Symmetries

❶ Strongly constrain the mathematical form of H

❷ Dictates quantum numbers of its eigenstates

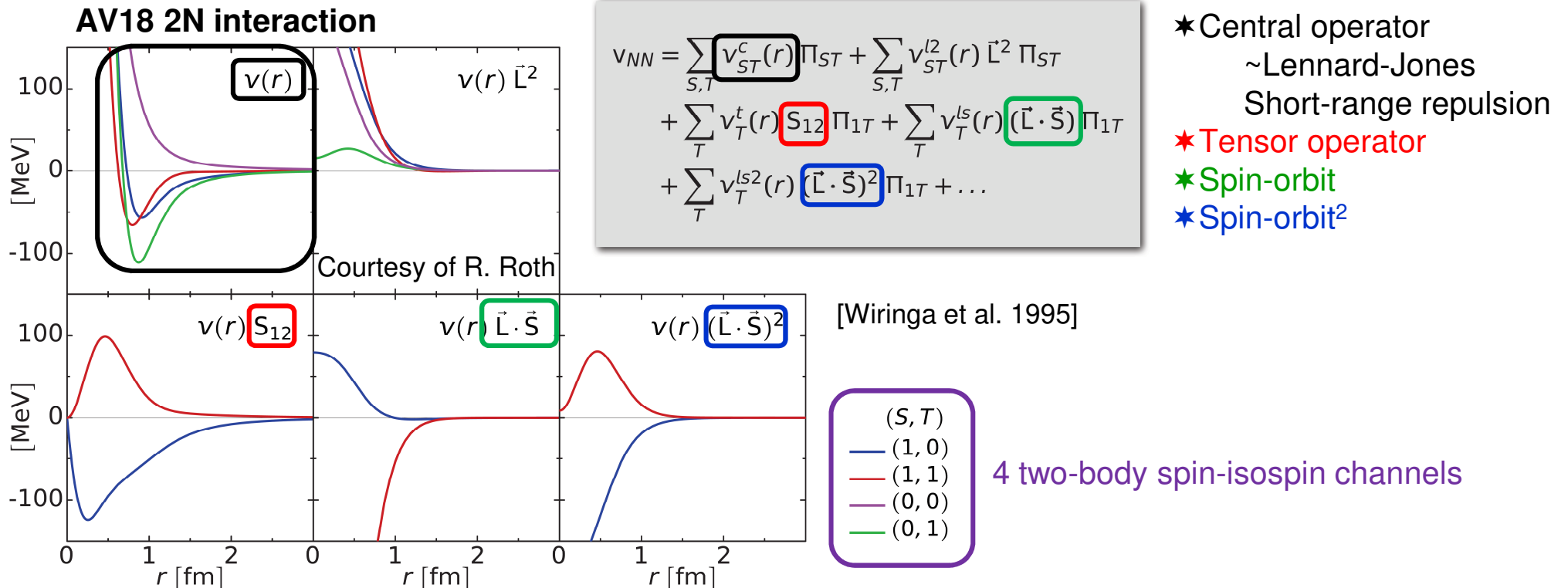
e.g. factorization of cm hard to ensure in practice

Phenomenology of inter-nucleon interactions

$$\begin{aligned}
 H &\equiv \sum_{i=1}^A \frac{\vec{p}_i^2}{2m} + \frac{1}{2} \sum_{i \neq j} V^{2N}(i,j) + \frac{1}{6} \sum_{i \neq j \neq k} V^{3N}(i,j,k) + \dots \\
 &= \sum_{\alpha\beta} t_{\alpha\beta} a_{\alpha}^{\dagger} a_{\beta} + \left(\frac{1}{2!}\right)^2 \sum_{\alpha\beta\gamma\delta} \bar{v}^{2N}_{\alpha\beta\gamma\delta} a_{\alpha}^{\dagger} a_{\beta}^{\dagger} a_{\delta} a_{\gamma} + \left(\frac{1}{3!}\right)^2 \sum_{\alpha\beta\gamma\delta\zeta\epsilon} \bar{v}^{3N}_{\alpha\beta\gamma\delta\zeta\epsilon} a_{\alpha}^{\dagger} a_{\beta}^{\dagger} a_{\gamma}^{\dagger} a_{\epsilon} a_{\zeta} a_{\delta} + \dots
 \end{aligned}$$

Interactions between **effective** **4-components** **point** fermions
 ↷ nucleons = $\pm 1/2$ isospin & $\pm 1/2$ spin projections

1. Complex operator structure in $r \otimes \sigma \otimes \tau$ spaces (constrained by symmetries)



⊗ AV18 model local but generally nuclear interactions are non-local in space

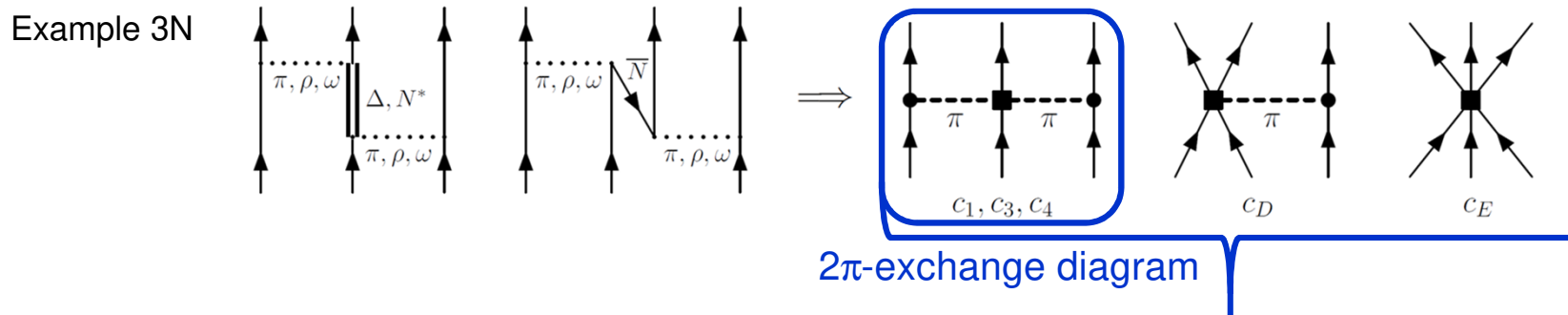
Phenomenology of inter-nucleon interactions

$$\begin{aligned}
 H &\equiv \sum_{i=1}^A \frac{\vec{p}_i^2}{2m} + \frac{1}{2} \sum_{i \neq j}^A V^{2N}(i,j) + \frac{1}{6} \sum_{i \neq j \neq k}^A V^{3N}(i,j,k) + \dots \\
 &= \sum_{\alpha\beta} t_{\alpha\beta} a_\alpha^\dagger a_\beta + \left(\frac{1}{2!}\right)^2 \sum_{\alpha\beta\gamma\delta} \bar{v}_{\alpha\beta\gamma\delta}^{2N} a_\alpha^\dagger a_\beta^\dagger a_\delta a_\gamma + \left(\frac{1}{3!}\right)^2 \sum_{\alpha\beta\gamma\delta\zeta\epsilon} \bar{v}_{\alpha\beta\gamma\delta\zeta\epsilon}^{3N} a_\alpha^\dagger a_\beta^\dagger a_\gamma^\dagger a_\epsilon a_\zeta a_\delta + \dots
 \end{aligned}$$

Interactions between **effective** 4-components **point** fermions
 ↻ nucleons = $\pm 1/2$ isospin & $\pm 1/2$ spin projections

2. Dominant 2-nucleon + sub-leading (but mandatory) 3-nucleon and (minor?) 4-nucleon forces

« Integrating out » DOFs lead to multi-nucleon forces



First contributions to 3N interaction in chiral-EFT (N^2LO)

Example of analytical expression

$$\begin{aligned}
 \langle \vec{p}'_1 \vec{p}'_2 \vec{p}'_3 | V_{2\pi N^2LO}^{3N} | \vec{p}_1 \vec{p}_2 \vec{p}_3 \rangle &= \frac{g_A^2}{8F_\pi^4} \frac{\boxed{\vec{\sigma}_1 \cdot \vec{q}_1 \vec{\sigma}_3 \cdot \vec{q}_3}}{[q_1^2 + m_\pi^2][q_3^2 + m_\pi^2]} \left[\vec{\tau}_1 \cdot \vec{\tau}_3 \left(\boxed{2c_3} \vec{q}_1 \cdot \vec{q}_3 - \boxed{4c_1} m_\pi^2 \right) \right. \\
 &\quad \left. + \boxed{c_4} \vec{\tau}_1 \times \vec{\tau}_3 \cdot \vec{\tau}_2 \boxed{\vec{q}_1 \times \vec{q}_3 \cdot \vec{\sigma}_2} \right] \delta(\vec{P}' - \vec{P}) \\
 &\quad + \text{all permutations of } (1,2,3)
 \end{aligned}$$

ME in plane-wave basis of \mathcal{H}_3
 $\vec{q}_i = \vec{p}'_i - \vec{p}_i \quad \vec{P} = \sum_{i=1}^3 \vec{p}_i$

Low-Energy Constants (LECs)



Fixed on π -nucleon scatt. exp.

Modern constructive approach = effective field theory

1. Use **separation of scales to define d.o.f** & expansion parameter [Weinberg, Gasser, Leutwyler, van Kolck, ..]

Typical momentum at play $\leftarrow Q/\Lambda \rightarrow$ High energy scale (physics beyond not included explicitly)

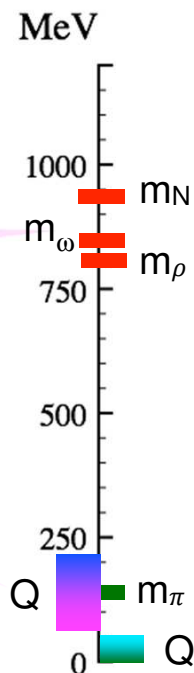
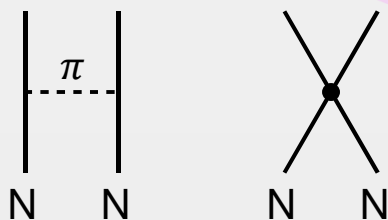
2. Parametrize physics beyond Λ + write $\#^\infty$ terms allowed by **(broken) symmetries of underlying QCD**
3. Order by size all possible terms \rightarrow **systematic expansion** (“power counting”) \rightarrow theoretical error
4. Truncate at a given order and **adjust low-energy constants (LECs) via underlying theory or data**
5. Regularize UV divergences and (hopefully) **achieve order-by-order renormalization of observables**

Chiral EFT

\Leftrightarrow Expand around $Q \sim m_\pi$

High-energy via contact interactions

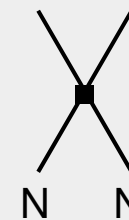
Keep pion dynamic explicit



Pionless EFT

\Leftrightarrow Expand around $Q \sim 0$

Integrate out pions too
 \rightarrow only contact terms



Chiral effective field theory = Weinberg power counting

- 1) Interaction diagrams are made out of
- a) nucleon and pion propagators
 - b) pion-nucleon and (derivative) k-nucleon contact vertices

Goal of PC: estimate the power ν of the law $(Q/\Lambda_\chi)^\nu$ with which each diagram scales

- 2) Naive Dimensional Analysis
- a) nucleon propagator carries Q^{-1}
 - b) pion propagator carries Q^{-2}
 - b) derivative operator carries Q
 - c) loop integration brings Q^4
- $\frac{1}{m_\omega^2 + Q^2} \approx \frac{1}{m_\omega^2} \left(1 - \frac{Q^2}{m_\omega^2} + \frac{Q^4}{m_\omega^4} - + \dots \right)$
 Fits with PC in powers of $Q/m_\omega \approx Q/\Lambda_\chi$

Connected diagrams

$$\nu = 2k - 4 + 2L + \sum_i \Delta_i$$

with $\Delta_i \equiv d_i + \frac{n_i}{2} - 2$

k = k-nucleon sector

L = # of loops

d_i = # of derivatives/pion masses at vertex i

n_i = # of nucleon fields at vertex i



Hierarchy of k-body forces: 3N (4N) starts 2 (4) orders after 2N

$$\Delta_i \geq 0$$

$$\nu \geq 0$$

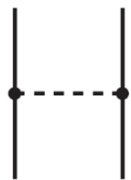
Chiral symmetry



Finite # at given order

Weinberg PC for interaction potential **Insert into dynamical, i.e. A-body Schroedinger, equation to access observables**

- 3) Examples: diagrams in 2-nucleon sector at Leading Order (LO) with $\sim Q^0$ ($\nu = 0$ from $k=2, L=0, \Delta_i=0$)



$$V_{1\pi}^{(0)}(\mathbf{p}', \mathbf{p}) = -\frac{g_A^2}{4f_\pi^2} \boldsymbol{\tau}_1 \cdot \boldsymbol{\tau}_2 \frac{\boldsymbol{\sigma}_1 \cdot \mathbf{q} \boldsymbol{\sigma}_2 \cdot \mathbf{q}}{q^2 + m_\pi^2}$$

Tensor operator



$$V_{ct}^{(0)}(\mathbf{p}', \mathbf{p}) = C_S + C_T \boldsymbol{\sigma}_1 \cdot \boldsymbol{\sigma}_2$$

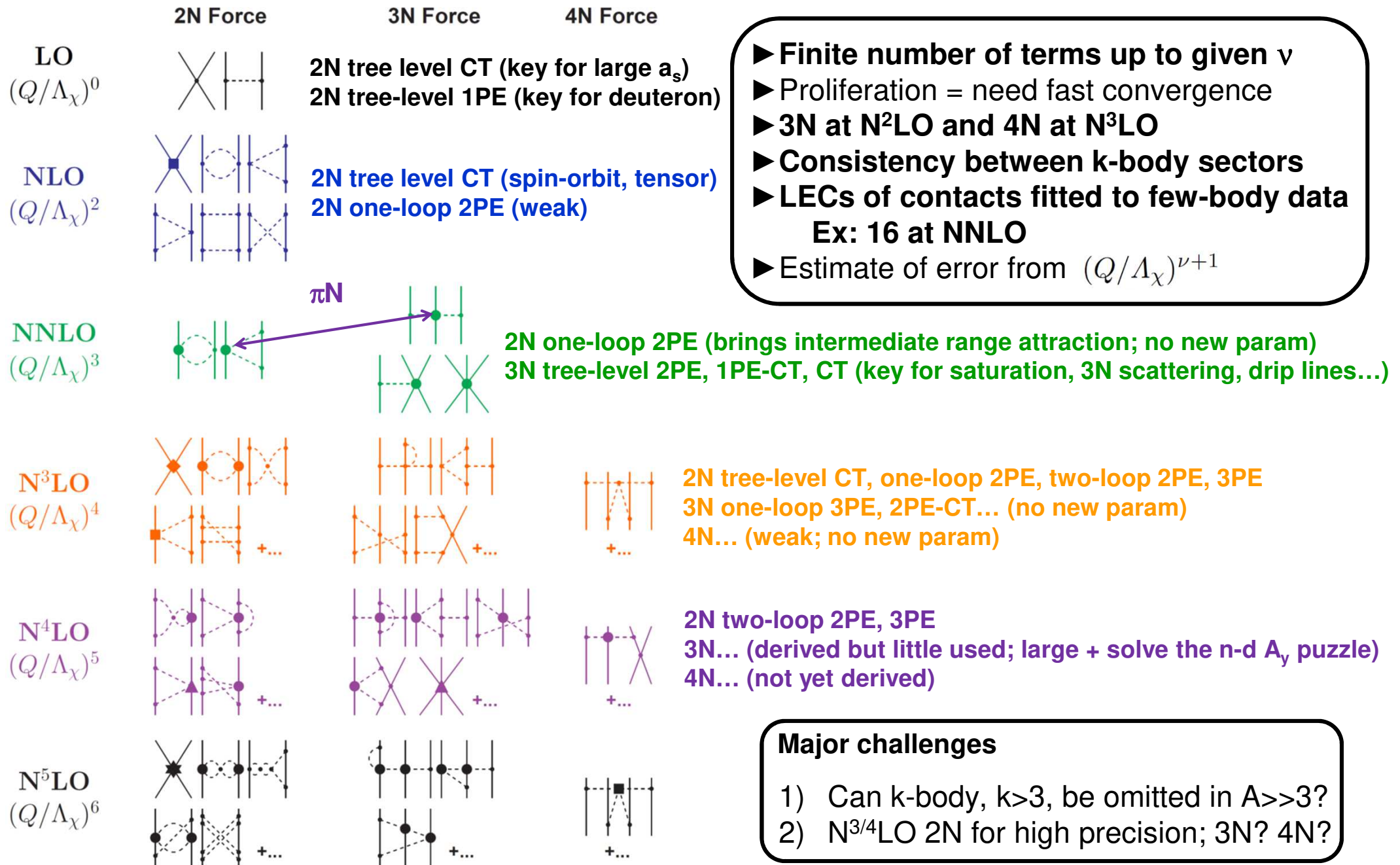
Central operator (no q dependence)

1 π exchange (1PE)

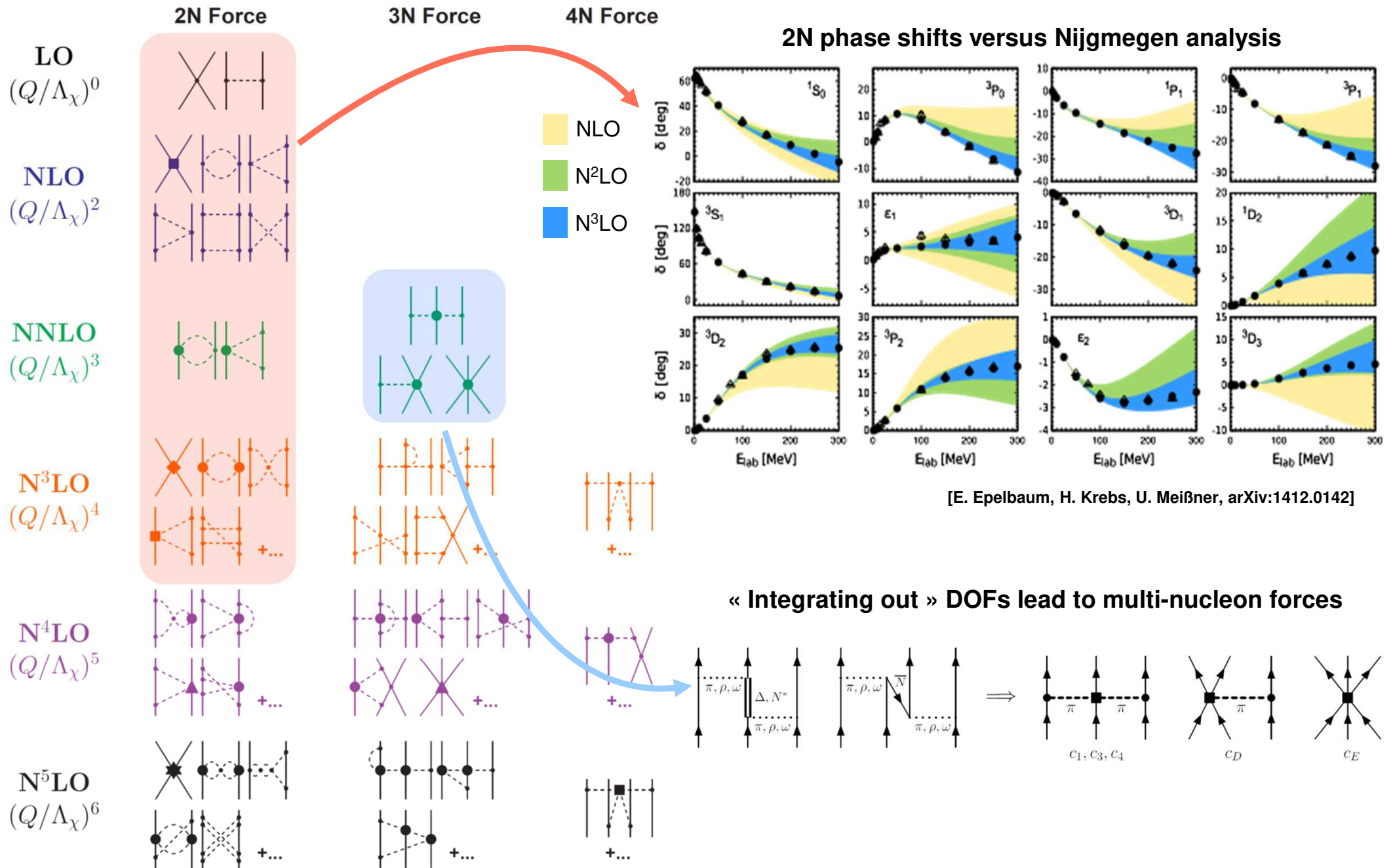
Pure contact term (CT)

- 4) Consistent construction of other operators (e.g. coupling to electroweak or WIMP probes)

Chiral effective field theory = interactions expansion



Chiral effective field theory = interactions expansion



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Nuclear many-body problem

Memory load for JT-coupled matrix elements

Transform to JT-coupled matrix elements for storage (on-the-fly decoupling)

→ SRG evolved in mass $A \sim 50$ ($e1_{max} = 13$ / $e2_{max} = 26$ / $e3_{max} = 16$)

$$\langle pq|V|rs\rangle \longrightarrow \langle \tilde{p}\tilde{q}; J; T | V | \tilde{r}\tilde{s}; J; T \rangle$$

→ typical reduction by factor ~ 30

$$\langle pq|W|stu\rangle$$

$$3NF \sim 25GB$$

$$\longrightarrow \langle \tilde{p}\tilde{q}\tilde{r}; J_{pq} J_{pq} T_{pq} | W | \tilde{s}\tilde{t}\tilde{u}; J_{st} J_{st} T_{st} \rangle$$

Ex: H_{N^2LO} SRG evolved in mass $A \sim 100$ ($e1_{max} = 15$ / $e2_{max} = 30$ / $e3_{max} = 20$) of the operator

$$2NF \sim 7GB$$

$$3NF \sim 350GB$$

More needed to reduce the load to go beyond $A \sim 100$

A-body Schrödinger Equation

$$H_{N^2LO} |\Psi_k^{JMNZ}\rangle = E_k^{JNZ} |\Psi_k^{JMNZ}\rangle$$

HO single-particle basis

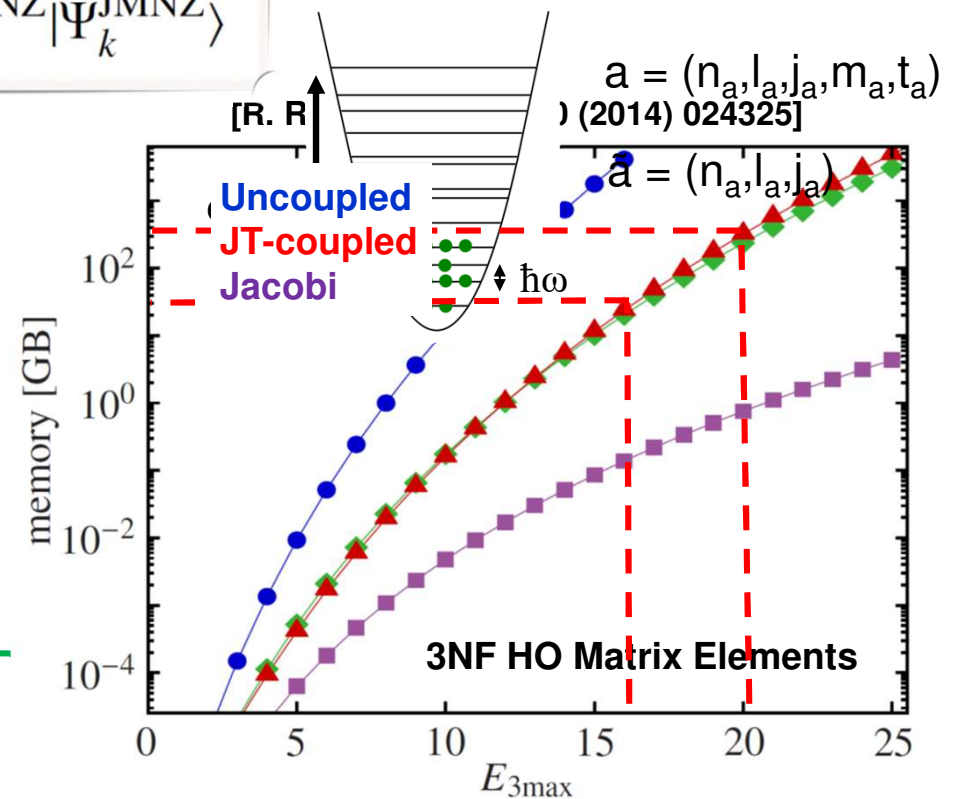
Second-quantized form

$$H \equiv \frac{1}{(1!)^2} \sum_{pq} t_{pq} c_p^\dagger c_q$$

Four-index tensor →
$$+ \frac{1}{(2!)^2} \sum_{pqrs} \bar{v}_{pqrs} c_p^\dagger c_q^\dagger c_s c_r$$

Six-index tensor →
$$+ \frac{1}{(3!)^2} \sum_{pqrstu} \bar{w}_{pqrstu} c_p^\dagger c_q^\dagger c_r^\dagger c_u c_t c_s$$

+ ...



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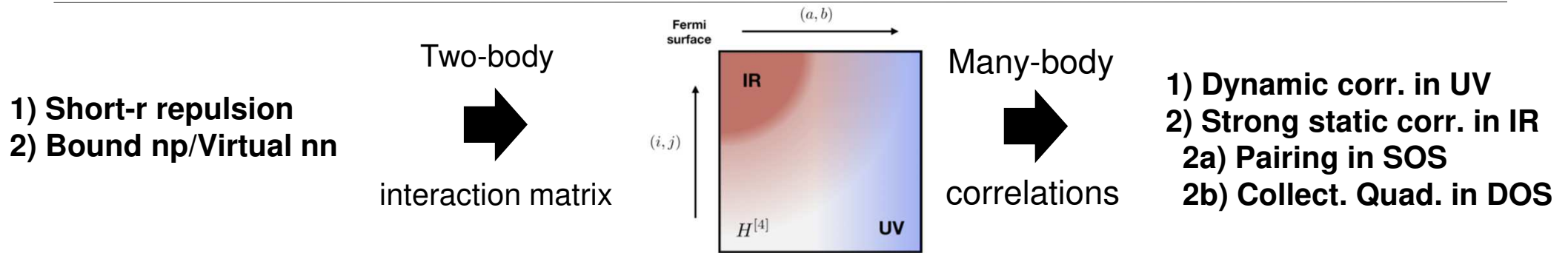
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Pre-processing of short-range correlations



1) Taming down the short-range/coupling to UV in the Hamiltonian

Unitary **Similarity Renormalization Group** (SRG) transformation $H(s) \equiv U(s)HU^\dagger(s) = T + V^{2N}(s) + V^{3N}(s) + \dots$

◆ Parameterize the *change* of the Hamiltonian $\frac{dH(s)}{ds} = [\eta(s), H(s)]$

Anti-hermitian generator $\eta(s) = \frac{dU(s)}{ds}U^\dagger(s)$ specifies the transformation

$H \equiv H_D + H_{OD} \Rightarrow \eta(s) \equiv [H_D, H(s)] \Rightarrow \frac{d}{ds}H(s) = 0$ when $[H_D, H(s)] = 0$

Trivial fixed point

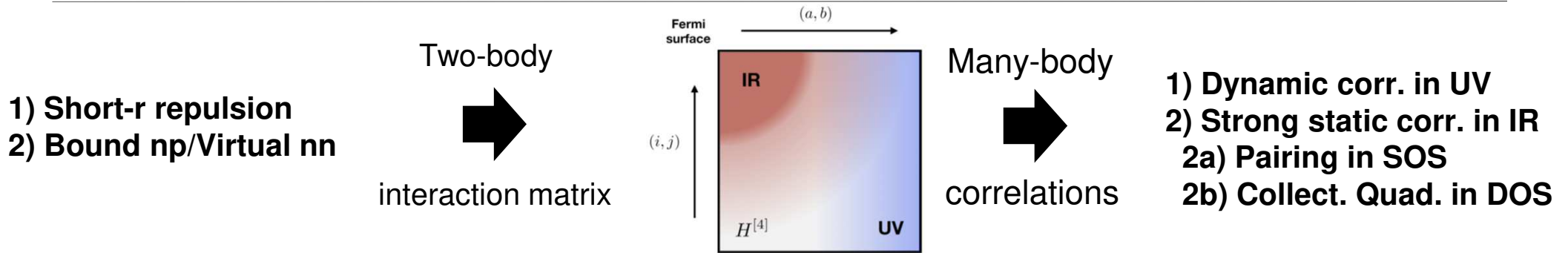
$H(s)$ diagonal

◆ To tame short-range choose $H_D \equiv T$ = diagonal in momentum space basis

◆ Do not go all the way to fixed point because $[\eta(s), H(s)]$ **induces multi-body operators in $H(s)$**

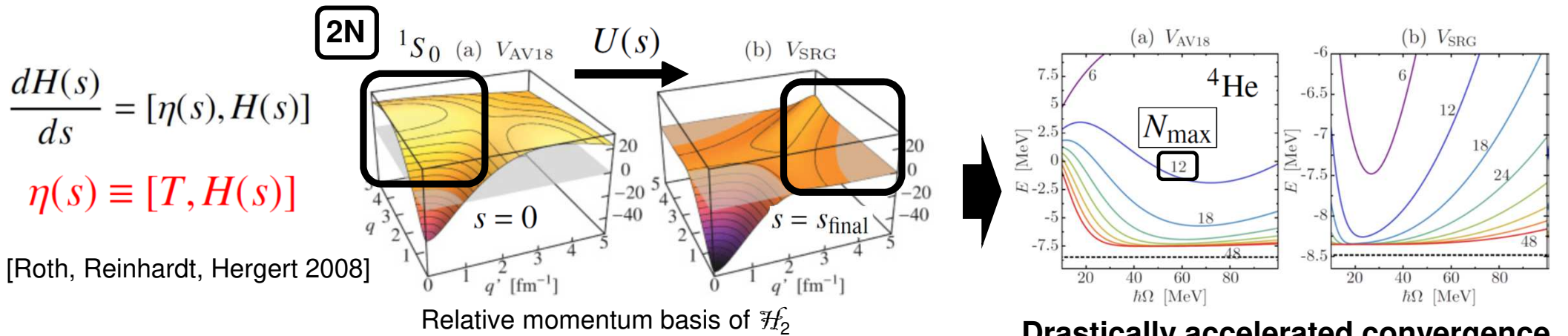
Run until appropriate s_{final} = pre-diagonalization

Pre-processing of short-range correlations



1) Taming down the short-range/coupling to UV in the Hamiltonian

Unitary **Similarity Renormalization Group (SRG)** transformation



Drastically accelerated convergence
More perturbative behavior in the UV

$$V^{2N}(s)(q, q') \approx V^{2N}(0)(q, q') e^{-s(q^2 - q'^2)^2}$$

Low-to-high off-diagonal matrix elements suppressed

⇒ Similar SRG procedure and achievement for 3N in \mathcal{H}_3

Pre-processed nuclear many-body problem

SRG
 $U(s)$ \rightarrow

A-body Schrödinger Equation

$$H_{N^2LO} |\Psi_k^{JMNZ}\rangle = E_k^{JNZ} |\Psi_k^{JMNZ}\rangle$$

Rather strong coupling to UV

Ex: $H_{N^2LO} = T + V_{N^2LO}^{2N} + V_{N^2LO}^{3N} + \emptyset$ **because of the truncation of chiral-EFT expansion of the operator**

Pre-processed nuclear many-body problem

$$\rho_k^{\text{JMNZ}}(\vec{r}_1, \vec{r}_2, \vec{r}_3, \vec{r}_4) \equiv \langle \Psi_k^{\text{JMNZ}} | c^\dagger(\vec{r}_1) c^\dagger(\vec{r}_2) c(\vec{r}_3) c(\vec{r}_4) | \Psi_k^{\text{JMNZ}} \rangle \quad \text{Two-body density matrix}$$

$$= \langle \Psi_k^{\text{JMNZ}}(s) | U(s) c^\dagger(\vec{r}_1) c^\dagger(\vec{r}_2) c(\vec{r}_3) c(\vec{r}_4) U^\dagger(s) | \Psi_k^{\text{JMNZ}}(s) \rangle$$

$$\neq \langle \Psi_k^{\text{JMNZ}}(s) | c^\dagger(\vec{r}_1) c^\dagger(\vec{r}_2) c(\vec{r}_3) c(\vec{r}_4) | \Psi_k^{\text{JMNZ}}(s) \rangle$$

Sum of up to A-body operator/density matrices

► discussion AV18 vs χ EFT on tuesday

given that $|\Psi_k^{\text{JMNZ}}(s)\rangle \equiv U(s) |\Psi_k^{\text{JMNZ}}\rangle$

A-body Schrödinger Equation

$$H_{\text{N}^2\text{LO}}(s) |\Psi_k^{\text{JMNZ}}(s)\rangle = E_k^{\text{JNZ}} |\Psi_k^{\text{JMNZ}}(s)\rangle$$

« Soft » Hamiltonian

=

reduced coupling to UV

A-body observables independent of s

Ex: $H_{\text{N}^2\text{LO}}(s) = T + V_{\text{N}^2\text{LO}}^{2\text{N}}(s) + V_{\text{N}^2\text{LO}}^{3\text{N}}(s) + \dots$ to be tractable $\Rightarrow \frac{d}{ds} E_k^{\text{JNZ}} \neq 0$ violate unitarity

Induced k-body forces ($k \leq A$)



Choose truncation & s

$$\frac{d}{ds} E_k^{\text{JNZ}} \sim 0$$

SRG transformation is a compromised between

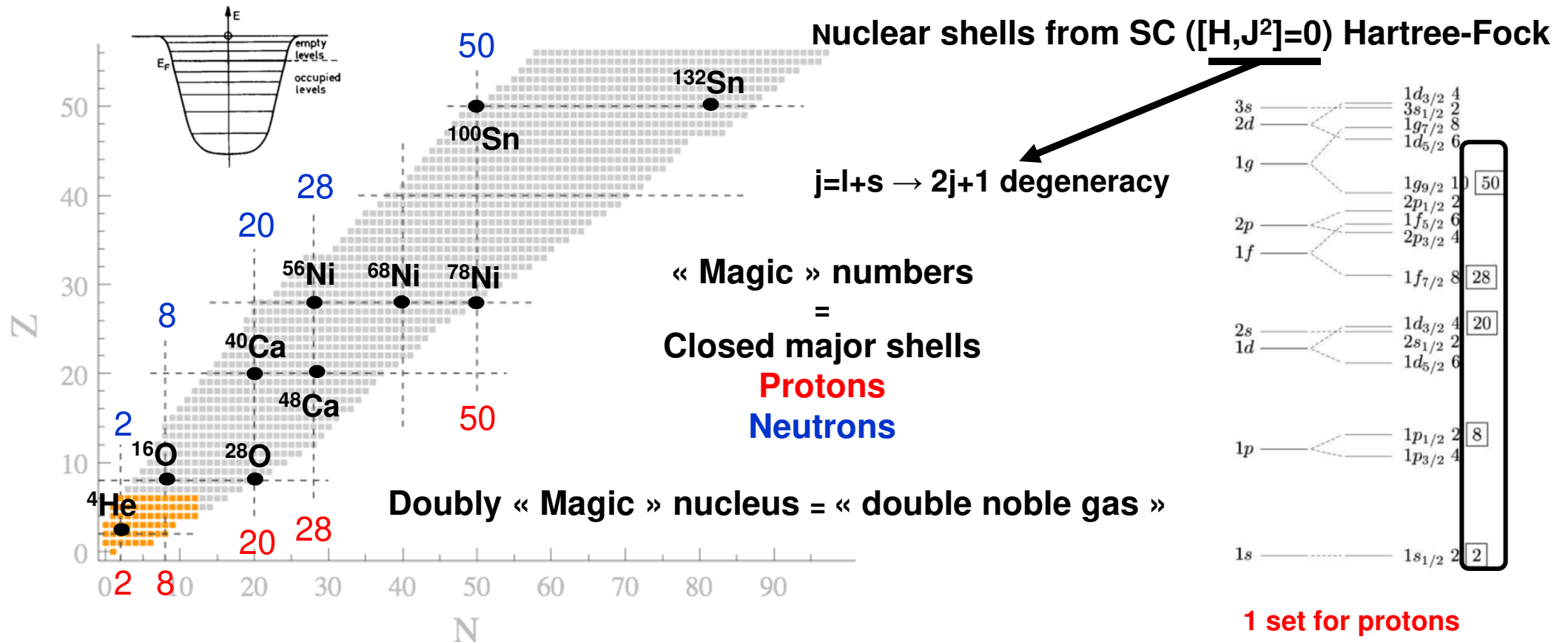
⇒ Reduction of coupling to UV

⇒ Size of induced k-body interactions that cannot be handled

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Categories of nuclei vs correlations vs expansion method



1 set for protons
 1 set for neutrons

Counting even-even nuclei belonging to each category

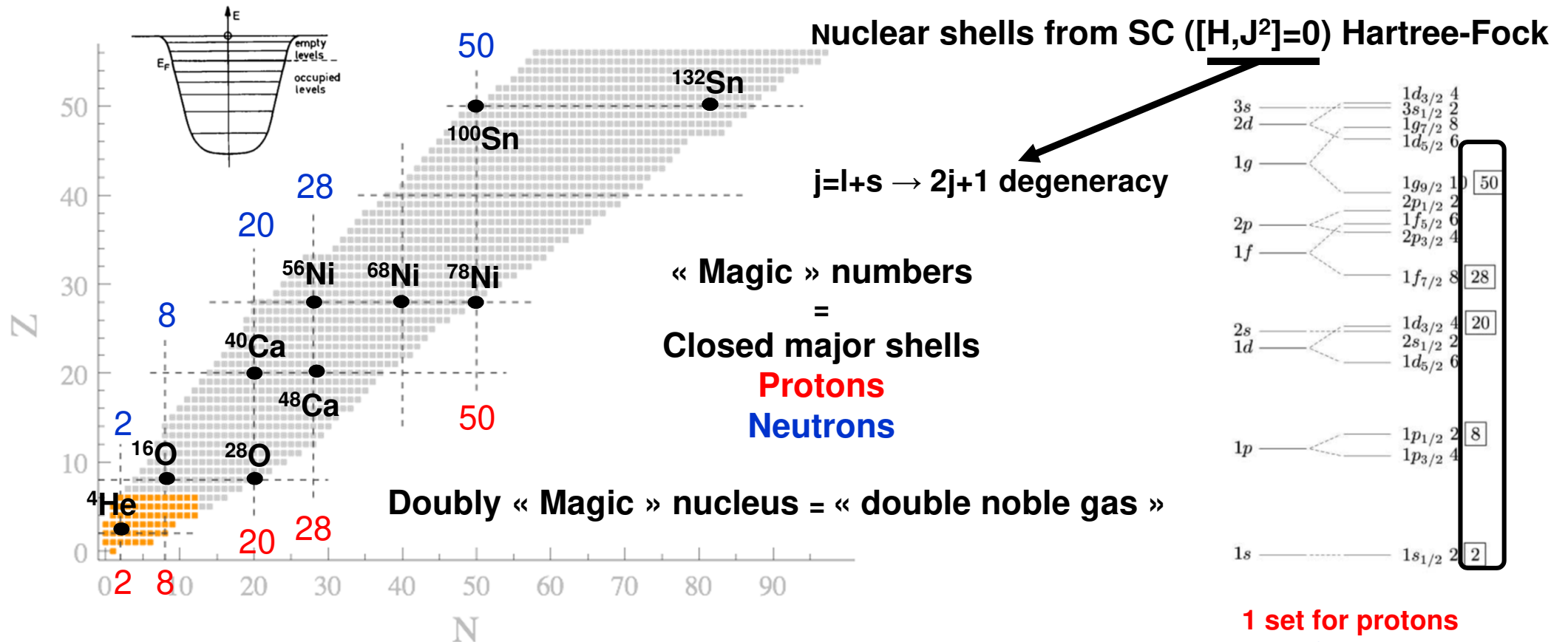
Even-even nuclei	Number estimated	Percentage estimated
Total	2075	100%
Doubly closed-shell	16	0.8%
Singly open-shell	246	11.9%
Doubly open-shell	1813	87.3%

99.2%

» correlations

Table: Based on nuclear shells from a Hartree-Fock calculation of ^{16}O . Courtesy of B. Bally.

Categories of nuclei vs correlations vs expansion method



1 set for protons
 1 set for neutrons

More pertinent categorization

Even-even nuclei	Number estimated	Percentage estimated
Total	2075	100%
Doubly closed-(sub)shell	181	8.7%
Singly open-(sub)shell	838	40.4%
Doubly open-(sub)shell	1056	50.9%

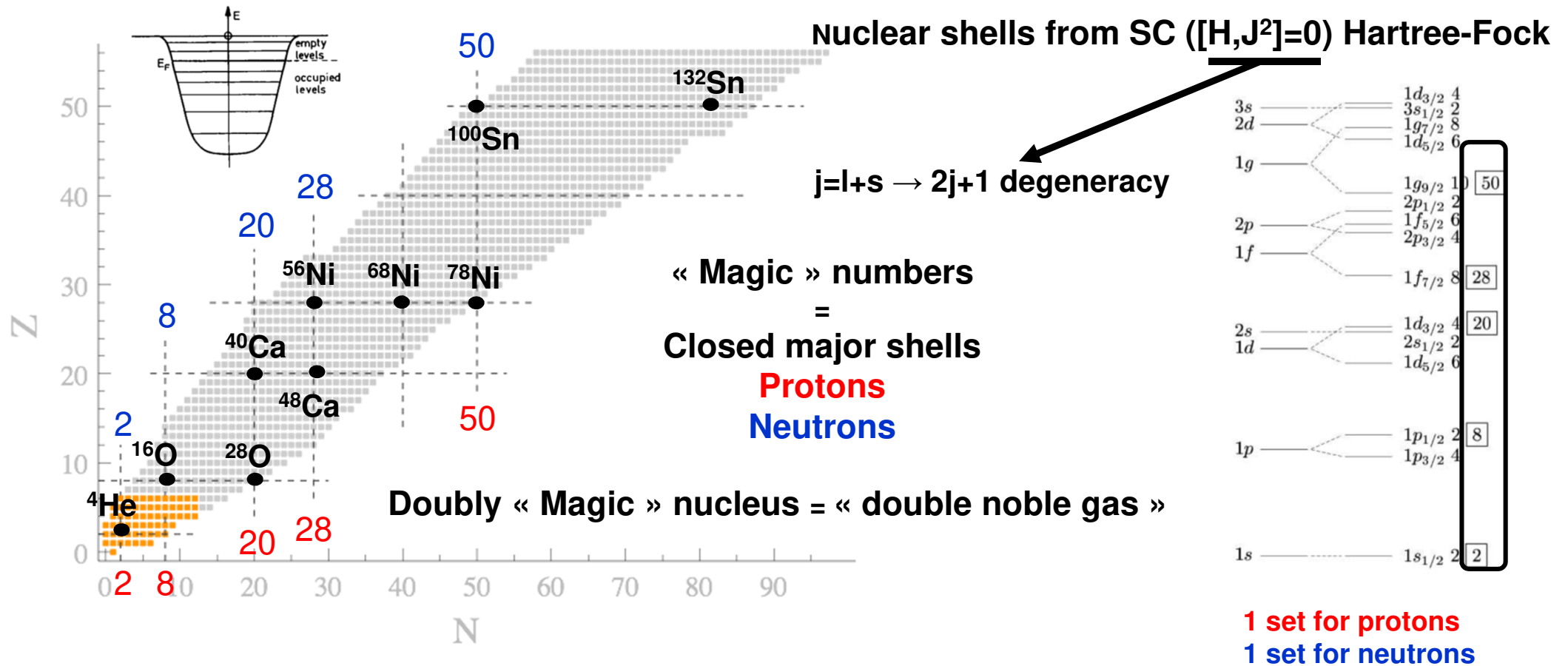
91.3%

Nuclei	Number
Odd-even	4050
odd-odd	2014

Via particle-attached methods

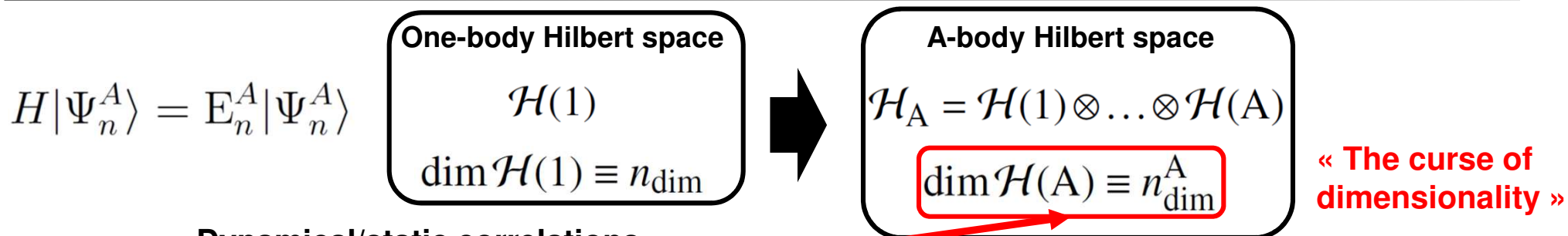
Table: Based on nuclear shells from a Hartree-Fock calculation of ^{16}O . Courtesy of B. Bally.

Categories of nuclei vs correlations vs expansion method



Any « universal » (expansion) method must deal with static and dynamical correlations
Consistently (no double counting)
Efficiently (at reasonable polynomial cost)

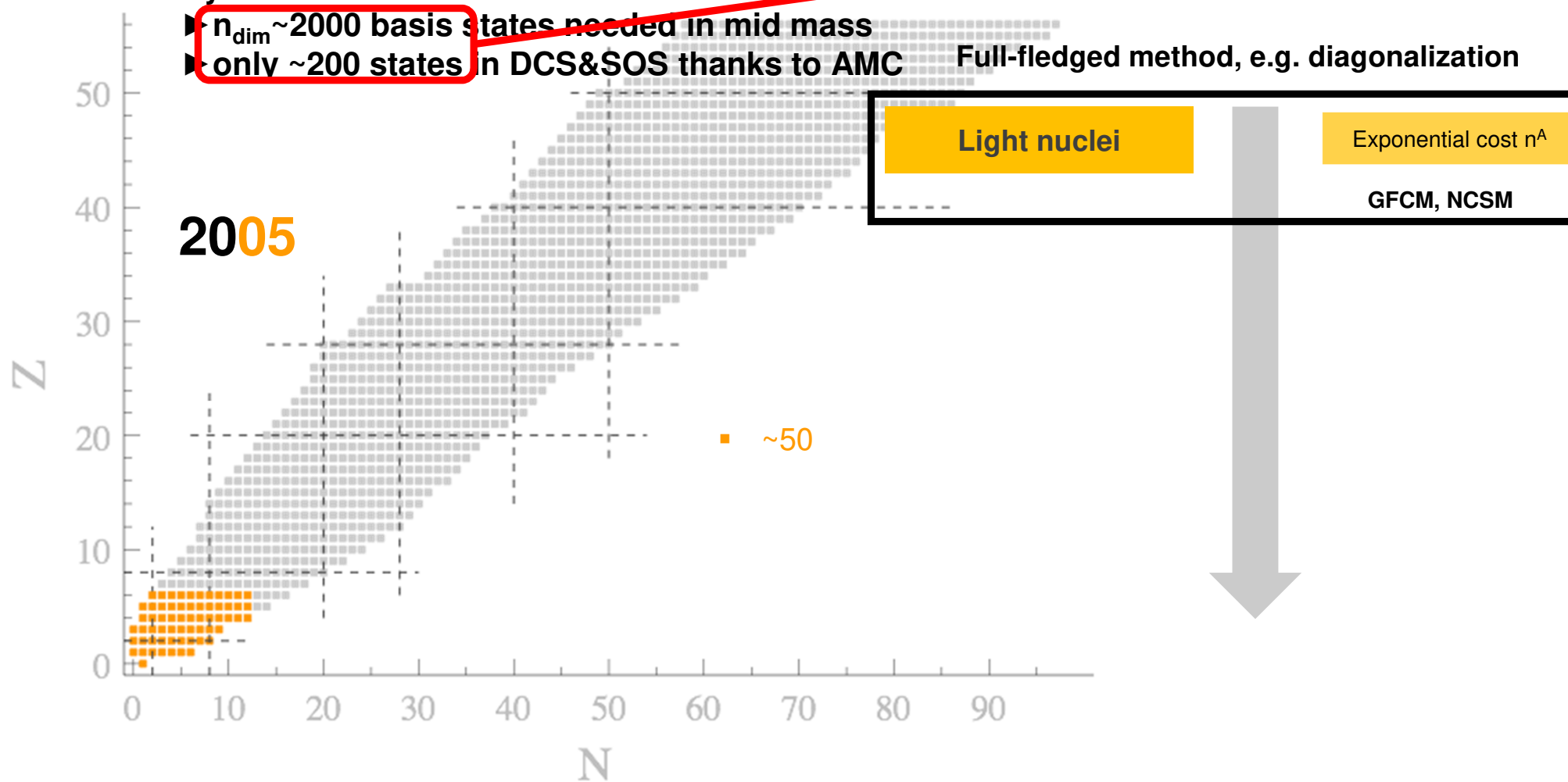
Evolution of ab initio nuclear chart vs type of method



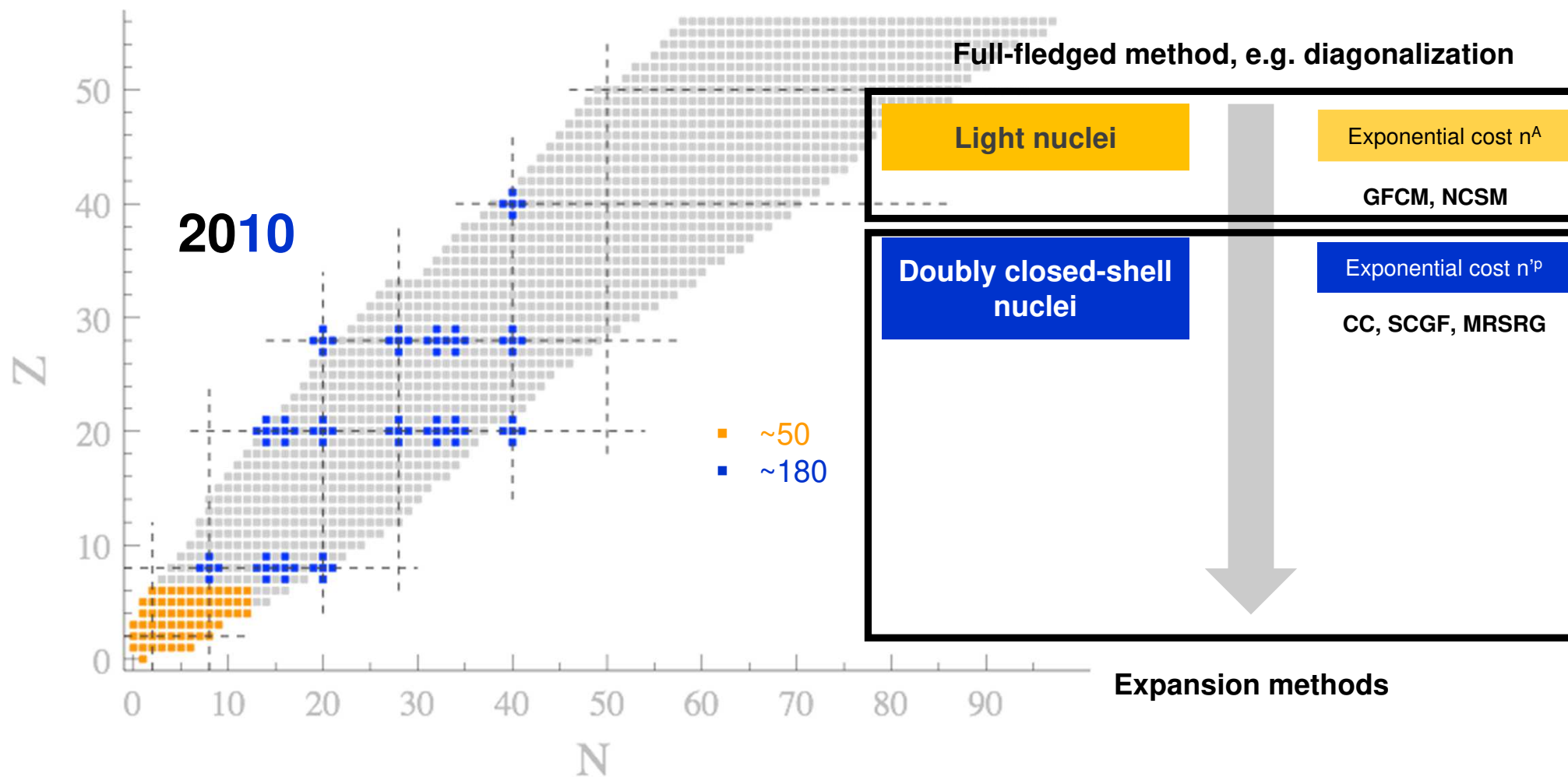
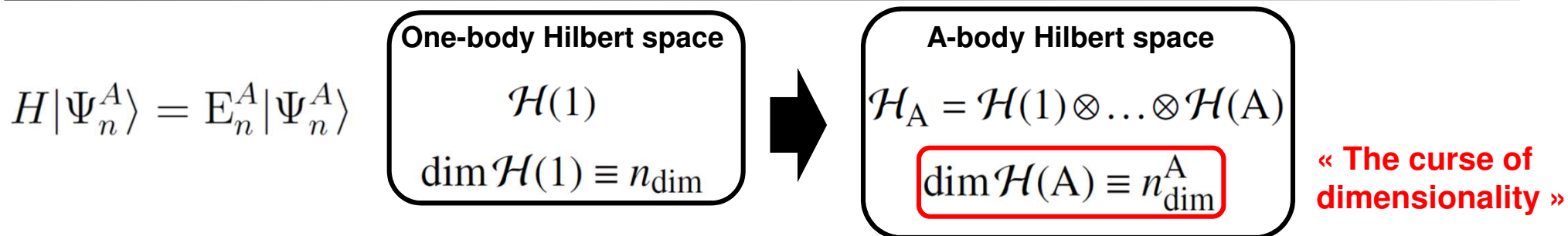
Dynamical/static correlations

- ▶ $n_{\text{dim}} \sim 2000$ basis states needed in mid mass
- ▶ ~ 200 states in DCS&SOS thanks to AMC

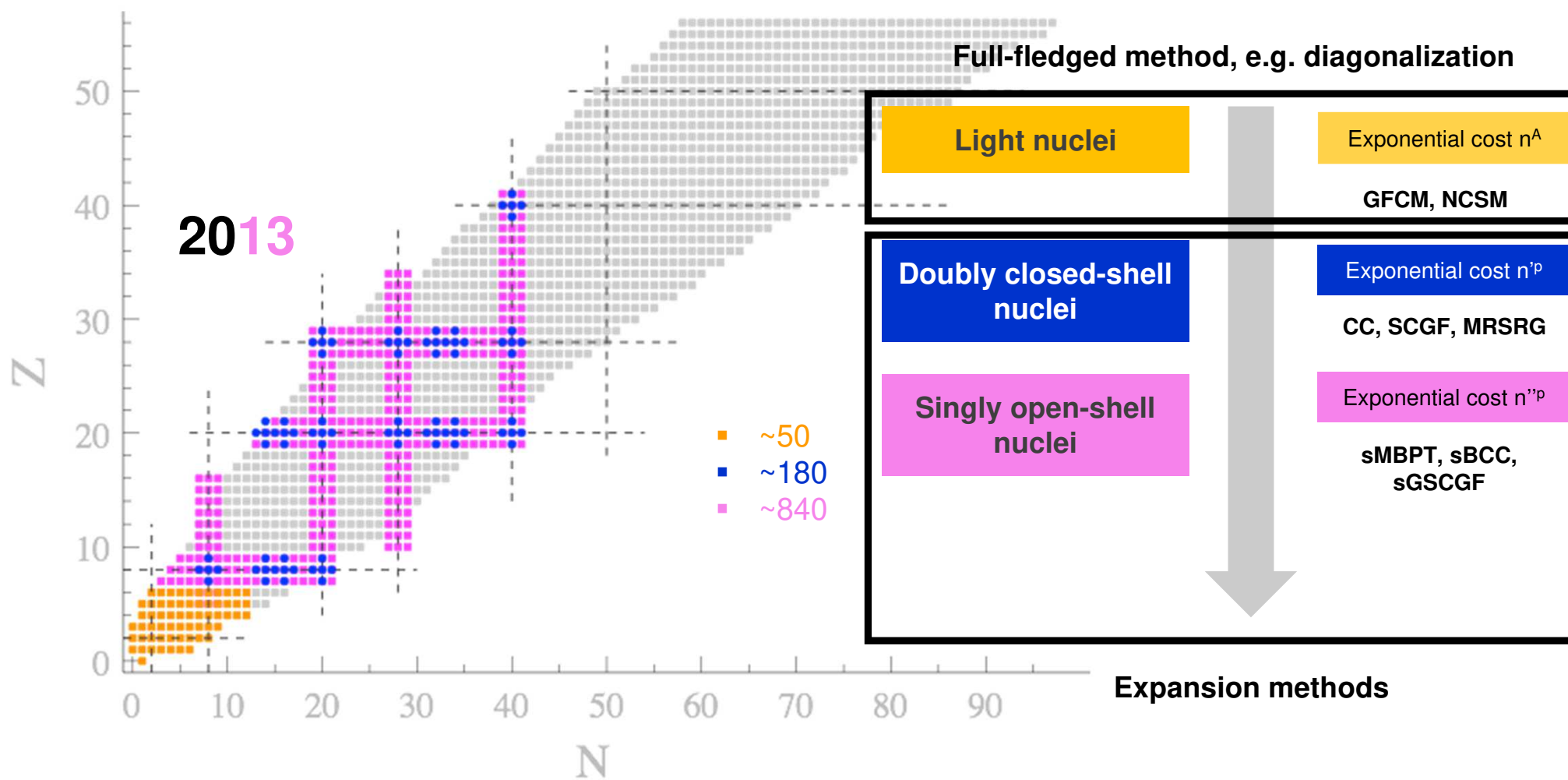
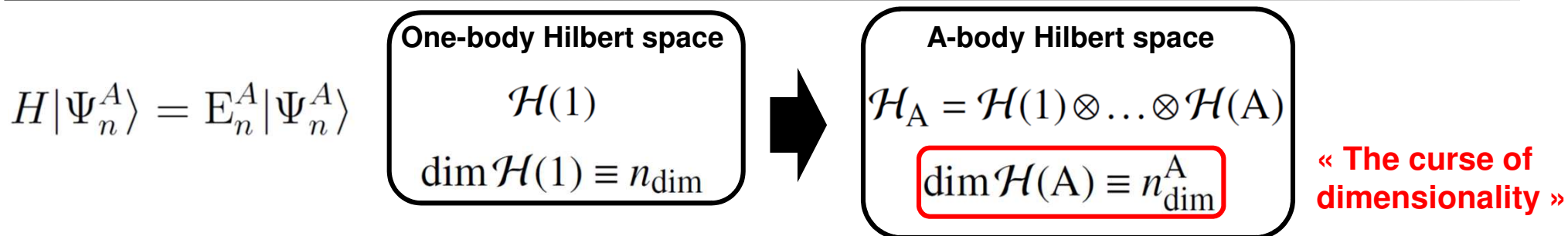
Full-fledged method, e.g. diagonalization



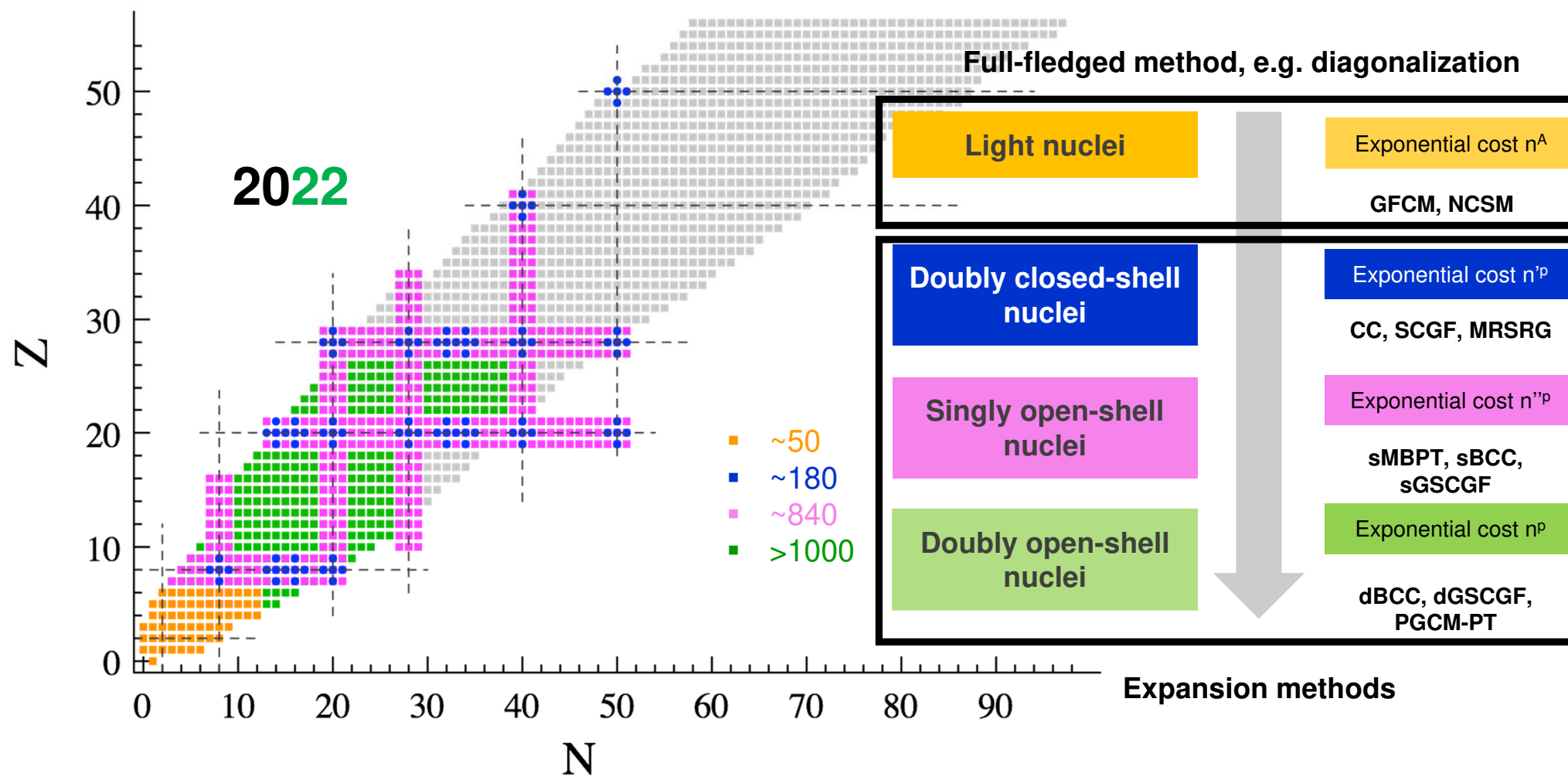
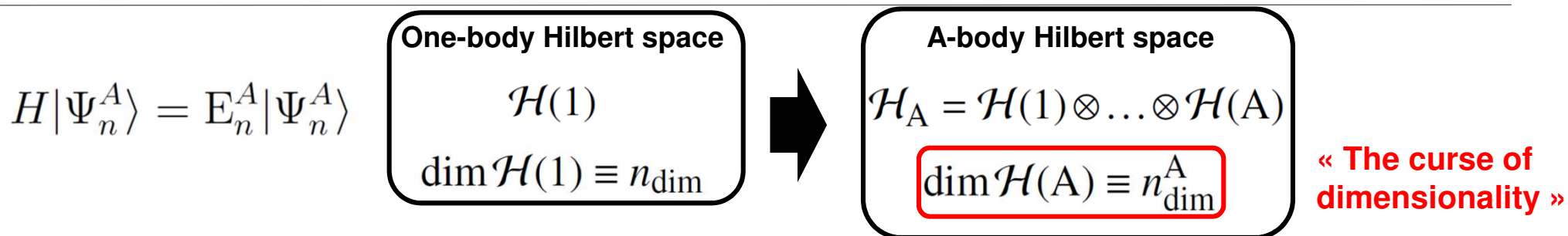
Evolution of ab initio nuclear chart vs type of method



Evolution of ab initio nuclear chart vs type of method



Evolution of ab initio nuclear chart vs type of method



Expansion many-body methods: general rationale

$$H$$

$$[H, R(\theta)] = 0$$

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

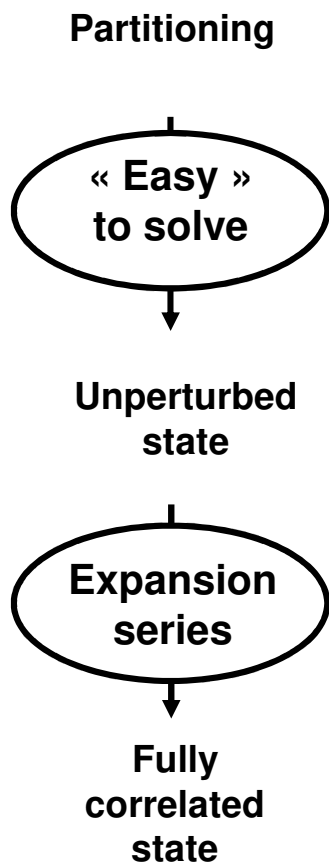
Hamiltonian **Good neutron/proton number N/Z**
 Symmetries (U(1), SU(2)...) **Good angular momentum (J², J_z)**
 Secular equation

Solution to static correlations lies here

$$H = H_0 + H_1$$

$$H_0|\Theta^{(0)}\rangle = E^{(0)}|\Theta^{(0)}\rangle$$

$$|\Psi\rangle = \Omega|\Theta^{(0)}\rangle$$



Key questions

- Unperturbed state
 - what nature for which systems?
 - what about symmetries?
 - how « simple »/low-cost can it remain?
- Nature of the expansion
 - perturbative? non-perturbative?
 - formulation depends on unperturbed state?**

Impacts algebraic&numerical complexity there

Closed-shell systems

$$H$$

$$[H, R(\theta)] = 0$$

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

$H = H_0 + H_1$

No correlations

Dynamical correlations

$H_0|\Theta^{(0)}\rangle = E^{(0)}|\Theta^{(0)}\rangle$

$|\Psi\rangle = \Omega|\Theta^{(0)}\rangle$

Closed-shell

$$[H_0, R(\theta)] = 0$$

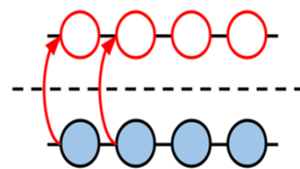
Spherical Hartree Fock

$$|\Theta^{(0)}\rangle \equiv |\Phi\rangle \text{ (sHF)}$$

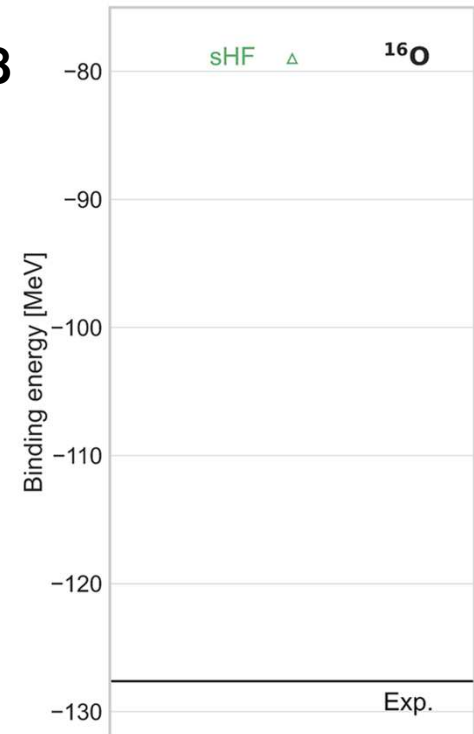
Controlled np-nh expansion

sMBPT, sCC, sDSCGF...

- 1) Partition
- 2) Expand



Z=8, N=8



$$|\Phi_{h_1 \dots}^{p_1 \dots}\rangle$$

$$|\Phi\rangle$$

$$\delta E_{h_1 \dots}^{p_1 \dots} > 0$$



Slater determinant reference state and normal ordering

Slater determinant unperturbed state

$$b_\alpha \equiv \sum_l U_{l\alpha}^* c_l \quad |\Phi^A\rangle \equiv \prod_{i=1}^A b_i^\dagger |0\rangle$$

Particle states a,b,c...
Hole states i,j,k...

Ritz variational principle

$$\delta \frac{\langle \Phi^A | H | \Phi^A \rangle}{\langle \Phi^A | \Phi^A \rangle} = 0$$

HF one-body eigenvalue problem

Normal ordering via Wick's theorem with respect to $|\Phi^A\rangle$

$$H \equiv \Lambda^{00}$$

$$+ \frac{1}{1!1!} \sum_{l_1 l_2} \Lambda_{l_1 l_2}^{11} : b_{l_1}^\dagger b_{l_2} :$$

$$+ \frac{1}{2!2!} \sum_{l_1 l_2 l_3 l_4} \Lambda_{l_1 l_2 l_3 l_4}^{22} : b_{l_1}^\dagger b_{l_2}^\dagger b_{l_4} b_{l_3} :$$

$$+ \frac{1}{3!3!} \sum_{l_1 l_2 l_3 l_4 l_5 l_6} \Lambda_{l_1 l_2 l_3 l_4 l_5 l_6}^{33} : b_{l_1}^\dagger b_{l_2}^\dagger b_{l_3}^\dagger b_{l_6} b_{l_5} b_{l_4} :$$

Anti-symmetric fields Λ^{ij} function of

$$t_{pq} \quad \bar{v}_{pqrs} \quad \bar{w}_{pqrst} \quad U_{pk}$$

➔ **Six-index tensor**

Too expensive to handle

➔ **NO2B approximation**

1-3% error in closed shell

[R. Roth *et al.*, PRL 109 (2012) 052501]

➔ **Effective 2-body operators**

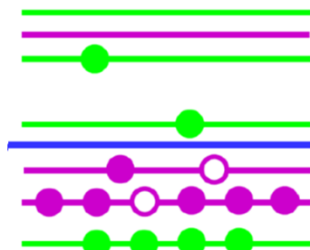
Captures essential of 3-body

Many-body method with 2-body

Spherical coupled cluster expansion method

Slater determinant reference state

$$|\Phi^A\rangle \equiv \prod_{i=1}^A b_i^\dagger |0\rangle$$



Individual excitations

$$|\Phi^\mu\rangle \equiv |\Phi_{ij\dots}^{ab\dots}\rangle \equiv b_a^\dagger b_{a_n}^\dagger \dots b_j b_i |\Phi^A\rangle$$

np-nh excitations of the vacuum
Orthonormal basis of \mathcal{H}_A

CC ansatz

CC wave operator Ω

$$|\Psi_0^A\rangle \equiv e^{T^A} |\Phi^A\rangle$$

$$\text{with } \begin{cases} T^A \equiv \sum_{n=1}^A T_n^A \\ T_n^A \equiv \frac{1}{(n!)^2} \sum_{ijk\dots abc\dots} T_{ijk\dots}^{abc\dots} b_a^\dagger b_b^\dagger b_c^\dagger \dots b_k b_j b_i \end{cases}$$

Cluster amplitudes
Unknowns of the problem

$T_1^A |\Phi\rangle \rightarrow |\Phi_i^a\rangle$ $T_2^A |\Phi\rangle \rightarrow |\Phi_{ij}^{ab}\rangle$

n-tuple connected cluster operator

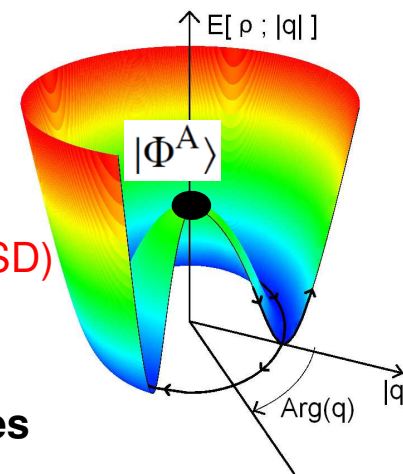
Energy and amplitude equations

$$H|\Psi_0^A\rangle = E_0^A |\Psi_0^A\rangle \Rightarrow E_0^A = \langle \Phi^A | H e^{T^A} | \Phi^A \rangle_C$$

$$0 = \langle \Phi^\mu | H e^{T^A} | \Phi^A \rangle_C$$

Pure excitation operators

Truncate, e.g. $T^A = T_1^A + T_2^A$ (CCSD)
Solve for $n=1,2$



Connected = terminating exponential

Algebraic expression through Wick's theorem/diagrammatic rules

Ex: for the energy

$$E_0^A = \Lambda^{00} + \sum_{ia} \Lambda_{ia}^{11} T_i^a + \frac{1}{2} \sum_{ijab} \Lambda_{ijab}^{22} T_i^a T_j^b + \frac{1}{4} \sum_{ijab} \Lambda_{ijab}^{22} T_{ij}^{ab}$$

Unperturbed

Dynamical correlations

Open-shell systems - 1

$$H$$

$$[H, R(\theta)] = 0$$

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

What to do?

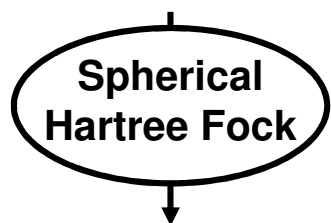
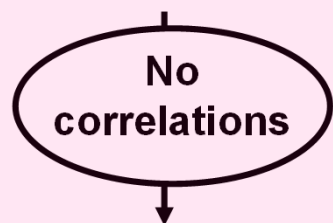
- can one keep the simplicity of a single-reference method?
- if so, is there a price to play?

Open-shell

$$[H_0, R(\theta)] = 0$$

Symmetry-conserving single-reference expansion
 ▶ state misses crucial IR static correlations

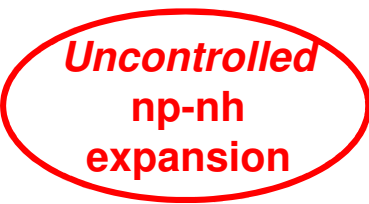
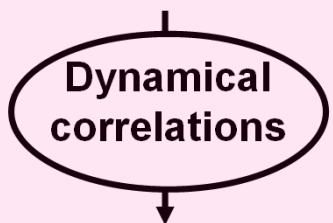
$$H = H_0 + H_1$$



$$H_0|\Theta^{(0)}\rangle = E^{(0)}|\Theta^{(0)}\rangle$$

$$|\Theta^{(0)}\rangle \equiv |\Phi\rangle \text{ (sHF)}$$

$$\begin{array}{c} \text{---} \\ \text{---} \\ \text{---} \end{array} |\Phi_{h_1 \dots}^{p_1 \dots}\rangle$$



$$\begin{array}{c} \text{---} \\ \text{---} \\ \text{---} \end{array} |\Phi\rangle$$

$$\delta E_{h_1 \dots}^{p_1 \dots} \sim 0$$

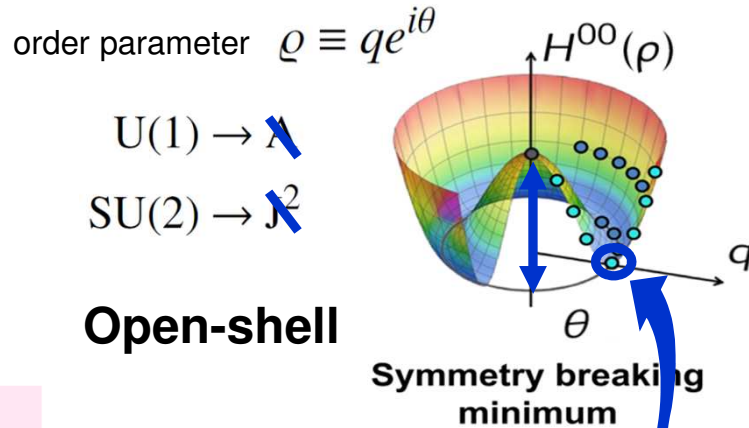
Degenerate unperturbed Slater determinant

$$|\Psi\rangle = \Omega|\Theta^{(0)}\rangle$$

$$\text{Ex: } \Delta E_{\text{MBPT}}^{(2)} = -\frac{1}{4} \sum_{ijab} \frac{|h_{ijab}^{(2)}|^2}{e_a + e_b - e_i - e_j} = 0$$

Open-shell systems - 2

H
 $[H, R(\theta)] = 0$
 $H|\Psi\rangle = E|\Psi\rangle$



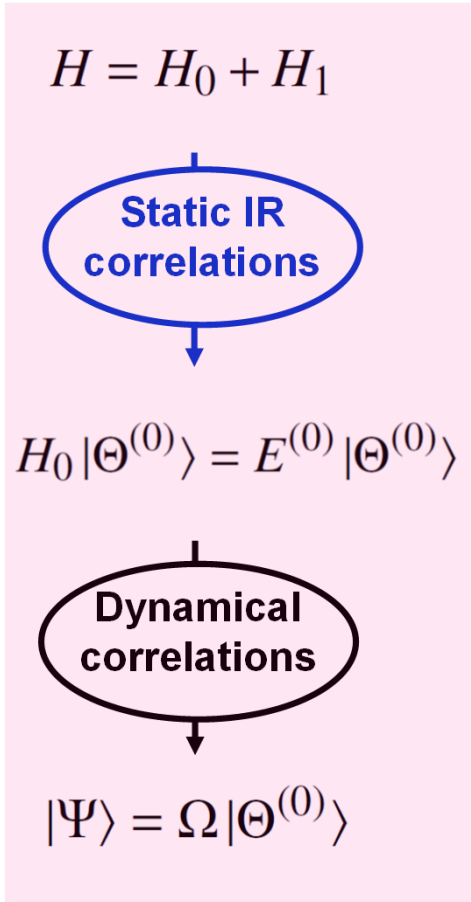
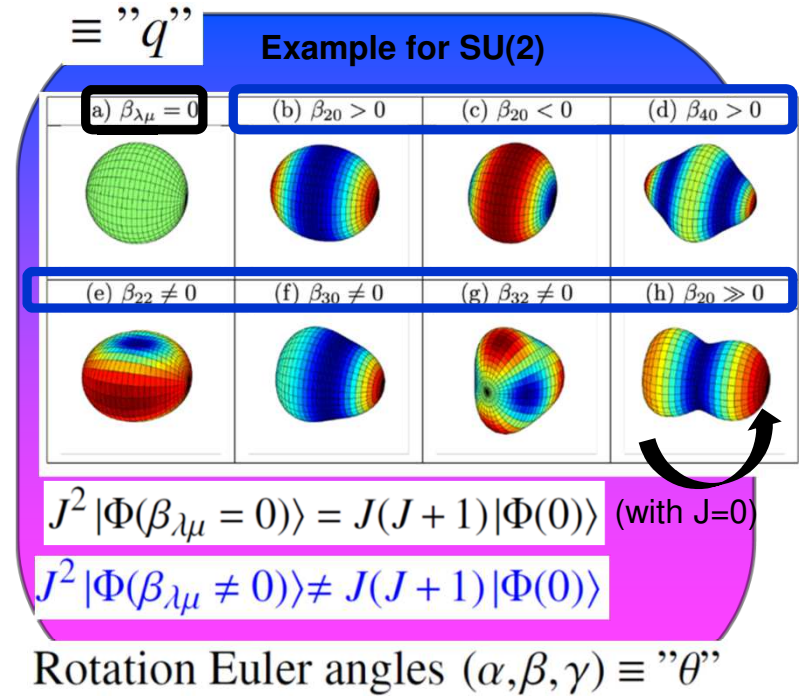
Open-shell

$[H_0, R(\theta)] \neq 0$

Deformed Hartree Fock Bogoliubov

$|\Theta^{(0)}\rangle \equiv |\Phi(q)\rangle$ (dHFB)

$q \neq 0$



Bogoliubov transformation **Bogoliubov Vacuum**

$\beta_k(q) \equiv \sum_l U_{lk}^*(q) c_l + V_k^{*l}(q) c_l^\dagger$
 $\beta_k^\dagger(q) \equiv \sum_l U^{lk}(q) c_l^\dagger + V_l^k(q) c_l$

$|\Phi(q)\rangle, / \beta_k(q) |\Phi(q)\rangle = 0 \quad \forall q$
 Product state as Slater determinant

Symmetry breaking

$A|\Phi(q)\rangle \neq A|\Phi(q)\rangle$
 $J^2 |\Phi(q)\rangle \neq J(J+1) |\Phi(q)\rangle$

Elementary excitations

$\beta_{k_1}^\dagger(q) \cdots \beta_{k_n}^\dagger(q) |\Phi(q)\rangle = |\Phi^{k_1 \cdots k_n}(q)\rangle$ Generalize np-nh:excitations

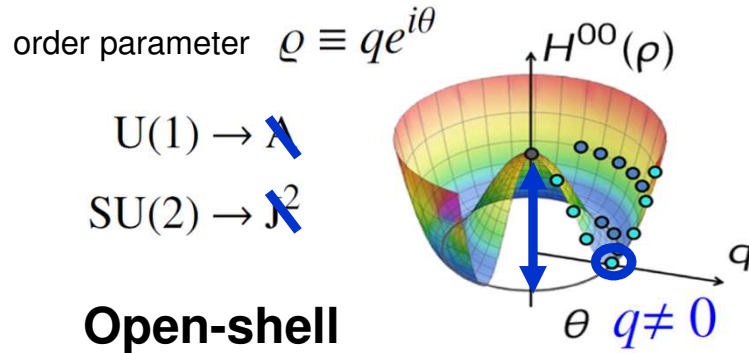
Sum over different j

Open-shell systems - 2

$$H$$

$$[H, R(\theta)] = 0$$

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



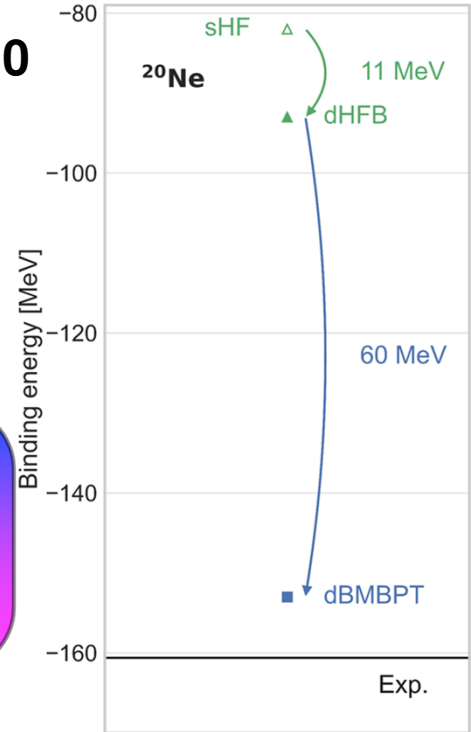
$Z=10, N=10$

Open-shell

Symmetry breaking minimum

$$[H_0, R(\theta)] \neq 0$$

Deformed Hartree Fock Bogoliubov



$$H = H_0 + H_1$$

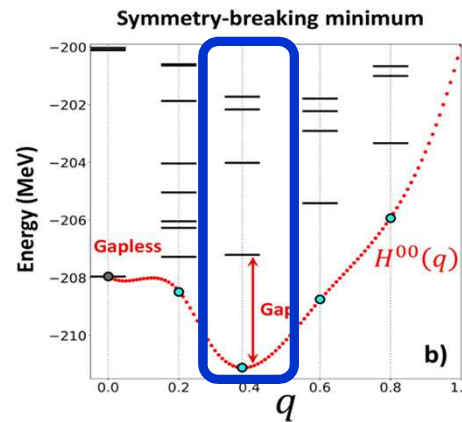
Static IR correlations

$$H_0|\Theta^{(0)}\rangle = E^{(0)}|\Theta^{(0)}\rangle \quad |\Theta^{(0)}\rangle \equiv |\Phi(q)\rangle \text{ (dHFB)}$$

Dynamical correlations

$$|\Psi\rangle = \Omega|\Theta^{(0)}\rangle$$

Controlled qp expansion



Non-degenerate unperturbed Bogoliubov state

dMBPT, dBCC, dGSCGF...

1) Break - partition

2) Expand

$$\frac{1}{4!} \sum_{k_1 k_2 k_3 k_4} \frac{|\Omega_{k_1 k_2 k_3 k_4}^{40}|^2}{E_{k_1} + E_{k_2} + E_{k_3} + E_{k_4}} > 0$$

Bogoliubov reference state and normal ordering

Bogoliubov reference state

$$\beta_k = \sum_p U_{pk}^* c_p + V_{pk}^* c_p^\dagger$$

$$\beta_k^\dagger = \sum_p U_{pk} c_p^\dagger + V_{pk} c_p$$

$$|\Phi\rangle \equiv C \prod_k \beta_k |0\rangle$$

$$\Omega \equiv H - \lambda A$$

$q_{U(1)} \neq 0$ a priori and reduce to SD otherwise

$q_{SU(2)}$ omitted everywhere for simplicity

Ritz variational principle

$$\delta \frac{\langle \Phi | \Omega | \Phi \rangle}{\langle \Phi | \Phi \rangle} = 0$$

HFB eigenvalue problem

Normal ordering via Wick's theorem with respect to $|\Phi\rangle$ in quasi-particle basis

$$H \equiv \sum_{n=0}^3 \sum_{i+j=2n} \frac{1}{i!j!} \sum_{l_1 \dots l_{i+j}} H_{l_1 \dots l_{i+j}}^{ij} \beta_{k_1}^\dagger \dots \beta_{k_i}^\dagger \beta_{k_{i+j}} \dots \beta_{k_{i+1}}$$

H^{ij} matrix elements function of
 $t_{pq} \bar{v}_{pqrs} \bar{w}_{pqrst} U_{pk} V_{pk}$

$$\equiv H^{00} + [H^{20} + H^{11} + H^{02}] + [H^{40} + H^{31} + H^{22} + H^{13} + H^{04}] + \sum_{i+j=6} H^{ij}$$

$$\equiv \sum_{n=0}^2 H^{[2n]} + H^{[6]} \quad \text{6-qp operators}$$

Similarly for A and $\Omega = H - \lambda A$

➔ **Six-index tensors**
Too expensive to handle

➔ **NO2B approximation**
Simply remove $H^{[6]}$?

PNO2B approximation
[Ripoche, Tichai, Duguet, EPJA 2020]
SC rank-reduction
[Frosini et al. EPJA 2021]

Deformed Bogoliubov coupled cluster expansion method

Bogoliubov reference state

$$|\Phi\rangle \equiv C \prod_k \beta_k |0\rangle$$

Quasi-particle excitations

$$|\Phi^\mu\rangle \equiv |\Phi^{k_1 \dots k_{2n}}\rangle \equiv \beta_{k_1}^\dagger \dots \beta_{k_{2n}}^\dagger |\Phi\rangle$$

Orthonormal basis of Fock space

Bogoliubov CC ansatz

$$|\Psi_0^A\rangle \equiv e^T |\Phi\rangle \quad \text{with} \quad \begin{cases} T = \sum_{n=1} T_n \\ T_n \equiv \frac{1}{(2n)!} \sum_{k_1 \dots k_{2n}} T_{k_1 \dots k_{2n}}^{2n0} \beta_{k_1}^\dagger \dots \beta_{k_{2n}}^\dagger \end{cases}$$

as soon as T is truncated
 ↪ symmetry contamination
 ↪ but « simple » theory with n^p cost

Reduces to nph excit. in closed-shell
 Cluster a $T_1|\Phi\rangle \rightarrow |\Phi^{k_1 k_2}\rangle T_2|\Phi\rangle \rightarrow |\Phi^{k_1 k_2 k_3 k_4}\rangle$
 Unknowns of the problem

n-tuple connected cluster operator

Energy and amplitude equations

$$H|\Psi_0^A\rangle = E_0^A |\Psi_0^A\rangle$$

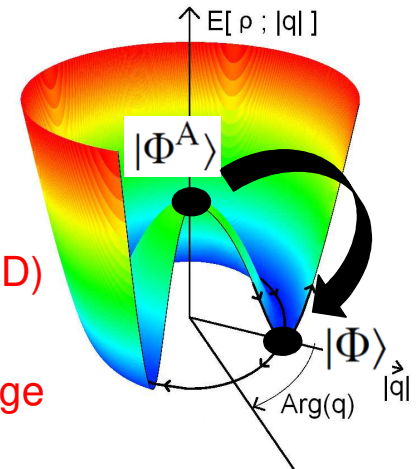
$$A|\Psi_0^A\rangle = A|\Psi_0^A\rangle$$

$$\begin{cases} \langle \Phi | \cdot | \Phi \rangle : E_0^A = \langle \Phi | H e^T | \Phi \rangle_C \\ \langle \Phi^\mu | \cdot | \Phi \rangle : 0 = \langle \Phi^\mu | H e^T | \Phi \rangle_C \\ \langle \Phi | \cdot | \Phi \rangle : \Lambda = \langle \Phi | A e^T | \Phi \rangle_C \end{cases}$$

Pure excitation operators

Truncate, e.g. $T = T_1 + T_2$ (BCCSD)
 Solve for $n=1,2$

Constrained to be true in average



Connected = terminating exponential

Algebraic expression through Wick's theorem/diagrammatic rules

$$E_0^A = H^{00} - \frac{1}{2} \sum_{k_1 k_2} H_{k_1 k_2}^{02} T_{k_1 k_2}^{20} + \frac{1}{8} \sum_{k_1 k_2 k_3 k_4} H_{k_1 k_2 k_3 k_4}^{04} T_{k_1 k_2}^{20} T_{k_3 k_4}^{20} + \frac{1}{4!} \sum_{k_1 k_2 k_3 k_4} H_{k_1 k_2 k_3 k_4}^{04} T_{k_1 k_2 k_3 k_4}^{40}$$

Unperturbed

Open-shell systems - 2

$$H$$

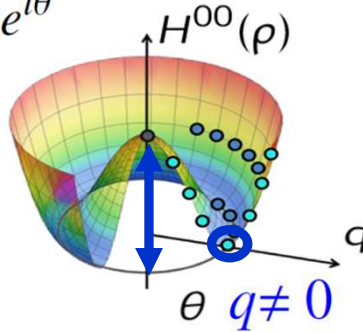
$$[H, R(\theta)] = 0$$

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

order parameter $\varrho \equiv qe^{i\theta}$

$$U(1) \rightarrow \mathbb{R}$$

$$SU(2) \rightarrow \mathbb{R}^2$$

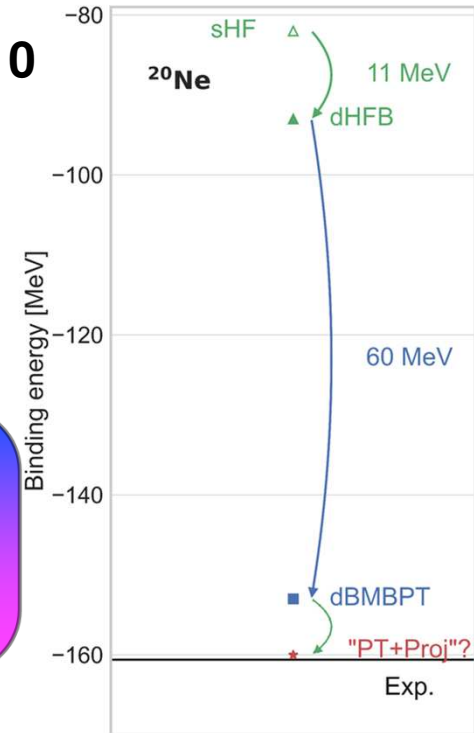


$Z=10, N=10$

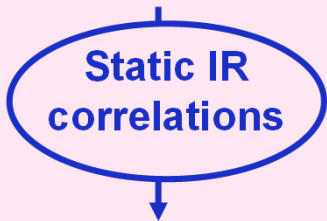
Open-shell

Symmetry breaking minimum

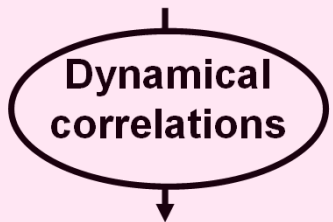
$$[H_0, R(\theta)] \neq 0$$



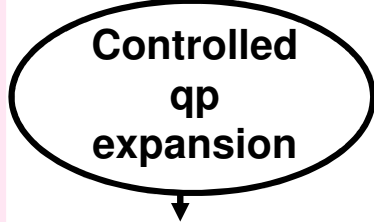
$$H = H_0 + H_1$$



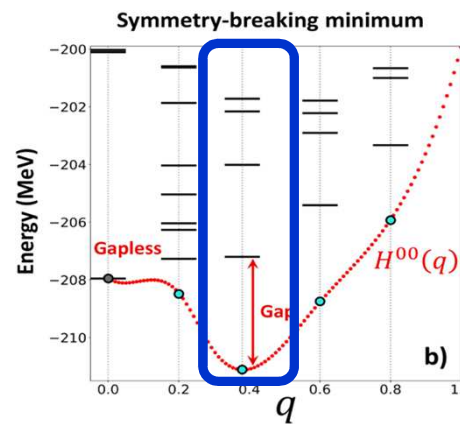
$$H_0|\Theta^{(0)}\rangle = E^{(0)}|\Theta^{(0)}\rangle \quad |\Theta^{(0)}\rangle \equiv |\Phi(q)\rangle \text{ (dHFB)}$$



$$|\Psi\rangle = \Omega|\Theta^{(0)}\rangle$$



dBMBPT, dBCC, dGSCGF...



Non-degenerate unperturbed Bogoliubov state

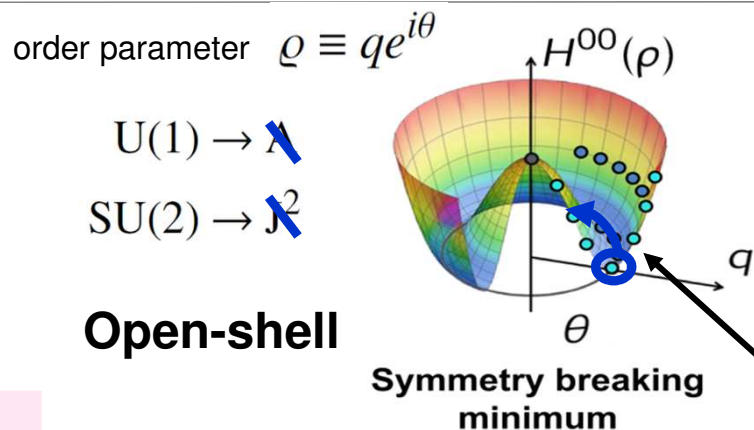
- 1) Break - partition
- 2) Expand

Open-shell systems - 3

$$H$$

$$[H, R(\theta)] = 0$$

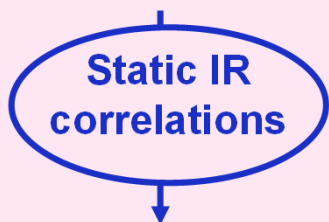
$$H|\Psi\rangle = E|\Psi\rangle$$



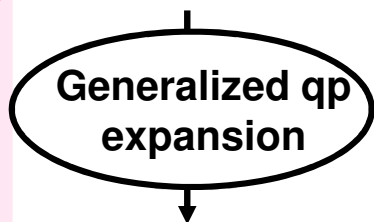
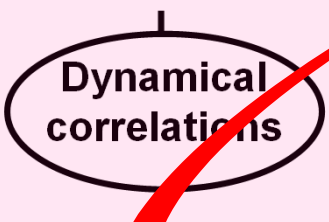
Open-shell

$$[H_0, R(\theta)] \neq 0$$

$$H = H_0 + H_1$$



$$H_0|\Theta^{(0)}\rangle = E^{(0)}|\Theta^{(0)}\rangle \quad |\Theta^{(0)}\rangle \equiv |\Phi(q)\rangle \text{ (dHFB)}$$



$$|\Psi\rangle = \Omega|\Theta^{(0)}\rangle$$

PBMBPT, PBCC

- 1) Break - partition
- 2) Expand - **Project**

Insert into expanded energy:

- ▶ keep same partitioning and expansion of Ω
- ▶ P superfluous/impactful if Ω exact/truncated

Further capture static correlations

Successful novel approach
Natural access to rotational excitations

Particle-number projected BCC formalism

Projection operator on good A

$$P^A \equiv \frac{1}{2\pi} \int_0^{2\pi} d\varphi e^{-iA\varphi} R(\varphi) \equiv e^{iA\varphi}$$

Rotation is gauge space

Projected BCC ansatz

$$|\Psi_{\text{PBCC}}^A\rangle \equiv P^A |\Psi_{\text{BCC}}^A\rangle \quad \text{Always true!}$$

Rotated state

$$\langle \Phi(\varphi) | = \langle \Phi | R(\varphi) = \langle \Phi(\varphi) | \Phi \rangle \langle \Phi | e^{Z(\varphi)}$$

Thouless operator

Known from (U,V,φ)

$$\text{with } Z(\varphi) \equiv \frac{1}{2} \sum_{k_1 k_2} Z_{k_1 k_2}^{02}(\varphi) \beta_{k_2} \beta_{k_1}$$

Pure de-excitation operator

Projected BCC energy

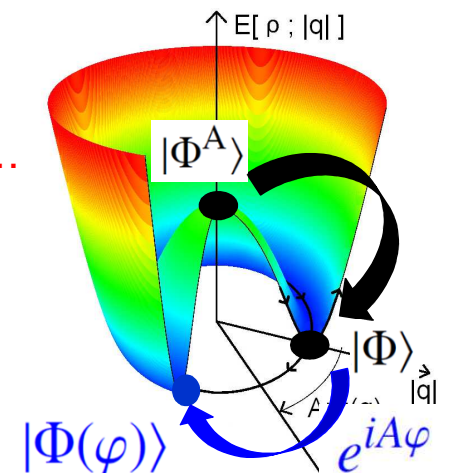
$$H|\Psi^A\rangle = E^A|\Psi^A\rangle \quad \Rightarrow \quad E^A = \frac{\int_0^{2\pi} d\varphi e^{-iA\varphi} \mathcal{H}(\varphi)}{\int_0^{2\pi} d\varphi e^{-iA\varphi} \mathcal{N}(\varphi)}$$

Similarity transformed operator

$$O_Z(\varphi) \equiv e^{Z(\varphi)} O e^{-Z(\varphi)}$$

Not a pure excitation operator...

$$\text{with } \begin{cases} \mathcal{N}(\varphi) \equiv \langle \Phi(\varphi) | e^U | \Phi \rangle = \langle \Phi(\varphi) | \Phi \rangle \langle \Phi | e^{U_Z(\varphi)} | \Phi \rangle \\ \mathcal{H}(\varphi) \equiv \langle \Phi(\varphi) | H e^U | \Phi \rangle = \langle \Phi(\varphi) | \Phi \rangle \langle \Phi | H_Z(\varphi) e^{U_Z(\varphi)} | \Phi \rangle \end{cases}$$



Particle-number projected BCC formalism

Disentangled cluster operators



Disantengling the algebra to extract pure excitation terms

$$e^{U_Z(\varphi)}|\Phi\rangle \equiv e^{W(\varphi)}|\Phi\rangle$$

- 1) Pure excitation operator **BUT contains a constant term**
- 2) Allows algebraic expressions of kernels later on following standard steps
- 3) Explicit relation between $W(\varphi)$ and $U_Z(\varphi)$ too complicated (need other approach)

$$W(\varphi) = \sum_{n=0} W_n(\varphi) \equiv \underbrace{W_0(\varphi)}_{\text{Constant}} + \underbrace{\mathcal{T}(\varphi)}_{\text{Standard cluster operator form}} \quad \text{with} \quad W_n(\varphi) \equiv \frac{1}{2n!} \sum_{k_1 \dots k_{2n}} W_{k_1 \dots k_{2n}}^{2n0}(\varphi) \beta_{k_1}^\dagger \dots \beta_{k_{2n}}^\dagger$$

Connected kernels and PBCC energy

$$\mathcal{N}(\varphi) \equiv e^{W_0(\varphi)} \langle \Phi(\varphi) | \Phi \rangle$$

$$h(\varphi) \equiv \frac{\mathcal{H}(\varphi)}{\mathcal{N}(\varphi)} = \langle \Phi | H_Z(\varphi) e^{\mathcal{T}(\varphi)} | \Phi \rangle_C$$

But how to determine $W(\varphi)$?

Norm kernel determined by $W_0(\varphi)$

Connected part of energy kernel determined by $\mathcal{T}(\varphi)$

Same algebraic/terminating form as standard BCC kernel!

$$E^A = \frac{\int_0^{2\pi} d\varphi e^{-iA\varphi} h(\varphi) \mathcal{N}(\varphi)}{\int_0^{2\pi} d\varphi e^{-iA\varphi} \mathcal{N}(\varphi)}$$

1) Reduction to BCC

$$\varphi = 0 \text{ in } h(\varphi)$$



$$E^A = \langle \Phi | H e^U | \Phi \rangle_C$$

2) Reduction to PHFB

$$W(\varphi) = 0$$



$$\mathcal{N}^{\text{PHFB}}(\varphi) \equiv \langle \Phi(\varphi) | \Phi \rangle$$

$$h^{\text{PHFB}}(\varphi) = \langle \Phi | H_Z(\varphi) | \Phi \rangle_C$$

Particle-number projected BCC formalism

Gauge-rotated cluster amplitudes $W_k(\varphi)$

Coupled ordinary differential equations

$$\frac{d}{d\varphi} \rightarrow e^{Z(\varphi)} e^U |\Phi\rangle = e^{W(\varphi)} |\Phi\rangle$$

$$\langle \Phi^\mu | \rightarrow$$

Kernel of particle number operator = generator of U(1)

$$\frac{d}{d\varphi} W_0(\varphi) = \frac{i}{2} \sum_{k_1 k_2} A_{k_1 k_2}^{02}(\varphi) W_{k_1 k_2}(\varphi)$$

$$\frac{d}{d\varphi} W_{k_1 k_2}(\varphi) = i \sum_{k_3 k_4} A_{k_3 k_4}^{02}(\varphi) \left[\frac{1}{2} W_{k_3 k_4 k_1 k_2}(\varphi) \right.$$

Initial conditions

$$W_0(0) = 0$$

$$W_k(0) = U_k$$

$$- W_{k_1 k_3}(\varphi) W_{k_2 k_4}(\varphi) \Big],$$

$$\frac{d}{d\varphi} W_{k_1 k_2 k_3 k_4}(\varphi) = i \sum_{k_5 k_6} A_{k_5 k_6}^{02}(\varphi) \left[\frac{1}{2} W_{k_5 k_6 k_1 k_2 k_3 k_4}(\varphi) \right.$$

Even when U truncated

All ranks in $W(\varphi)$ coupled

$$+ W_{k_1 k_5}(\varphi) W_{k_6 k_2 k_3 k_4}(\varphi)$$

$$+ W_{k_2 k_5}(\varphi) W_{k_1 k_6 k_3 k_4}(\varphi)$$

$$+ W_{k_3 k_5}(\varphi) W_{k_1 k_2 k_6 k_4}(\varphi)$$

$$+ W_{k_4 k_5}(\varphi) W_{k_1 k_2 k_3 k_6}(\varphi) \Big]$$

Second truncation on $W_k(\varphi)$



⋮

Integrate coupled ODEs and insert in PBCC energy

Open-shell systems - 3

$$H$$

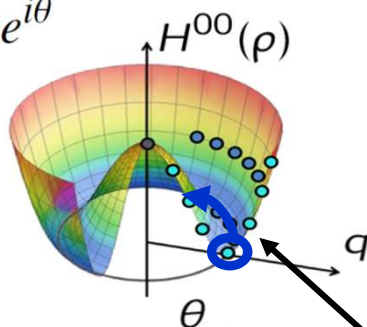
$$[H, R(\theta)] = 0$$

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

order parameter $\varrho \equiv qe^{i\theta}$

$$U(1) \rightarrow \mathbb{R}$$

$$SU(2) \rightarrow \mathbb{R}^2$$



Open-shell

Symmetry breaking minimum

$$H = H_0 + H_1$$

$$[H_0, R(\theta)] \neq 0$$

Static IR correlations

Deformed Hartree Fock Bogoliubov

$$H_0|\Theta^{(0)}\rangle = E^{(0)}|\Theta^{(0)}\rangle \quad |\Theta^{(0)}\rangle \equiv |\Phi(q)\rangle \text{ (dHFB)}$$

Dynamical correlations

Generalized qp expansion

Insert into expanded energy:

- ▶ keep same partitioning and expansion of Ω
- ▶ P superfluous/impactful if Ω exact/truncated

Further capture static correlations

$$|\Psi\rangle = \Omega|\Theta^{(0)}\rangle$$

PBMBPT, PBCC

- 1) Break - partition
- 2) Expand - **Project**

Successful novel approach
 Natural access to rotational excitations
 Projection however approximated
 Handling symmetry prior to partition?

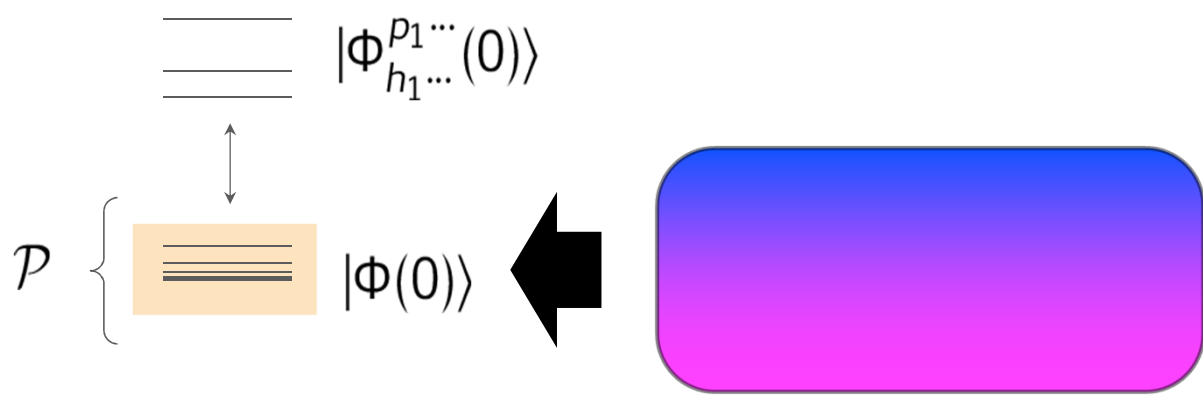
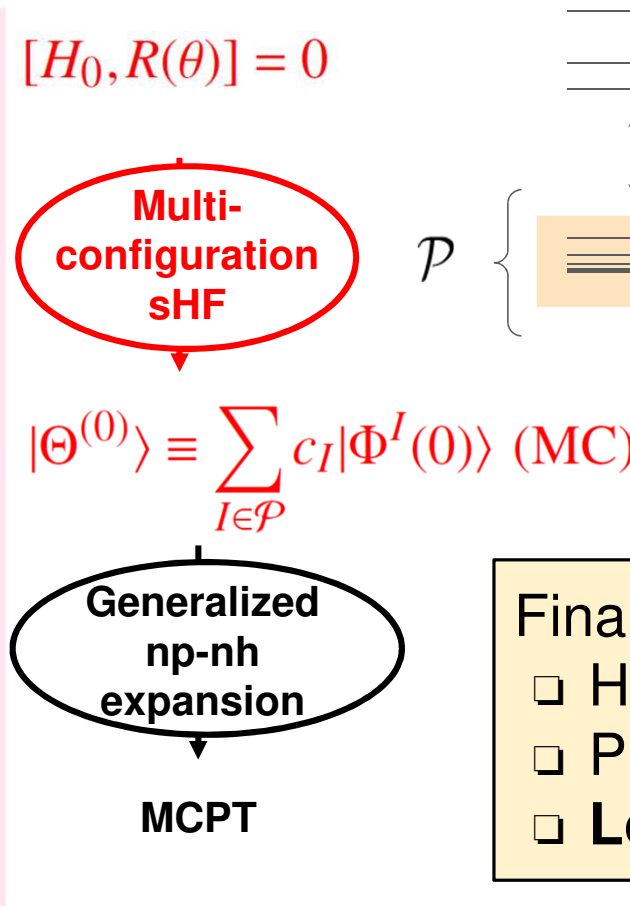
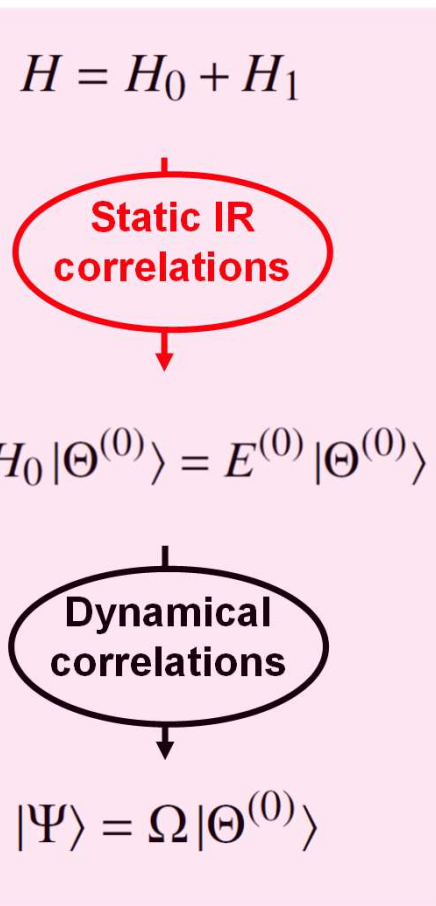
Open-shell systems - 4

$$H$$

$$[H, R(\theta)] = 0$$

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

Open-shell



- Final requirements for unperturbed state
- Handles **degeneracy**
 - Preserves **symmetry**
 - Low dimensionality**

Open-shell systems - 4

$$H$$

$$[H, R(\theta)] = 0$$

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

order parameter

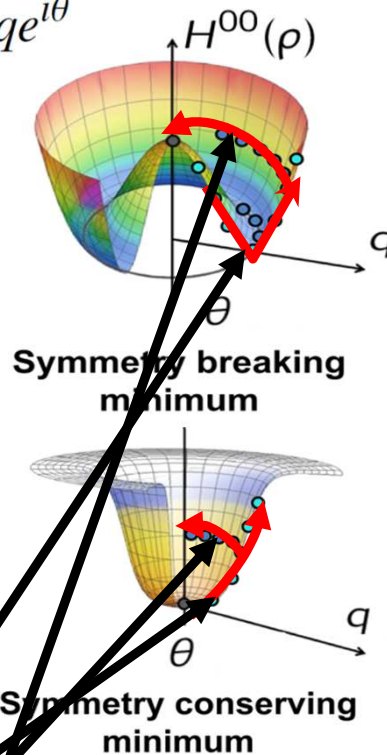
$$\varrho \equiv qe^{i\theta}$$

$$U(1) \rightarrow A$$

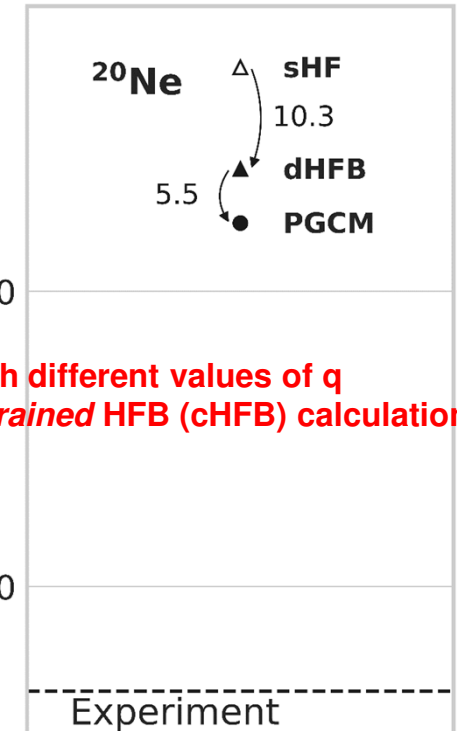
$$SU(2) \rightarrow J^2$$

Open-shell

$$[H_0, R(\theta)] = 0$$



Z=10, N=10



Set of HFB states with different values of q
 ► generated via *constrained* HFB (cHFB) calculations

$$H = H_0 + H_1$$

Static IR correlations

$$H_0|\Theta^{(0)}\rangle = E^{(0)}|\Theta^{(0)}\rangle$$

Dynamical correlations

$$|\Psi\rangle = \Omega|\Theta^{(0)}\rangle$$

PGCM

$$|\Theta^{(0)}\rangle \equiv \sum_q f(q) P\Phi(q) \text{ (PGCM)}$$

Projected generator coordinate method

Low dimensional mixing of non-orthogonal cHFB states

- Symmetry restored = fluctuation of angle θ of order parameter
- Further includes quantum fluctuations of norm q of order parameter

Perform low-dimensional diagonalization in *non-orthogonal basis*

- further include static ground-state correlations
- access both vibrational (q) and rotational (θ) excitations

Open-shell systems - 4

$$H$$

$$[H, R(\theta)] = 0$$

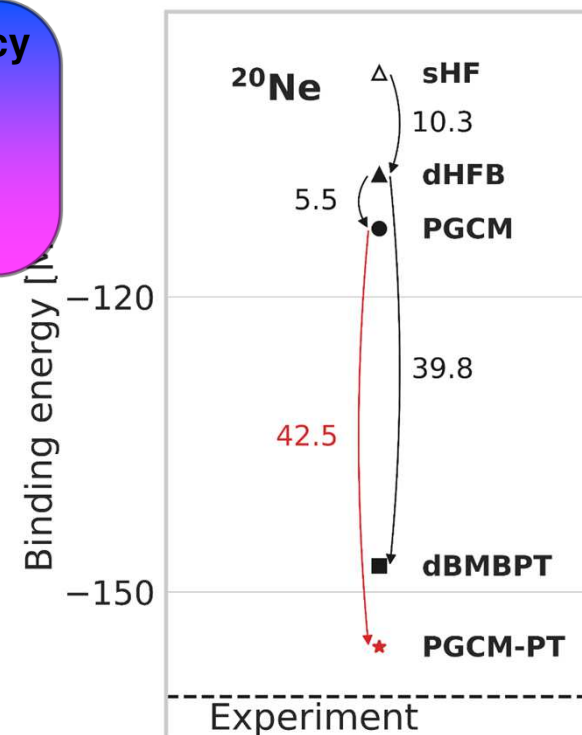
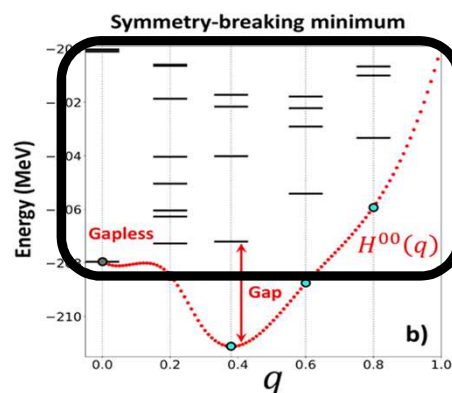
$$H|\Psi\rangle = E|\Psi\rangle$$

$$U(1) \rightarrow A$$

$$SU(2) \rightarrow J^2$$

Open-shell

Absolute energies: **1-2% accuracy**
 -improves over dBMBPT(2)
 Spectra: **20% accuracy**
 -Negligible PT corrections
-Enrich PGCM state?



$$H = H_0 + H_1$$

$$[H_0, R(\theta)] = 0$$

Static IR correlations

PGCM

$$H_0|\Theta^{(0)}\rangle = E^{(0)}|\Theta^{(0)}\rangle$$

$$|\Theta^{(0)}\rangle \equiv \sum_q f(q)P|\Phi(q)\rangle \text{ (PGCM)}$$

Dynamical correlations

Generalized multi vacua qp expansion

$$|\Psi\rangle = \Omega|\Theta^{(0)}\rangle$$

PGCM-PT

PGCM Perturbation Theory

Only weak remaining dynamical correlations to include
Multi copies of Fock space = large linear system to solve

▶ handling redundancies, intruders, large dimension

State-specific expansion for each PGCM state

▶ access ground-state and spectroscopy

- 1) Break - project - partition
- 2) Expand

Selected references

Symmetry-breaking single-reference expansion methods

- GSCGF [V. Somà, T. Duguet, C. Barbieri, PRC 84 (2011) 064317]
[V. Somà, A. Cipollone, C. Barbieri, P. Navratil, T. Duguet, PRC 89 (2014) 061301]
[C. Barbieri, T. Duguet, V. Somà, PRC 105 (2022) 044330]
- BMBPT [A. Tichai, P. Arthuis, T. Duguet, H. Hergert, V. Somà, R. Roth]
[P. Arthuis, T. Duguet, A. Tichai, R.-D. Lasserri, J.-P. Ebran, CPC 240 (2019) 202]
- BCC [A. Signoracci, T. Duguet, G. Hagen, G. R. Jansen, PRC 91 (2015) 064320]
[T. M. Henderson, G. E. Scuseria, J. Dukelsky, A. Signoracci, T. Duguet, PRC89 (2014) 054305]
[A. Tichai, P. Demol, T. Duguet, in preparation (2022)]

Symmetry-breaking and restored single-reference expansion methods

- PBMBPT [T. Duguet, JPG 42 (2015) 025107]
- PBCC [T. Duguet, A. Signoracci, JPG 44 (2016) 015103]
[Y. Qiu, T. M. Henderson, J. Zhao, and G. E. Scuseria, JCP 147 (2017) 064111]
[Y. Qiu, T. M. Henderson, T. Duguet, G. E. Scuseria, PRC 99 (2019) 044301]
[G. Hagen, S. J. Novario, Z. H. Sun, T. Papenbrock, G. R. Jansen, J. G. Lietz, T. Duguet, A. Tichai, PRC 105 (2022) 064311]

Symmetry-conserving multi-reference expansion method

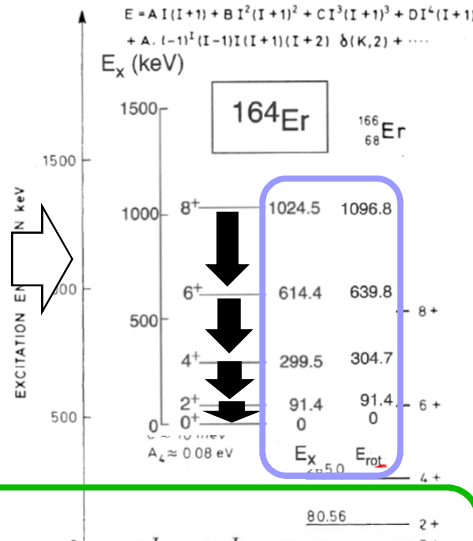
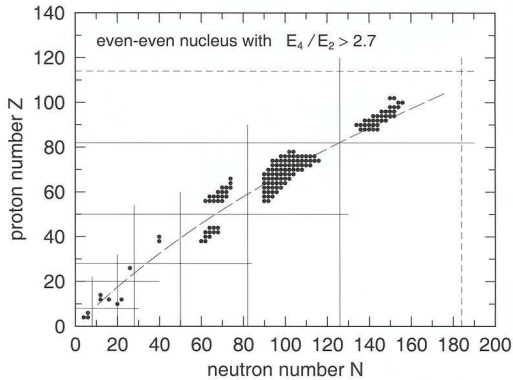
- PGCM-PT [M. Frosini, T. Duguet, J.-P. Ebran, V. Somà, EPJA 58 (2022) 62]
[M. Frosini, T. Duguet, J.-P. Ebran, B. Bally, T. Mongelli, T. R. Rodriguez, R. Roth, V. Somà, EPJA 58 (2022) 63]
[M. Frosini, T. Duguet, J.-P. Ebran, B. Bally, H. Hergert, T. R. Rodriguez, R. Roth, J. M. Yao, V. Somà, EPJA 58 (2022) 64]

Contents

- Introduction to low-energy nuclear physics
 - Phenomenology
 - Rationale from the theoretical viewpoint
- Strong inter-nucleon forces
 - Basic phenomenology and modelling
- The *ab initio* nuclear many-body problem
 - Pre-processing short-range correlations
 - Expansion methods handling both « weak/strong » dynamical/static correlations
 - Nuclear deformation from *ab initio* calculations
- Conclusions

Rotational properties: from experiment to theory

I. The phenomenology



II. The symmetry $SU(2) \equiv \{R(\Omega), \Omega \in D_{SU(2)}\}$

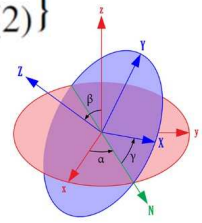
Symmetry

$$[H, R(\Omega)] = 0$$

$$H|\Psi_n^{JM}\rangle = E_n^J |\Psi_n^{JM}\rangle$$

$$\langle \Psi_n^{JM} | T_\mu^\lambda | \Psi_{n'}^{J'M'} \rangle \equiv (JM\lambda\mu | J'M')$$

IRREP $\langle \Psi_n^{JM} | R(\Omega) | \Psi_{n'}^{J'M'} \rangle \equiv \delta_{nn'} \delta_{JJ'} D_{MM'}^J(\Omega)$



A. Bohr, Nobel Lecture (1975)
Observable patterns

- Set of states
- Strong E2
- Happens for

Observable patterns dictated by SU(2) symmetry

Energies labeled by J and independent of M

Ab initio nuclear A-body problem viewpoint

Do rotational properties emerge from basic interactions between the nucleons?

- Non-trivial as $B \ll$ energy scale for individual excitations
- $2N$ (+ $3N$) are adjusted on 2-body (+3-body) systems

Do perturbations due to coupling to vibrations and individual dof emerge?

III. The model

$$|\Psi_{KM}^J\rangle \propto \int d\Omega$$

True eigenstate

Intrinsic state

Rotational motion

Features

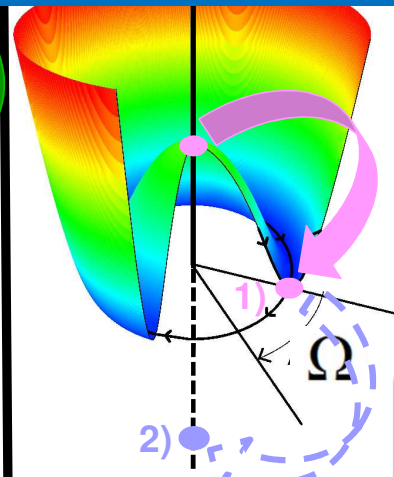
$$E_n^J = E_0^J + BJ(J+1) \quad \text{with} \quad B \equiv \frac{2}{2I}$$

$$Q(J) = [3K^2 - J(J+1)][(J+1)(2J+3)]^{-1} Q_0$$

$$B(E2; J \rightarrow J') = 5(16\pi)^{-1} (JK20 | J'K)(eQ_0)^2$$

Lessons

- Links a specific subset of states together
- Excellent account of idealized patterns
- Built in separation of rotational degrees of freedom
- Disturbed by coupling of rot. to vib. and ind. dynamics



Is not fully realized
Similar for other symmetries of H
Emerging lower $\sim Sp(3, R)$ symmetry

- Spontaneous breaking of SU(2)
 - GS has lower symmetry than H
 - GS = wave packet mixing IRREPs
 - Goldstone boson = rotations
 - Higgs modes = vibrations

- Finite system = breaking only emergent
 - SU(2) symmetry actually satisfied
 - Lower symmetry imprints excitations
 - Rotational bands and transitions

Symmetry breaking

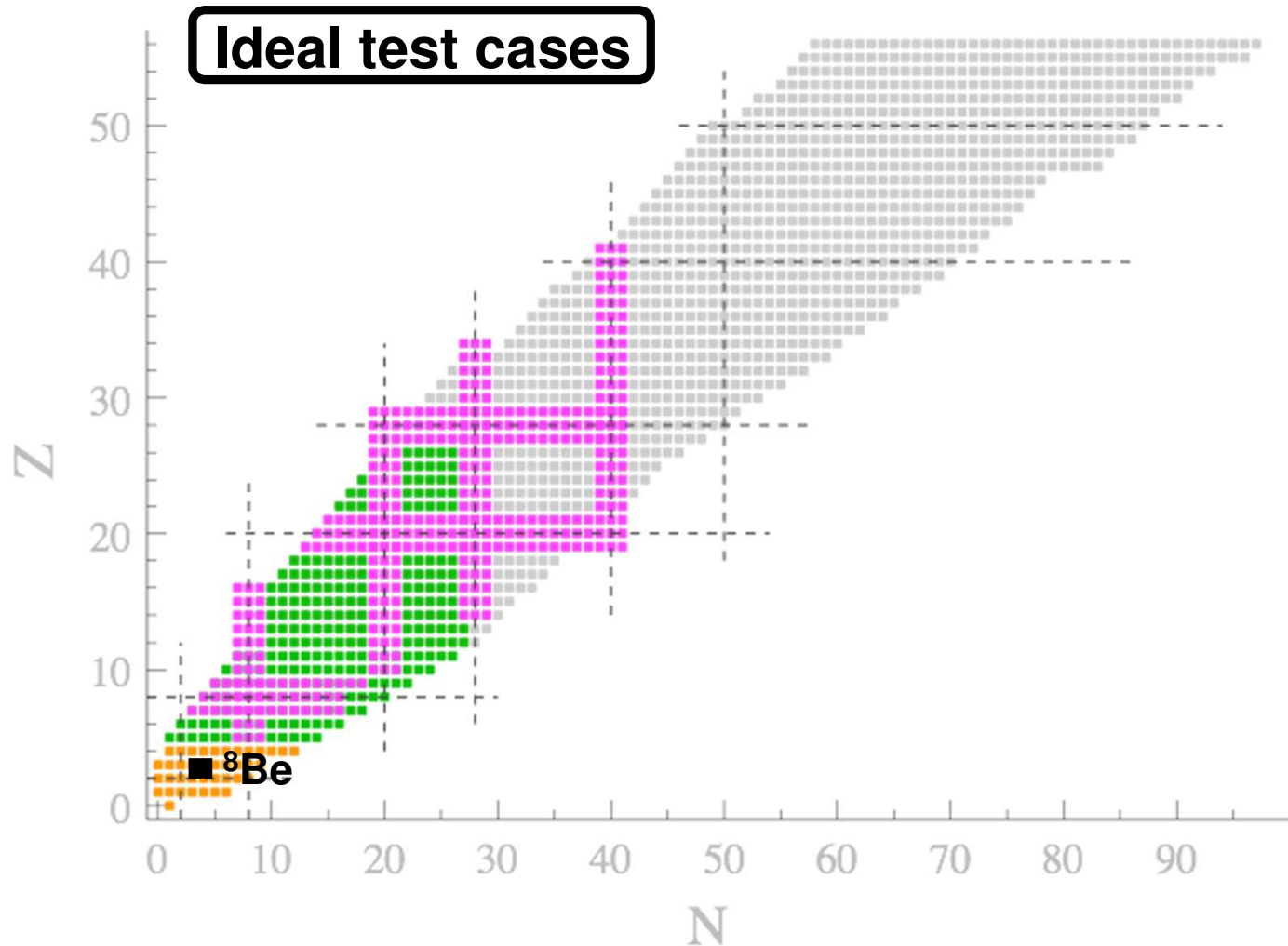
from dof + H

Ab initio many-body methods: rotational properties

$$H|\Psi_n^{JM}\rangle = E_n^J |\Psi_n^{JM}\rangle$$

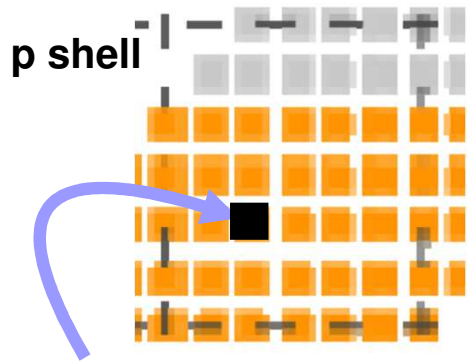
1) ${}^8\text{Be}$ [2015]

- No-core shell model
- **Symmetry conserving**



No-core shell model calculation of ${}^8\text{Be}$ isotopes

[M.A. Caprio *et al.*, JMPE 24 (2015) 1541002]

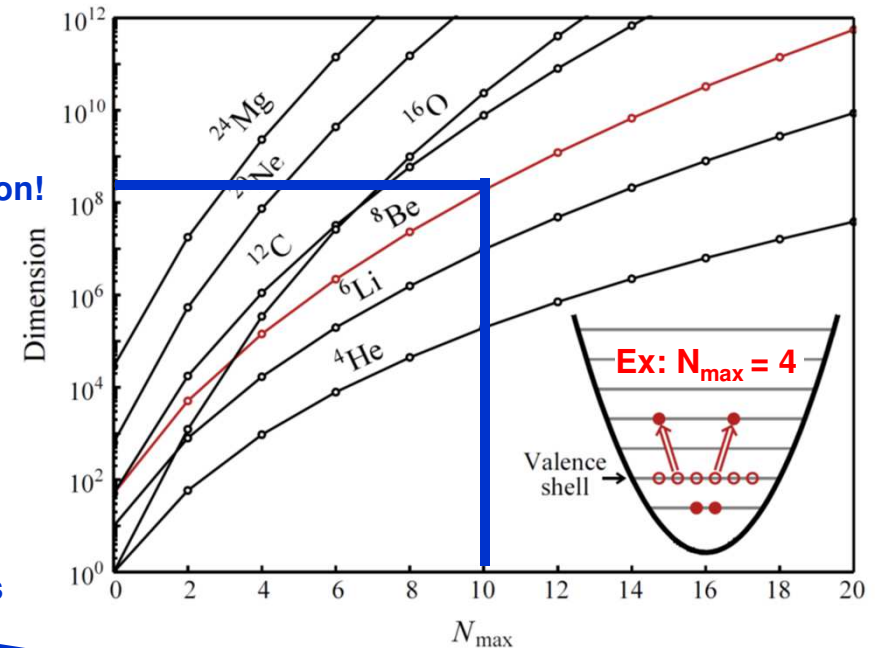


No core shell model calculation of ${}^8\text{Be}$

${}^8\text{Be}$ at $N_{\text{max}} = 10 \sim 2 \cdot 10^8$ matrix dimension!

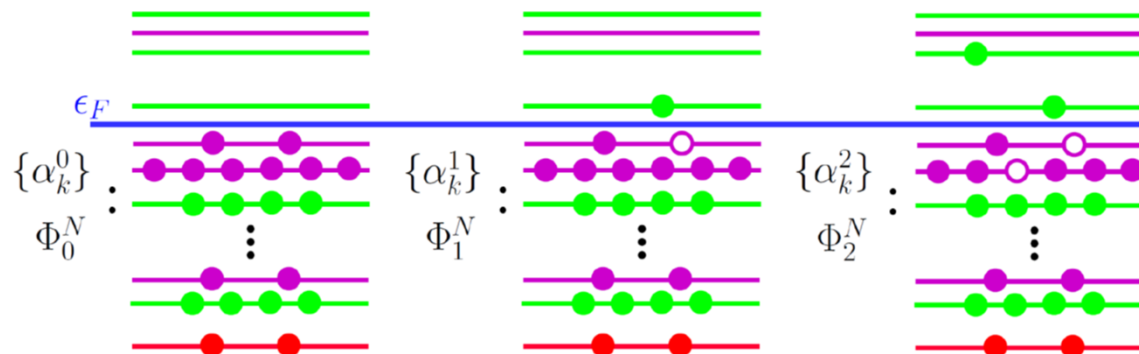
SD basis truncated according to N_{max}

From diagonalization of H in SD basis



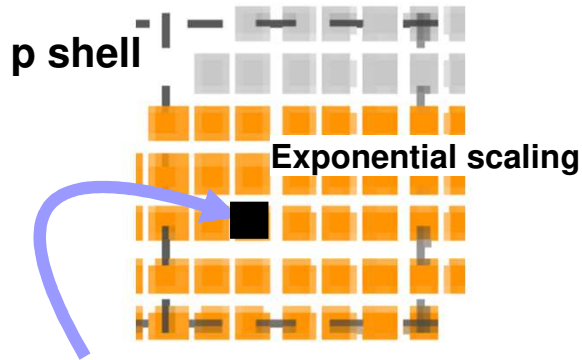
CI expansion over basis of symmetry conserving SD

$$|\Psi_0^N\rangle = |\Phi\rangle + \sum_{ai} C_i^a(0) |\Phi_i^a\rangle + \left(\frac{1}{2!}\right)^2 \sum_{abij} C_{ij}^{ab}(0) |\Phi_{ij}^{ab}\rangle + \left(\frac{1}{3!}\right)^2 \sum_{abcijk} C_{ijk}^{abb}(0) |\Phi_{ijk}^{abc}\rangle + \dots$$



No-core shell model calculation of ${}^8\text{Be}$ isotopes

[M.A. Caprio *et al.*, JMPE 24 (2015) 1541002]



No core shell model calculation of ${}^8\text{Be}$

Two-nucleon interactions

- Chiral 2N ($N^2\text{LO}$; $\Lambda_{2\text{NF}} = 500 \text{ MeV}/c$) [Ekstrom *et al.*, PRL 110 (2013) 192502]

Results

Rotational behavior emerge convincingly

- Energies, E2/M1 moments and transitions
- Converged quadrupole strength *ratios* (**absolute moment unsettled**)
- Null spin contribution to $\mu(J)$ consistent with α -clustering
- Similar for (un)natural parity/excited bands in ${}^7, {}^9\text{Be}$ (not shown)

Robust against (modest) variation of 2N interaction (not shown)

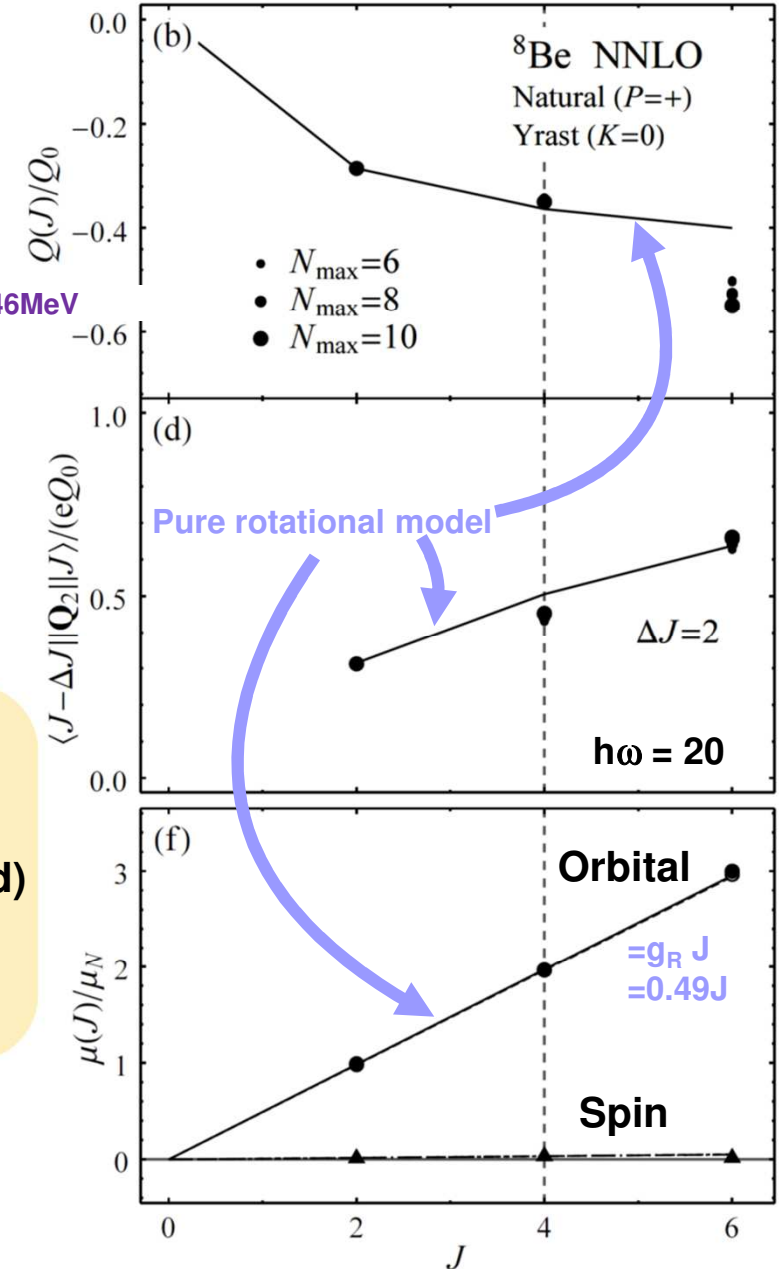
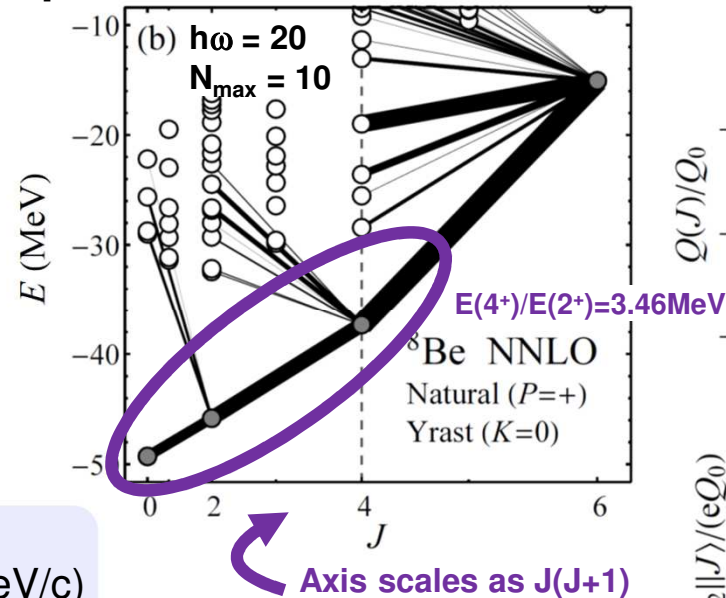
Perspectives

- Check in non-ideal rotor nuclei
- Add 3N interaction + test at various $N^k\text{LO}$ orders

Similar for GFMC calculations [R. B. Wiringa *et al.*, PRC62 (2000) 014001]

Yrast positive parity band

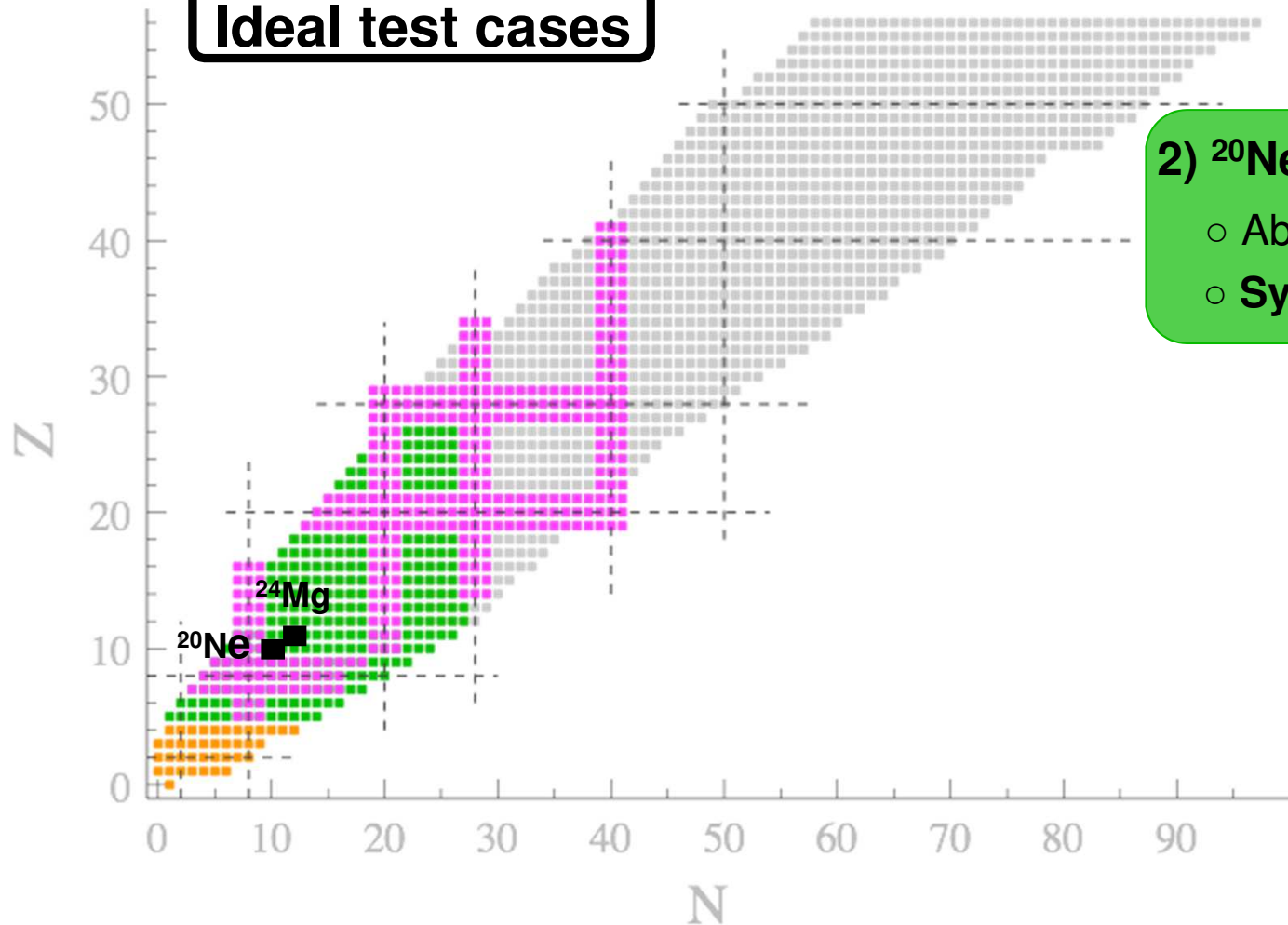
$J_{\text{max}}=4$ in pure p shell



Ab initio many-body methods: rotational properties

$$H|\Psi_n^{JM}\rangle = E_n^J |\Psi_n^{JM}\rangle$$

Ideal test cases



1) ^8Be [2015]

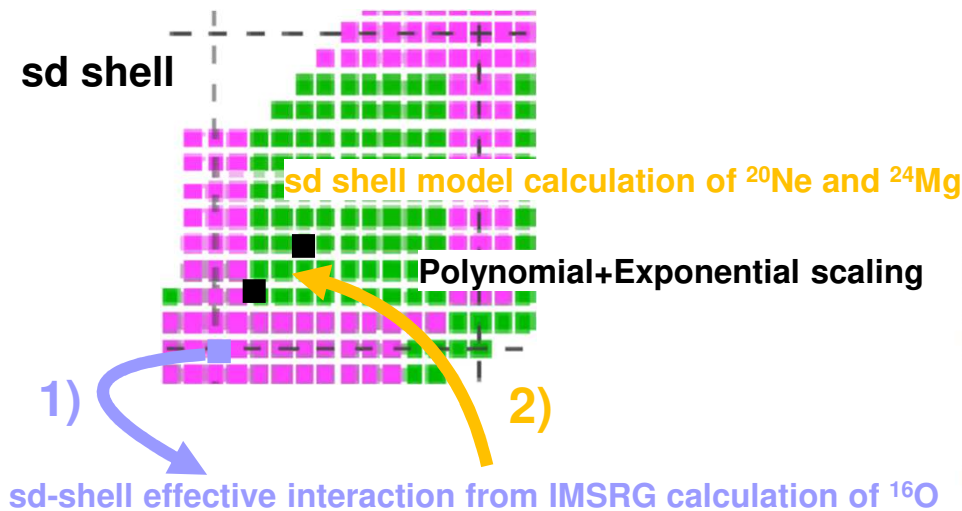
- No-core shell model
- **Symmetry conserving**

2) ^{20}Ne and ^{24}Mg [2016]

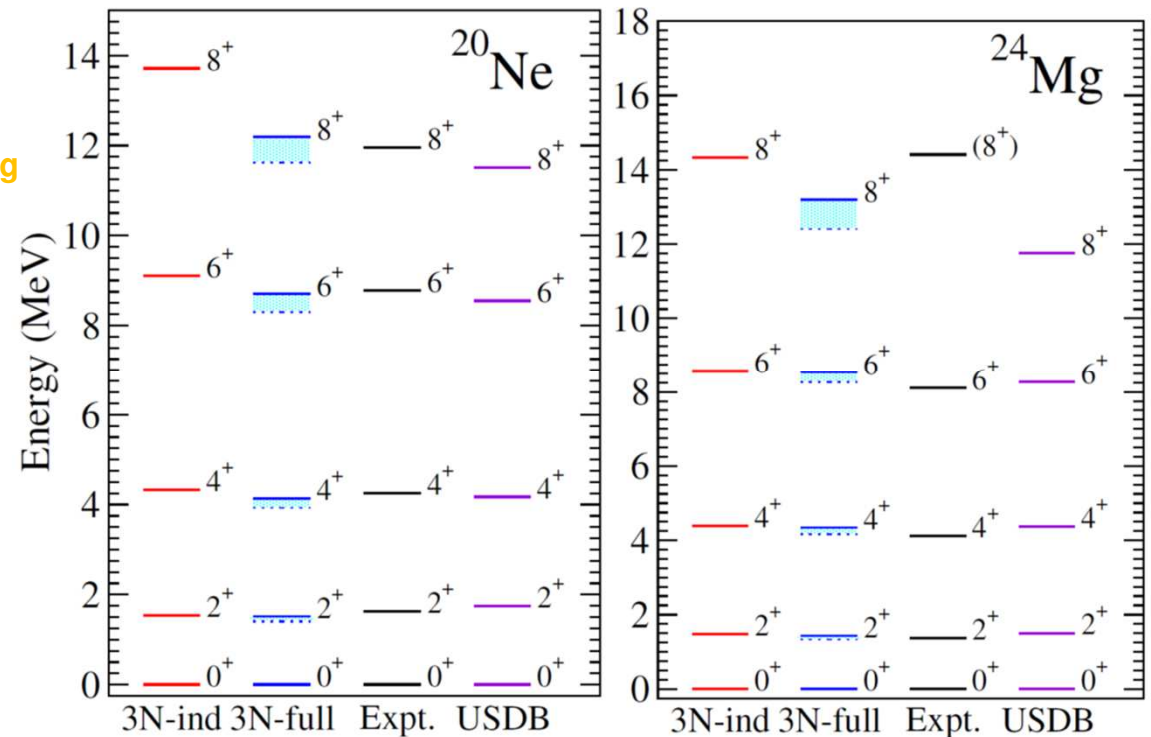
- Ab initio valence-space shell model
- **Symmetry conserving**

Valence-space shell model calculation of ^{20}Ne and ^{24}Mg

[S. R. Stroberg *et al.*, PRC93 (2016) 051301]



Yrast spectroscopy of ideal rotor nuclei



Inter-nucleon interactions

- Chiral 2N (N^3LO ; $\Lambda_{2\text{NF}} = 500 \text{ MeV}/c$)
[D.R. Entem, R. Machleidt, PRC 68, 041001 (2003)]
- Chiral 3N (N^2LO ; $\Lambda_{3\text{NF}} = 400 \text{ MeV}/c$)
[P. Navratil, FBS 41, 117 (2007)]
- SRG evolved down to $\lambda = 2.0 \text{ fm}^{-1}$

Perpectives

- Check in non-ideal rotor nuclei
- Various EFT orders and uncertainty propagation
- Investigate E2/M1 moments and transitions

Results

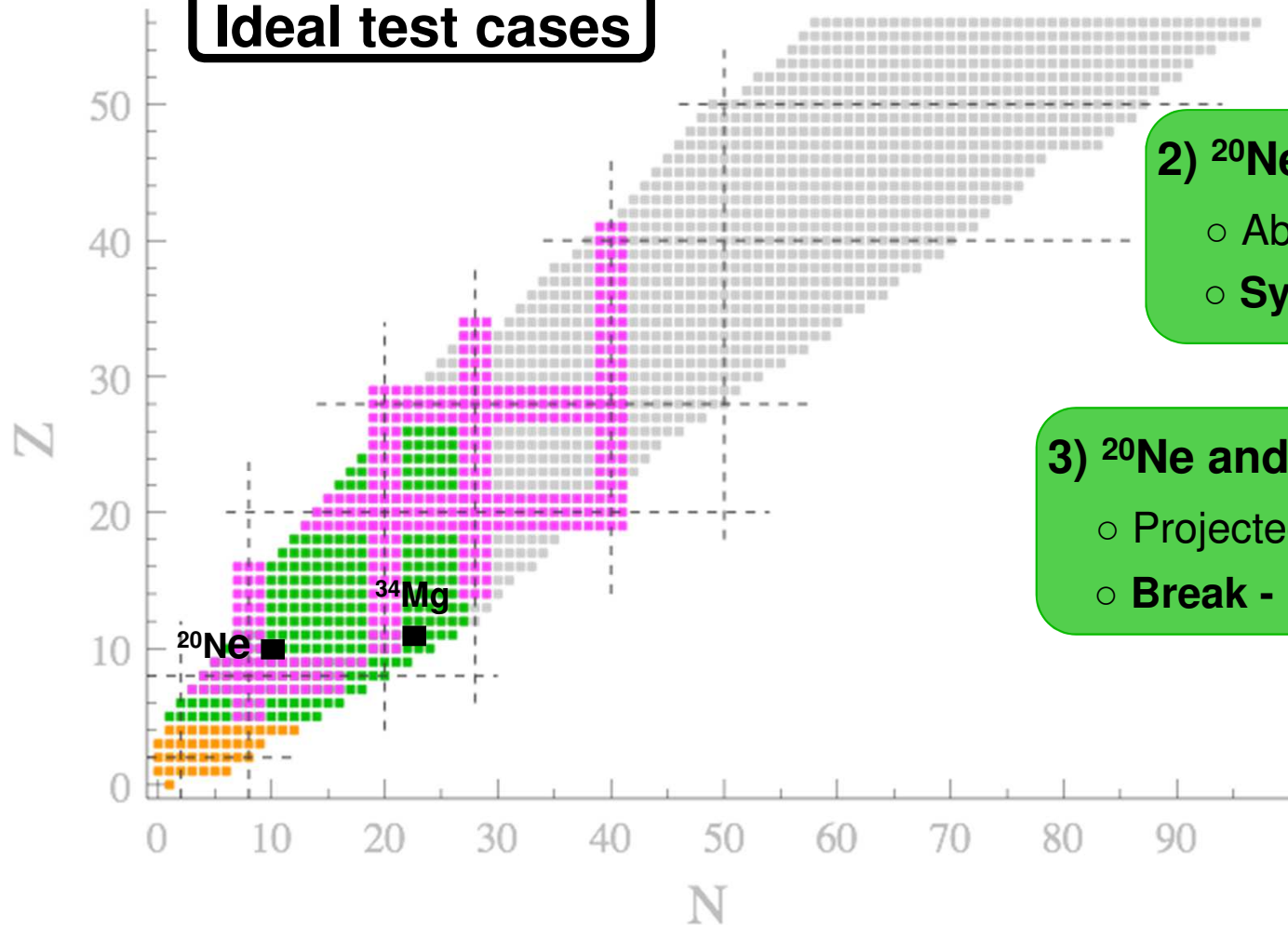
- Rotational bands emerge convincingly
- Quantitatively as good as empirical model
- Insensitive to 3N interaction at low spins
Unlike overall spectroscopy in sd shell

Similarly for CG-based valence-space shell model
[G. Hagen *et al.*, Phys. Scr. 91 (2016) 063006]

Ab initio many-body methods: rotational properties

$$H|\Psi_n^{JM}\rangle = E_n^J |\Psi_n^{JM}\rangle$$

Ideal test cases



1) ^8Be [2015]

- No-core shell model
- **Symmetry conserving**

2) ^{20}Ne and ^{24}Mg [2016]

- Ab initio valence-space shell model
- **Symmetry conserving**

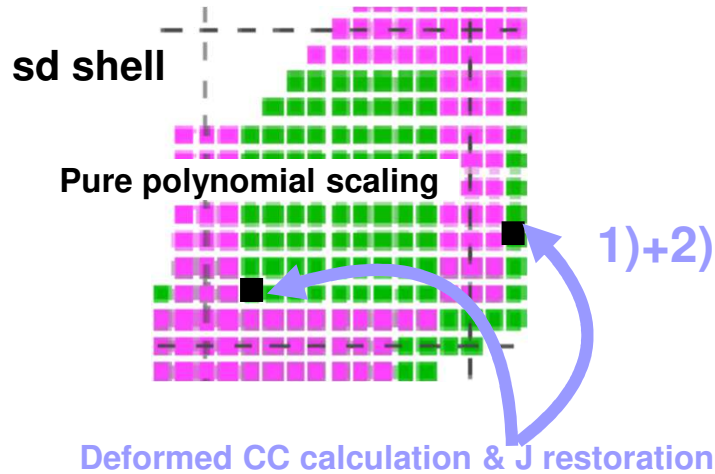
3) ^{20}Ne and ^{34}Mg [2022]

- Projected Coupled cluster theory
- **Break - Expand - Restore**

SU(2) broken & restored CC calculation of ^{20}Ne and ^{34}Mg

[T.Duguet. JPG 42 (2015) 025107]

[G. Hagen et al., PRC 105, 064311 (2022)]

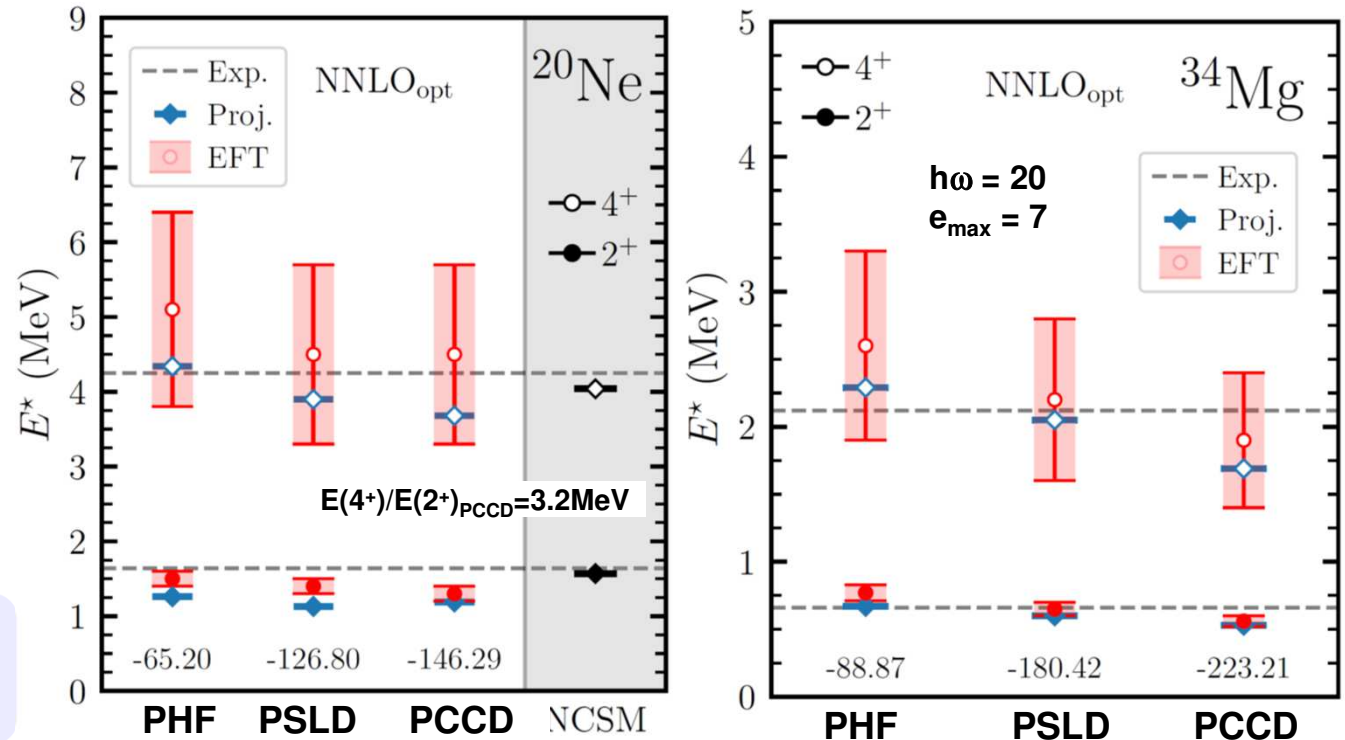


Two-nucleon interactions

➤ Chiral 2N (N^2LO ; $\Lambda_{2\text{NF}} = 500 \text{ MeV}/c$)

[Ekstrom et al., PRL 110 (2013) 192502]

SA-NCSM results in ^{20}Ne from [T. Dytrych et al., PRL124 (2020) 042501]



Perspectives

- Inclusion of 3N interaction (done)
- Better “bra state” (done)
- Check in non-ideal rotor nuclei
- EFT orders and uncertainty propagation
- E2/M1 moments and transitions

Results

Low-lying rotational states consistently described

- ▶ vs NCSM benchmark and experiment
- ▶ vs LO=RRM (+uncertainty) of EFT for deformed nuclei [T. Papenbrock, NPA 852, 36 (2011)]

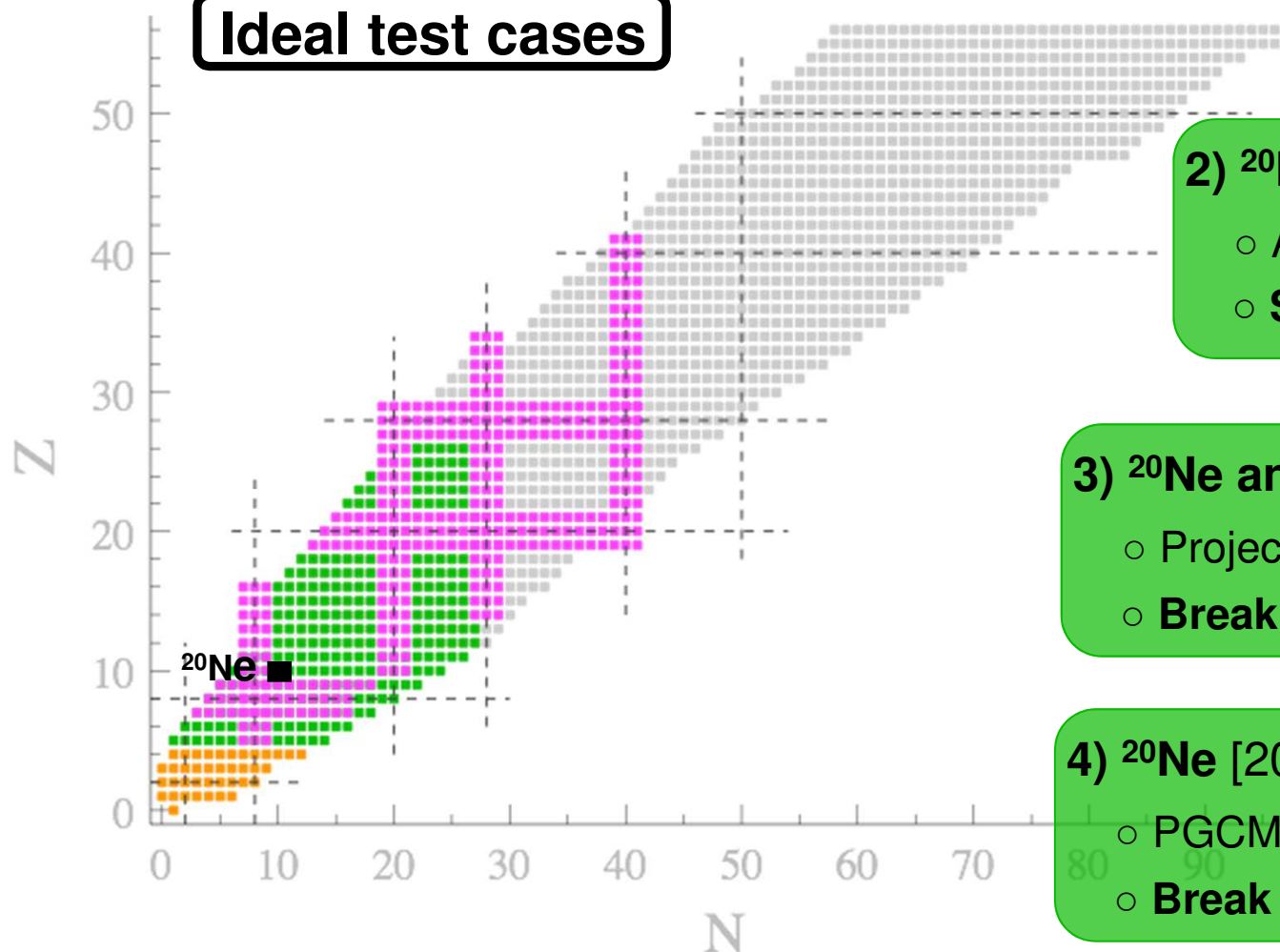
Dynamical correlations

- ▶ strongly impact absolute energies
- ▶ only slightly increase moment of inertia in ^{20}Ne
- ▶ impact ^{34}Mg more significantly

Ab initio many-body methods: rotational properties

$$H|\Psi_n^{JM}\rangle = E_n^J |\Psi_n^{JM}\rangle$$

Ideal test cases



1) ^8Be [2015]

- No-core shell model
- **Symmetry conserving**

2) ^{20}Ne and ^{24}Mg [2016]

- Ab initio valence-space shell model
- **Symmetry conserving**

3) ^{20}Ne and ^{34}Mg [2022]

- Projected Coupled cluster theory
- **Break - Expand - Restore**

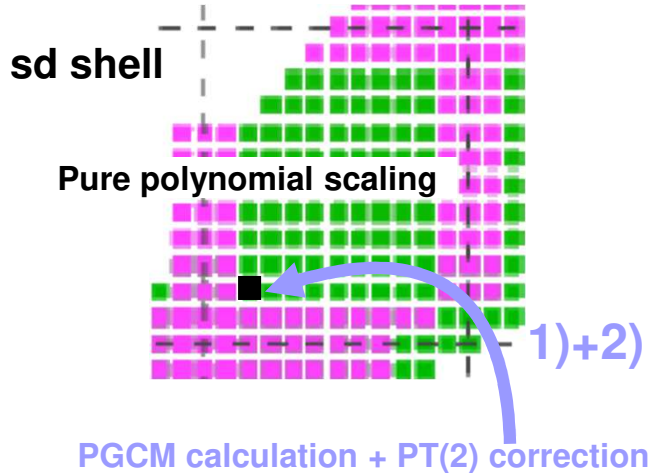
4) ^{20}Ne [2022]

- PGCM-Perturbation theory
- **Break - Restore - Expand**

PGCM-PT calculation of ^{20}Ne

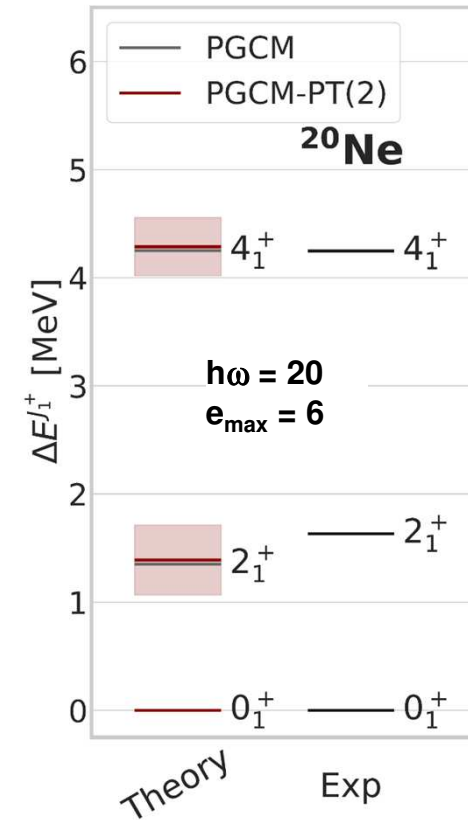
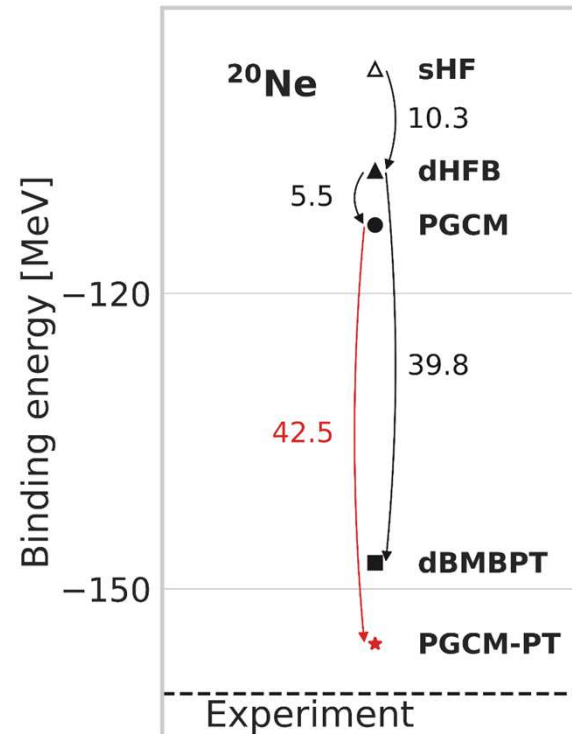
[M. Frosini et al., EPJA 58 (2022) 62]

[M. Frosini et al., EPJA 58 (2022) 64]



Inter-nucleon interactions

- Chiral 2N (N^3LO) $\lambda_{\text{SRG}} = 1.8 \text{ fm}^{-1}$
 - Chiral 3N (N^2LO ; $\Lambda_{3\text{NF}} = 2.0 \text{ fm}^{-1}$)
- [K. Hebeler et al., PRC 83, 031301 (2011)]



Perspectives

- Check in non-ideal rotor nuclei
- **EFT orders and uncertainty propagation**
- **E2/M1 moments and transitions**
- **Systematic comparisons with PCC**
- Study vibrational excitations

Results

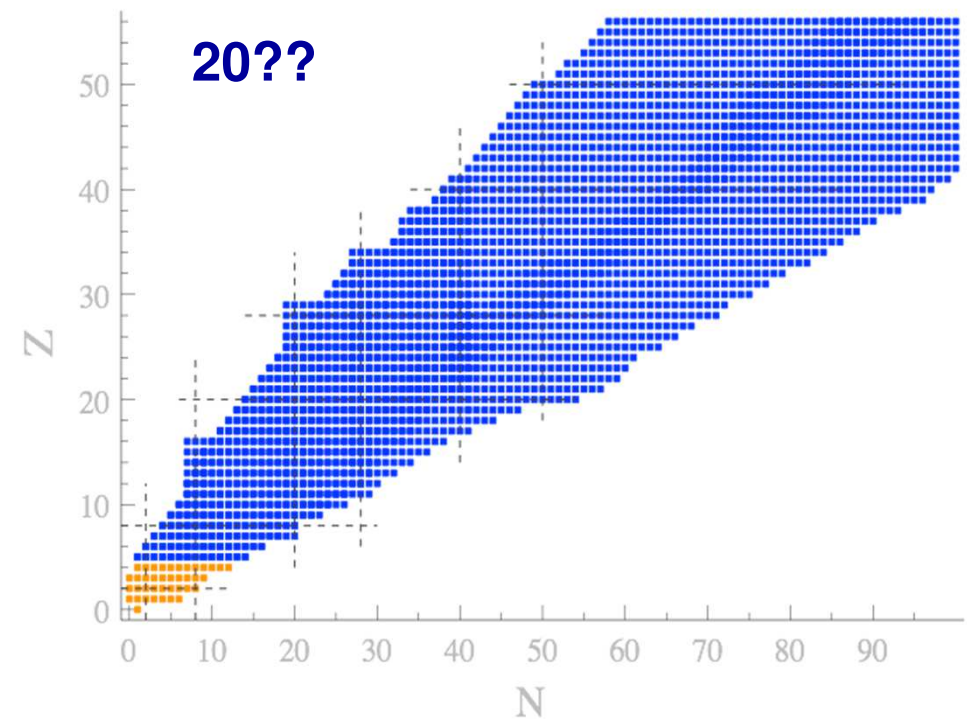
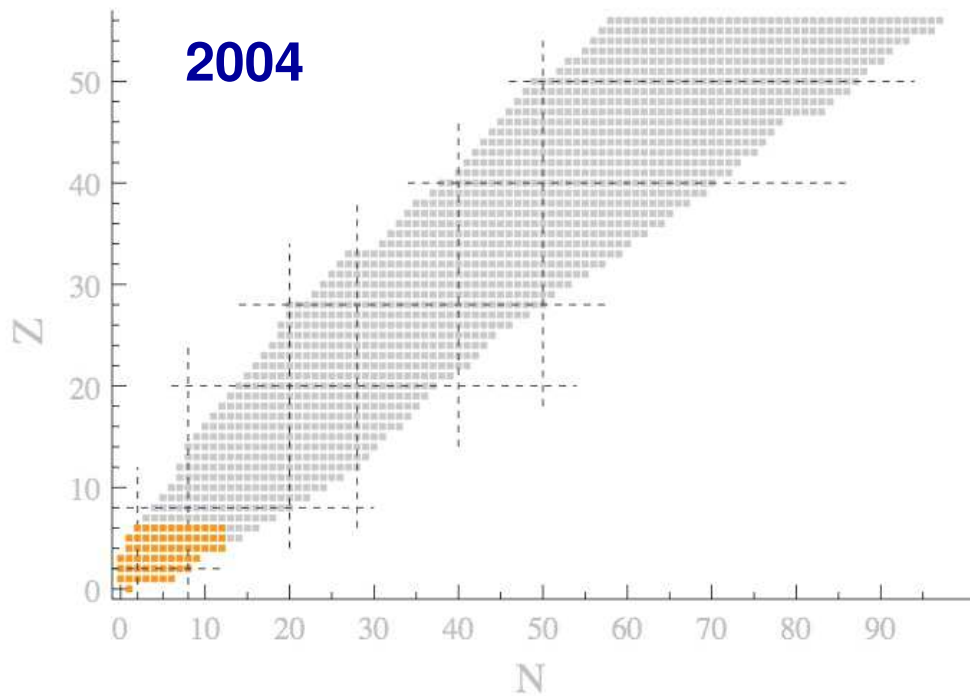
Low-lying rotational states

- ▶ consistently emerge
- ▶ reproduce well experimental data

Dynamical correlations

- ▶ strongly impact absolute energies
- ▶ do not impact moment of inertia in ^{20}Ne

Long-term perspectives of ab initio methods



Emergence from nucleons and their interactions?

- Binding, size, limit of existence, collectivity, superfluidity...

Limits of such a description with A in accuracy?

- Modified ab initio effective theory when A increases?
- More effective but explicitly connected approaches?

Detailed and systematic description of nuclei

Rotational properties

- ❖ Dominance of prolate over oblate?
- ❖ Superdeformation?
- ❖ Physics of transitional nuclei?
- ❖ Shape coexistence phenomenon?
- ❖ New features?

What specific features of AN interactions probed?

Contents

- Introduction to low-energy nuclear physics
 - Phenomenology
 - Rationale from the theoretical viewpoint
- Strong inter-nucleon forces
 - Basic phenomenology and modelling
- The ab initio nuclear many-body problem
 - Pre-processing short-range correlations
 - Expansion methods handling both « weak/strong » dynamical/static correlations
 - Nuclear deformation from ab initio calculations
- Conclusions

Conclusions
