Rooting the EDF method into the *ab initio* framework

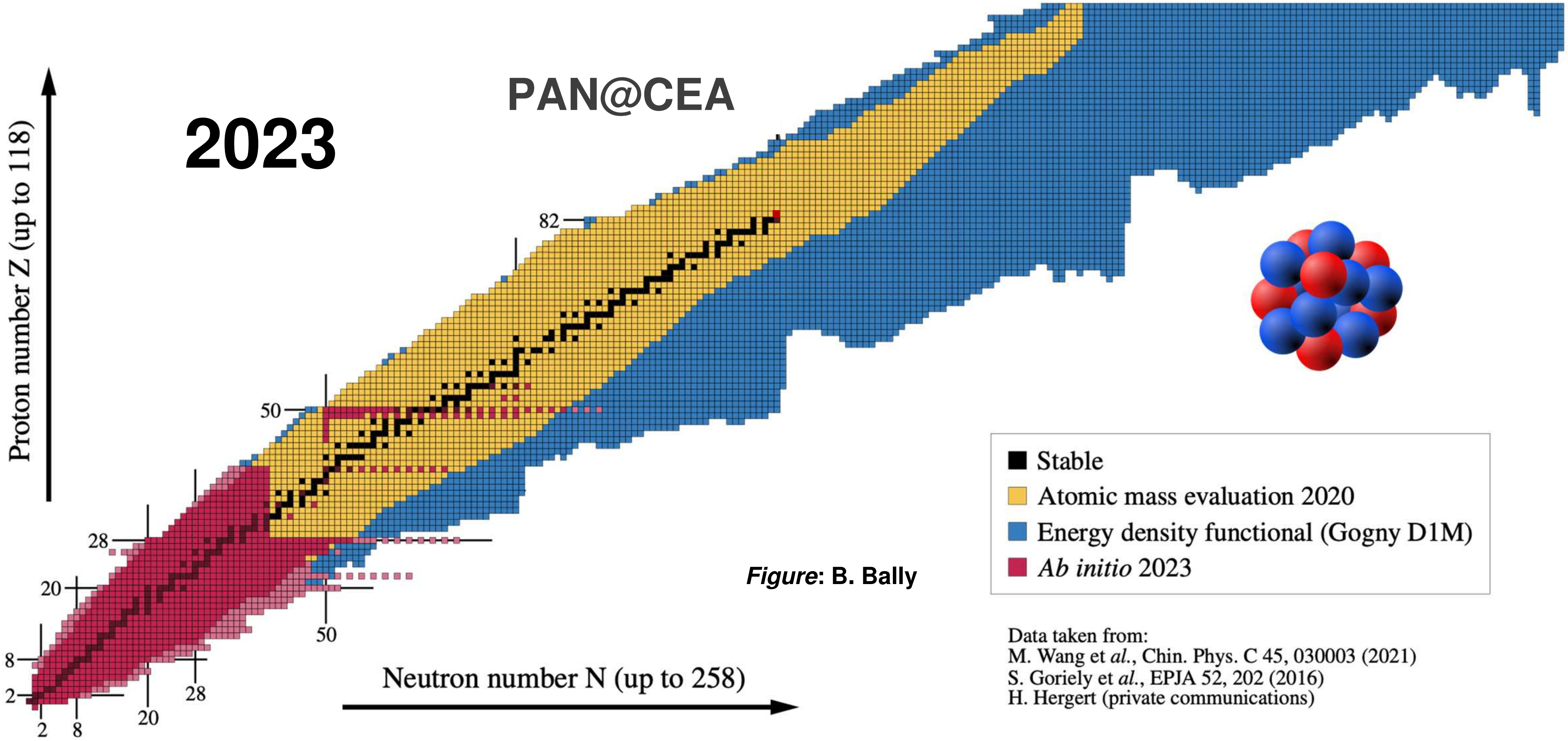

Figure: B. Bally

Nuclear energy density functional method: going beyond the minefield
ESNT Workshop, November 20-24, Saclay, France

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

Contents

- Ab initio expansion many-body methods
- Comparison of ab initio and EDF workflows
- Anchoring EDF methodology into ab initio methods
- Perspectives

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Ab initio endeavor

Can nuclear systems be described

1) From nucleons and their interactions (right balance between reductionism/emergence?)
2) Rooted in QCD (sound connection to underlying EFT?)
3) Systematically (complete phenomenology?)
4) Accurately enough (relevant to experimental uncertainty?)

Currently best realized by chiral effective field theory (χEFT) in A-body sector

$$H|\Psi_n^A\rangle = \mathrm{E}_n^A|\Psi_n^A\rangle$$

Systematic expansion of H

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

Systematic many-body expansion

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

Global philosophy

Approximate solution **systematically improvable** towards **well-defined limit**

+

Uncertainties evaluation, quantify what is missing

Expansion many-body methods

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

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

$$\mathcal{H}_{\text{A}} = \mathcal{H}(1) \otimes \ldots \otimes \mathcal{H}(\text{A})$$

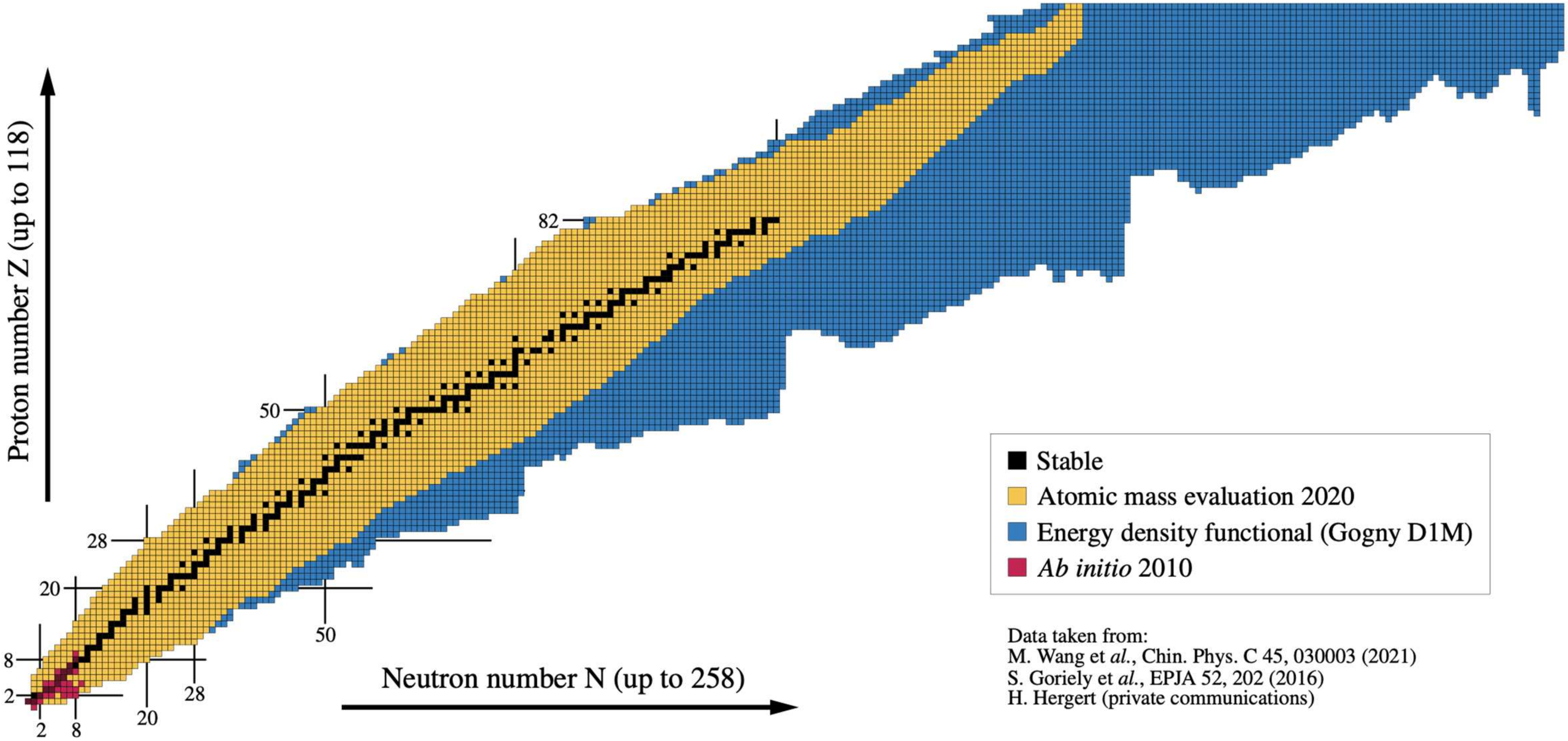
$$\boxed{\dim \mathcal{H}(\text{A}) \equiv n_{\text{dim}}^{\text{A}}}$$

« The curse of dimensionality »

Ground-state *ab initio* nuclear chart… then

Quasi-exact methods (>1990)

Examples: No core shell-model (NCSM)
Green's function monte carlo (GFMC)



2010

[*Figure*: B. Bally]

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« The curse of dimensionality »

Expansion many-body methods

Hamiltonian partitioning

$H = \boxed{H_0} + H_1$

« Easy » to solve

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

Unperturbed state

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

Symmetry?

Nature of the state?

Expansion many-body methods

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

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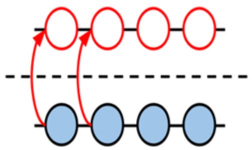

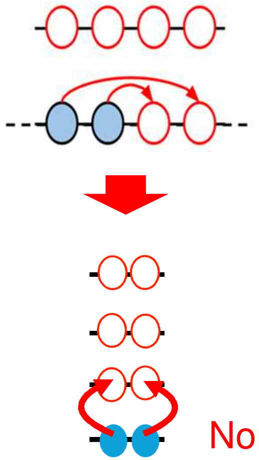

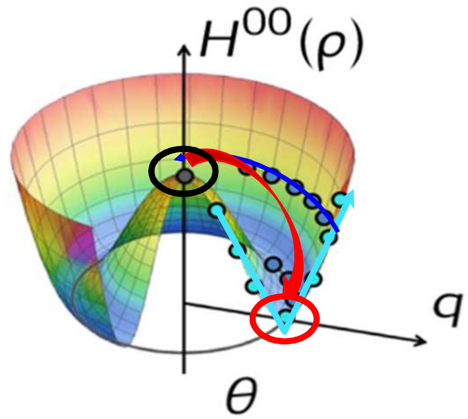

Symmetry breaking
Static correlations
Lost σ

Non-degenerate ind. excitations

Closed-shell nuclei

Open-shell nuclei

Partitioning	$[H_0,R(\theta)] = 0$	$[H_0,R(\theta)] \neq 0$
Single reference $\lvert\Theta_\mu^{(0)}\rangle$	sHF $\lvert\Phi^\sigma(0)\rangle$	dHFB $\lvert\Phi(q)\rangle$
Multi reference $\lvert\Theta_k^{(0)}\rangle$	PGCM $\lvert\Theta_k^\sigma\rangle \equiv \int dq\, f_k^{\tilde\sigma}(q)\, P_{M0}^{\tilde\sigma}\lvert\Phi(q)\rangle$	

Symmetry restoration
+
« Shape » mixing
Further static correlations
Recovered σ
Access collective excitations

Closed- & open-shell nuclei

Expansion many-body methods

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

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Hamiltonian partitioning

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

Unperturbed state

Hilbert-space partitioning

$$\mathcal{P}_k + \mathcal{Q}_k \equiv 1 \left\{ \begin{array}{l} \mathcal{P}_k \equiv |\Theta_k^{(0)}\rangle\langle\Theta_k^{(0)}| \\ \mathcal{Q}_k \equiv 1 - \mathcal{P}_k = \sum_{\mu\neq k} \boxed{|\Theta_\mu^{(0)}\rangle\langle\Theta_\mu^{(0)}|} \end{array} \right.$$

1-dimensional P space $|\Theta_k^{(0)}\rangle = \mathcal{P}_k|\Psi_k^\sigma\rangle$

Basis not necessarily known

- ► **SR expansions: known**
- ► **MR PGCM-PT : not known**

Frosini *et al.* (2023)

See Talk by M. Frosini on Tuesday

Expansion many-body methods

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Expansion many-body methods

Hamiltonian partitioning | **Unperturbed state** | **Fully correlated state**

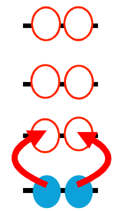
$H = H_0 + \boxed{H_1}$ → « Easy » to solve → $H_0|\Theta_k^{(0)}\rangle = E_k^{(0)}|\Theta_k^{(0)}\rangle$ → Expansion series → $|\Psi_k^\sigma\rangle = \boxed{\Omega_k}|\Theta_k^{(0)}\rangle$

Non-degenerate ind. excitations

Wave operator

Connects P to Q

Dynamical correlations due to H_1



Wave-operator expansion

Nature of the expansion?

Cost?

Expansion many-body methods

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Wave operator

Wave-operator expansion nature

$$\Omega_k \equiv \sum_{q=0}^{\cancel{\infty}\ q_{max}} c_q H_1^q$$ Perturbative

$$\Omega_k \equiv \sum_{q=0}^{\cancel{\infty}\ q_{max}} f_q(H_1)$$ Non-perturbative

$$|\Psi_k^{\sigma}\rangle = \sum_{q=0}^{\cancel{\infty}\ q_{max}} |\Theta_k^{(q)}\rangle$$

with

$$|\Theta_k^{(q)}\rangle = \sum_{\mu \neq k}^{\text{subset}(q)} \boxed{C_{k\mu}^{(q)}}|\Theta_\mu^{(0)}\rangle$$

When basis of Q-space known

Coefficients calculated at n_{dim}^{p} cost

- ► Tuncated expansion = n_{dim}^{p} **cost**
  → **Systematically improvable**
- ► Become quickly expansive as q ↗
  → **Typically $q_{max} \leq 3$**

Ground-state *ab initio* nuclear chart… then

Quasi-exact methods (>1990)

Examples: No core shell-model (NCSM)
Green's function monte carlo (GFMC)

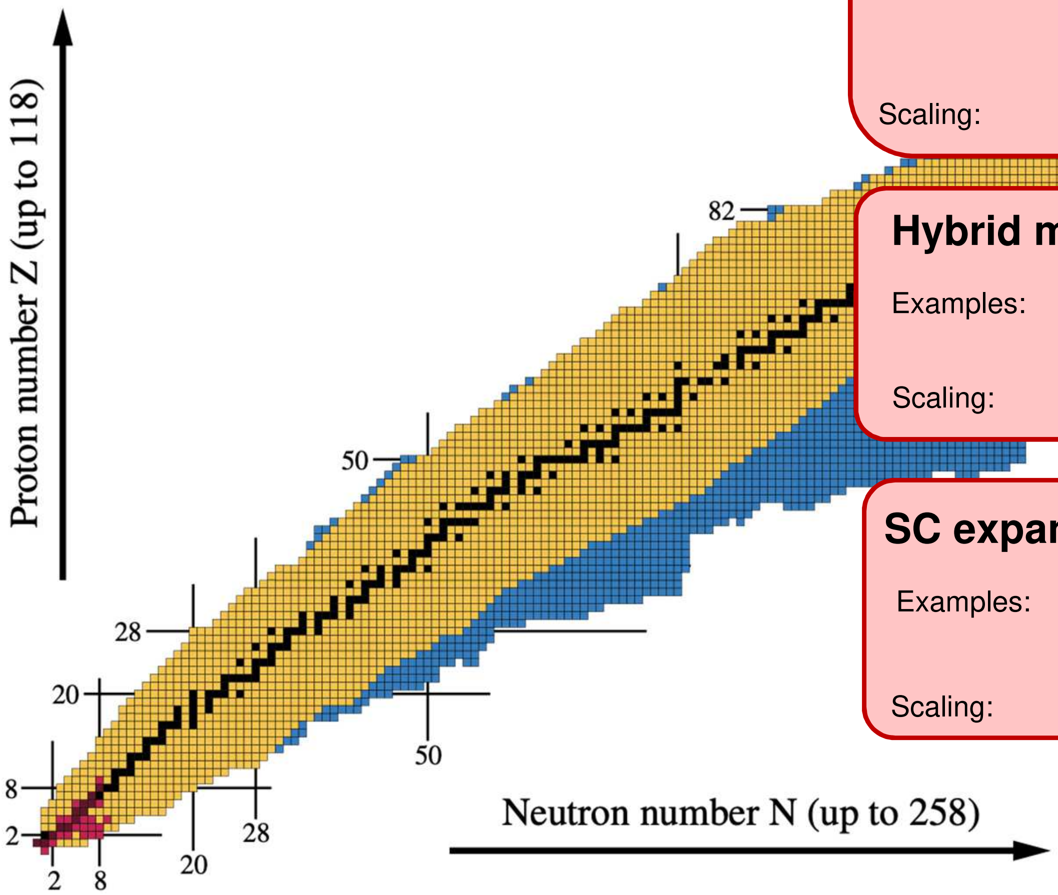
SC expansion methods for closed-shell (>2010)

Examples: Spherical many-body perturbation theory (sMBPT)
Spherical coupled cluster (sCC)
Spherical Dyson self consistent Green's function (sDSCGF)
Spherical in-medium similarity renormalization group (sIMSRG)

SB expansion methods for open-shell (>2013)

Examples: Deformed Bogoliubov many-body perturbation theory (dBMBPT)
Deformed Bogoliubov coupled cluster (dBCC)
Deformed Gorkov self-consistent Green's function (dGSCGF)
Deformed Bogoliubov in-medium similarity renormalization group (dBIMSRG)

Scaling: $O(A^n)$ → **CPU scalable (but memory limitations arise)**



Hybrid methods for open shell (>2015)

Examples: Valence-space in-medium similarity renormalization group (VS-IMSRG)
Multi-configuration perturbation theory (MCPT)

Scaling: $O(A^n) + O(A!)$ → **CPU not scalable**

SC expansion methods for open shell (>2022)

Examples: Projected Bogoliubov coupled cluster theory (PBCC)
Projected generator coordinate method perturbation theory (PGCM-PT)

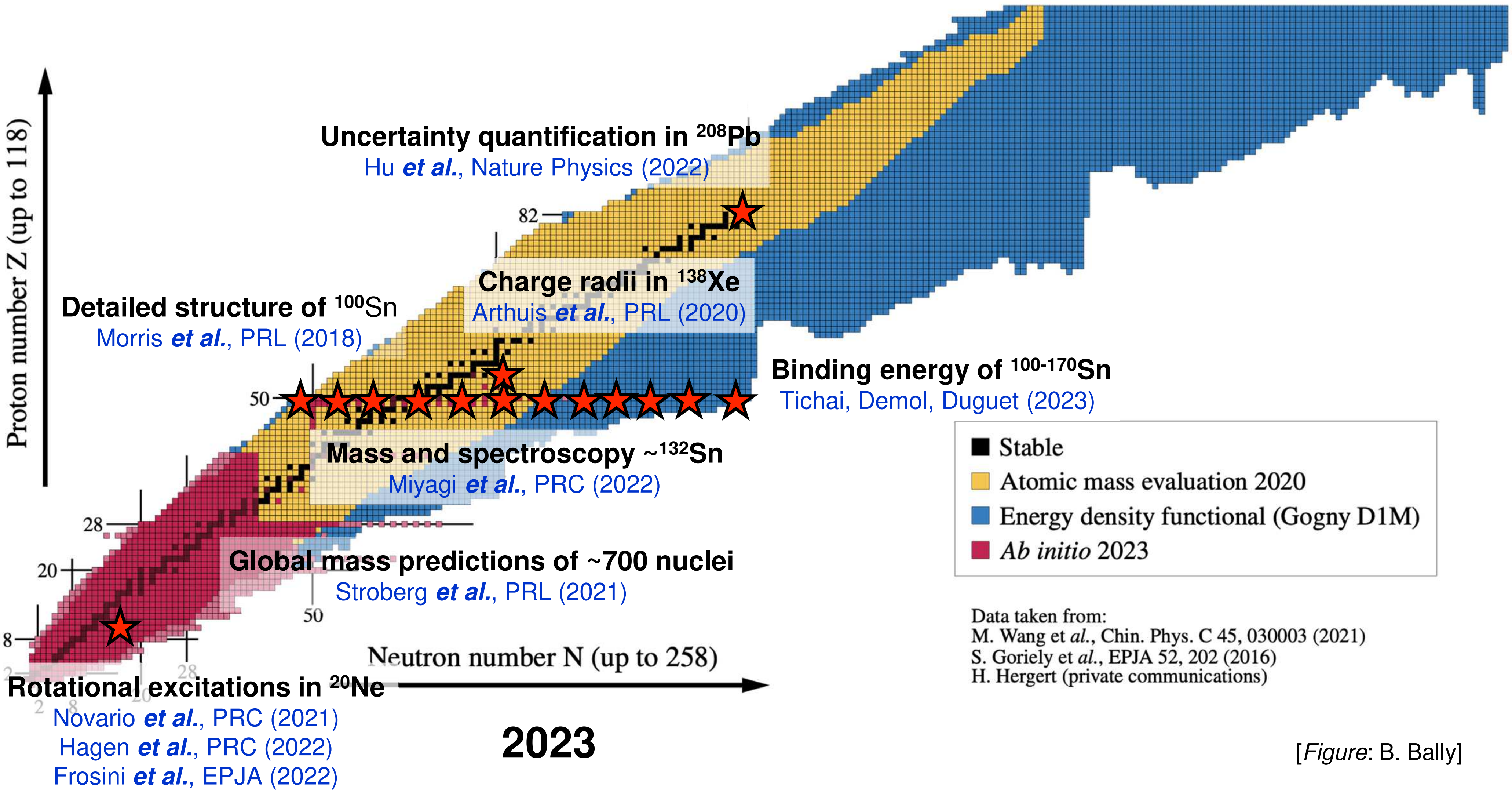
Scaling: $O(A^n)$ → **CPU scalable (but higher scaling)**

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)

2010

[*Figure*: B. Bally]

Ground-state *ab initio* nuclear chart… now!



2023

[*Figure*: B. Bally]

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Expansion many-body methods

Hamiltonian partitioning — $H = H_0 + H_1$ — « Easy » to solve →

Unperturbed state — $H_0|\Theta_k^{(0)}\rangle = E_k^{(0)}|\Theta_k^{(0)}\rangle$ — Expansion series →

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

Wave operator

Wave-operator expansion cost

CPU (naive) scaling

Mild scaling with A Bally, Bender (2021)

$q_{\max}$	(B)MBPT	(B)CC	(B)IMSRG	PGCM-PT
1	$O(\boxed{n_{\text{dim}}^4})$	$O(\boxed{n_{\text{dim}}^4})$	$O(\boxed{n_{\text{dim}}^4})$	$O(\boxed{n_{\text{proj}}n_{\text{gcm}}^2}\boxed{n_{\text{dim}}^4})$
2	$O(\boxed{n_{\text{dim}}^5})$	$O(n_{\text{dim}}^6)$	$O(n_{\text{dim}}^6)$	$O(n_{\text{proj}}n_{\text{gcm}}^2\boxed{n_{\text{dim}}^8})$
3	$O(n_{\text{dim}}^6)$	$O(\boxed{n_{\text{dim}}^8})$	$O(\boxed{n_{\text{dim}}^9})$	

Mean-field (like) cost

Impact of unperturbed state nature

Cost of high-precision (<1%)

Expansion many-body methods

$$H|\Psi^{\sigma}_{k}\rangle = E^{\tilde{\sigma}}_{k}|\Psi^{\sigma}_{k}\rangle$$ with $\sigma \equiv JM\Pi NZ \equiv \tilde{\sigma}M$

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Hamiltonian partitioning → « Easy » to solve → **Unperturbed state** → Expansion series → **Fully correlated state**

$$H = H_0 + H_1 \qquad H_0|\Theta^{(0)}_k\rangle = E^{(0)}_k|\Theta^{(0)}_k\rangle \qquad |\Psi^{\sigma}_{k}\rangle = \boxed{\Omega_k}|\Theta^{(0)}_k\rangle$$

Wave operator

Breaking SU(2), e.g. sBMBPT → Triax dBMBPT

Wave-operator expansion cost

<u>BMBPT(2)</u>

Spherical → Triaxial (e_{max}=12)

e_{max} = 6 → e_{max} = 12

sHO basis

↗ A

$e_{\max}$	$n_{\dim}$	$\tilde{n}_{\dim}$
2	40	12
4	140	30
6	336	56
8	660	90
10	1140	132
12	1820	182

m scheme j scheme

~x2 ~x2 ~x2 ~x2

~x10 at e_{max}=12

<u>BMBPT(2)</u>

~x2^5 = 32 each time

~x10^5 at e_{max}=12

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Wave-operator expansion cost

Eventually a memory bottleneck

► **3-body interaction requires $E_{3max} = 3e_{max}$**

-Recent major jump to $E_{3max} = 28$
-Jump from spherical ^{70}Ni to ^{208}Pb via e.g. sCC
…but not converged at $e_{max} = 14$

► **2-body tensors in doubly open-shell require m-scheme**

Ex: Nuclei A~70 converged with (e_{max}=12,E_{3max}=18)
-Axial dBMBPT(2) indeed ok with (12,18)
-Triaxial dBMBPT(2) nearly impossible with (8,14)

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m scheme j scheme

Techniques to alleviate n_{dim}^{p}

► Similarity renormalization group transformation

$H(\lambda) \equiv U(\lambda)HU^{\dagger}(\lambda)$ (to reduce n_{dim})

→ A-independent pre-processing of H

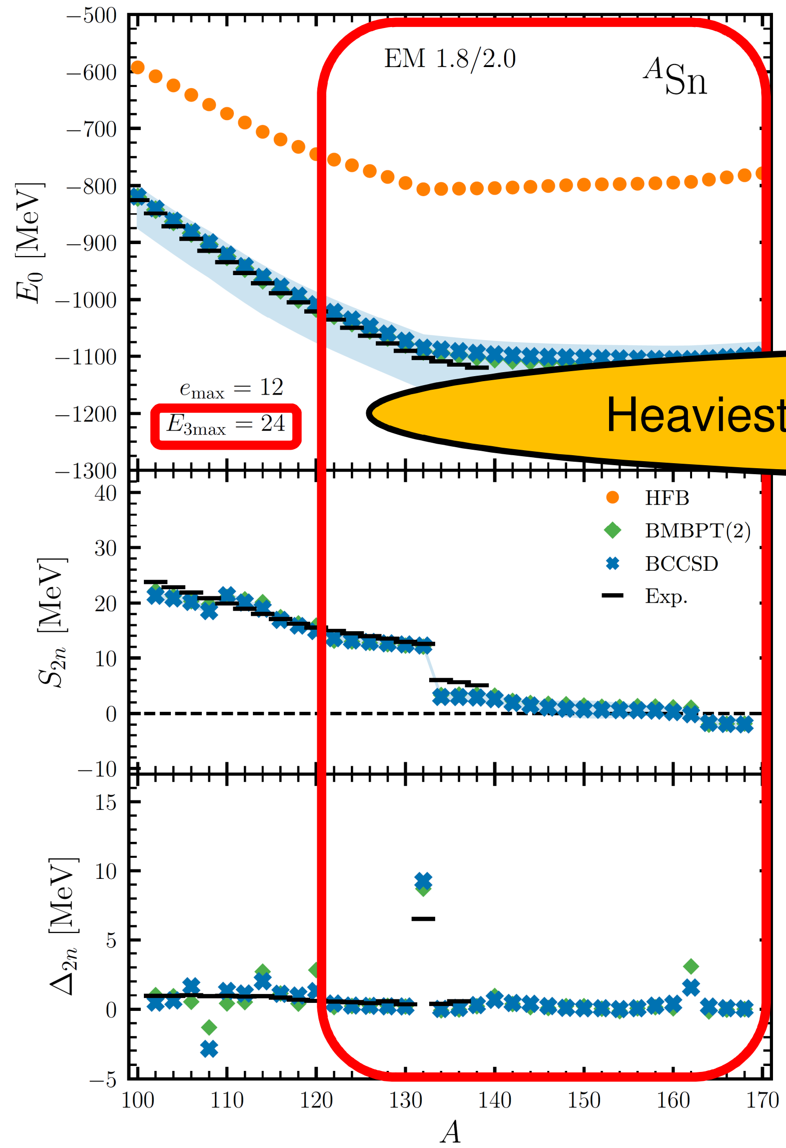
► Tensor factorization (to reduce p)

► Importance truncation (to reduce n_{dim})

► (B)MBPT natural orbital basis (to reduce n_{dim})

Example: ab initio calculation of tin open-shell isotopes

Tichai, Demol, Duguet (2023)



sHFB

$$|\Psi_k^A\rangle \equiv \boxed{\Omega_k}\boxed{|\Theta_k^{(0)}\rangle}$$

Break U(1)

Dynamical correlations

BMBPT **BCC**

∞

Heaviest open-shell nuclei computed ab initio so far

BMBPT	BCC
-q=0 : IQP	**-q=0 : IQP**
-q=1 : sHFB	**-q=1 : sBCCS = sHFB**
-q=2 : sBMBPT(2)	**-q=2 : sBCCSD** (BMBPT(3) complete)
-q=3 : sBMBPT(3)	**-q=3 : sBCCSDT**
⋮	⋮

Long semi-magic isotopic chain in A>100 accessible

- ► E_{3max} = 24 adapt Miyagi (2022) to Bogliubov-based method
- ► Significant uncertainty on S_{2n} for A>140 due to e_{max}=12

BCC uncertainty estimate due to missing triples

- ► Consistent with non-polynomial VS-IMSRG(2) in Ca
- ► **sBCCSD(T) + e_{max}=14 under way for drip-line prediction**

sBMBPT(2) ≈ sBCCSD because very « soft » interaction

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Global philosophy

Approximate solution **systematically improvable** towards **well-defined limit**

\+

Uncertainties evaluation, quantify what is missing

1) Is the ab initio EFT scheme the right way to go when futher increasing A?
2) Should one formulate another EFT anchored into the ab initio EFT?
3) **Can the EDF method as we know it (but revisited) be a good candidate?**

Ab initio versus EDF

Static correlations

Refined/Explicit description → **Ab initio EFT**

Refined/Explicit description → **EDF**

Ab initio EFT

- − High computational cost
  - → Limited reach
- + Systematically improvable
- + High predictive power

EDF

- + Low computational cost
  - → Mass table accessible
- − Not straightforwardly improvable
- − Limited predictive power

Refined/Explicit description → Ab initio EFT

Averaged/Implicit description → EDF

Dynamical correlations

Can the current version be improved?

Can anchoring it into ab initio help?

Need consistent formal scheme

Ab initio roadmap

Ab initio $H \equiv T + V + W$

χEFT Hamiltonian at N^{k}LO contains up to, e.g. 3NF

$$H(\lambda) \equiv U(\lambda) H U^{\dagger}(\lambda) = T + V(\lambda) + W(\lambda) + \cancel{\cdots}$$

Vacuum SRG transformed H truncated up to, e.g., 3NF

→ A-*independent* pre-processing of H

$$H \equiv \bar{h}^{(0)}[\rho] + \bar{h}^{(1)}[\rho] + \bar{h}^{(2)}[\boxed{\rho}] + \cancel{\bar{h}^{(3)}}[\rho]$$

See Talk by M. Frosini on Tuesday

Frosini *et al.* (2023)

Rank-reduction up to, e.g., 2N operator

→ A-*dependent* Hamiltonian $\bar{H}[\rho]$ (generalizes NO2B)

Symmetry-conserving one-body density matrix of auxiliary, e.g. sHFB, state

dHFB state → start for symmetry-*breaking* SR expansion

PGCM state → start for symmetry-*conserving* MR expansion

$\left(|\Theta_k^{(0)}\rangle, H_0\right)$ **by mininimizing** $\mathcal{E}_k = \langle \Theta_k^{(0)} | H | \Theta_k^{(0)} \rangle$

Unperturbed state including static correlations

→ Mean-field-like cost

Effective Hamiltonien $H^{\text{eff}}_{|\Theta_k^{(0)}\rangle}$ in 1d P space

$$E_k^{\tilde{\sigma}} \equiv \frac{\langle \Theta_k^{(0)} | H | \Psi_k^{\sigma} \rangle}{\boxed{\langle \Theta_k^{(0)} | \Psi_k^{\sigma} \rangle}} = \langle \Theta_k^{(0)} | \boxed{H\Omega_k} | \Theta_k^{(0)} \rangle = \sum_{q=0}^{2} \langle \Theta_k^{(0)} | \boxed{H f_k^{(q)}(H_1)} | \Theta_k^{(0)} \rangle$$

=1 intermediate normalization

e.g. PT(2)

(truncated) expansion including dynamical correlations

→ Polynomial cost (potentially high)

▶ High-cost nucleus-dependent $H^{\text{eff}}_{|\Theta_k^{(0)}\rangle}$

▶ Unperturbed-state (e.g. P-space) dependent

→ dHFB vs PGCM and ground vs excited state

→ Different beast depending on [P,R(θ)]=0 or not

Frosini *et al.* (2023)

→ Doable for PGCM P-space for the first time

→ At second order in perturbation theory (PGCM-PT(2))

EDF roadmap

EDF

Functional « generator »

→ Zero cost

$$H^{\text{gen}} \equiv T + \sum_i c_i V_i^{\text{gen}} + \sum_j c_j W_j^{\text{gen}}$$

dHFB state → symmetry-*breaking* SR EDF realization
PGCM state → symmetry-*conserving* MR EDF realization

Hopefully exact

Unperturbed state including static correlations

→ Mean-field-like cost

$|\Theta_k^{(0)}\rangle$ **by mininimizing** $E_k^{\tilde{\sigma}} = \langle \Theta_k^{(0)} | H^{\text{gen}} | \Theta_k^{(0)} \rangle$

Explicitly handles quickly varying static correlations

Implicitly mocks up slowly varying dynamical correlations

Ab initio versus EDF

Ab initio

$$H \equiv T + V + W$$

$$H(\lambda) \equiv U(\lambda) H U^{\dagger}(\lambda) = T + V(\lambda) + W(\lambda) + \cancel{\ldots}$$

$$H \equiv \bar{h}^{(0)}[\rho] + \bar{h}^{(1)}[\rho] + \bar{h}^{(2)}[\rho] + \cancel{\bar{h}^{(3)}}[\rho]$$

$\left(|\Theta_k^{(0)}\rangle, H_0\right)$ **by mininimizing** $\mathcal{E}_k = \langle\Theta_k^{(0)}|H|\Theta_k^{(0)}\rangle$

$$E_k^{\sigma} \equiv \frac{\langle\Theta_k^{(0)}|H|\Psi_k^{\sigma}\rangle}{\langle\Theta_k^{(0)}|\Psi_k^{\sigma}\rangle} = \langle\Theta_k^{(0)}|\underbrace{\boxed{H\Omega_k}}_{H^{\text{eff}}_{|\Theta_k^{(0)}\rangle}}|\Theta_k^{(0)}\rangle = \sum_{q=0}^{\infty}\langle\Theta_k^{(0)}|H f_k^{(q)}(H_1)|\Theta_k^{(0)}\rangle$$

EDF

$$H^{\text{gen}} \equiv T + \sum_i c_i V_i^{\text{gen}} + \sum_j c_j W_j^{\text{gen}}$$

Obviously not the same

$|\Theta_k^{(0)}\rangle$ **by mininimizing** $E_k^{\sigma} = \langle\Theta_k^{(0)}|\boxed{H^{\text{gen}}}|\Theta_k^{(0)}\rangle$

Dependence of $H^{\text{eff}}_{|\Theta_k^{(0)}\rangle}$ on P-space character

<u>Option 1</u>: SR EDF realization = potentially exact

$\rightarrow$ $H^{\text{gen}}_{\text{SR}} = H^{\text{gen}}_{\text{MR}}$ has no formal justification

$\rightarrow$ Not only fit but also formal content

<u>Option 2</u>: SR EDF realization = approximation to MR one

$\rightarrow$ $H^{\text{gen}} \equiv H^{\text{gen}}_{\text{MR}}$ is the only relevant object

Time for EDF practitioners to clarify this long-running story!

Contents

Concretely anchoring EDF into the ab initio EFT

Option 1: use ab initio results as pseudo-data to constrain parameters of pre-defined empirical ansatz of H^{gen}

► Infinite-matter equation of state at the SR level — Chabanat *et al.* (1997), …, Marino *et al.* (2021)

► Finite-nuclei binding energies at the SR level — Salvioni *et al.* (2020)

→ **If performed at SR level cannot be then employed at MR level**

→ **Ab initio predictions must be accurate enough (some *differential* quantities such as S_{2n} OK today)**

→ **Ansatz for H^{gen} must be rich/flexible enough (to model A-dependent dynamical correlations): probably not today**

Option 2: use ab initio expansion method to derive educated analytical form of H^{gen}

► MBPT(2) in INM at SR level $H^{\text{eff}}_{\text{SR}} \approx (H + H R H_1)_{|\Phi_{\text{INM}}\rangle}$ — Moghrabi *et al.* (2010)

► Many-body-based in low-density INM at SR level $H^{\text{eff}}_{\text{SR}} \approx (H\,\Omega)_{|\Phi_{\text{ldINM}}\rangle}$ — Yang et al. (2016), …, Burrello *et al.* (2021)

► DME in finite nuclei at SR level $H^{\text{eff}}_{\text{SR}} \approx (H_{\text{DME}} + \Delta H^{\text{gen}})_{|\Phi\rangle}$ — Stoitsov *et al.* (2010), …, Zurek *et al.* (2023)

See Talk by L. Zurek on Wednesday

Option 2 bis: use ab initio expansion method to compute full-fledged numerical $H^{\text{eff}}_{|\Theta^{(0)}_k\rangle}$ to be matched on H^{gen} ansatz

► MBPT(2) in finite nuclei **at MR level** $H^{\text{eff}}_{\text{MR}} \approx (H + H R H_1)_{|\Theta^{\sigma}_k\rangle}$ — Duguet *et al.* (2023)

Connecting MR-EDF to ab initio in ^{20}Ne

PGCM-PT(2)
- ► H = N^3LO 2N + VSRG (λ_{srg}=1.88 fm^{-1}) + N^2LO 3N (Λ_{3N} = 2 fm^{-1})
- ► H → H[ρ] via rank-reduction method

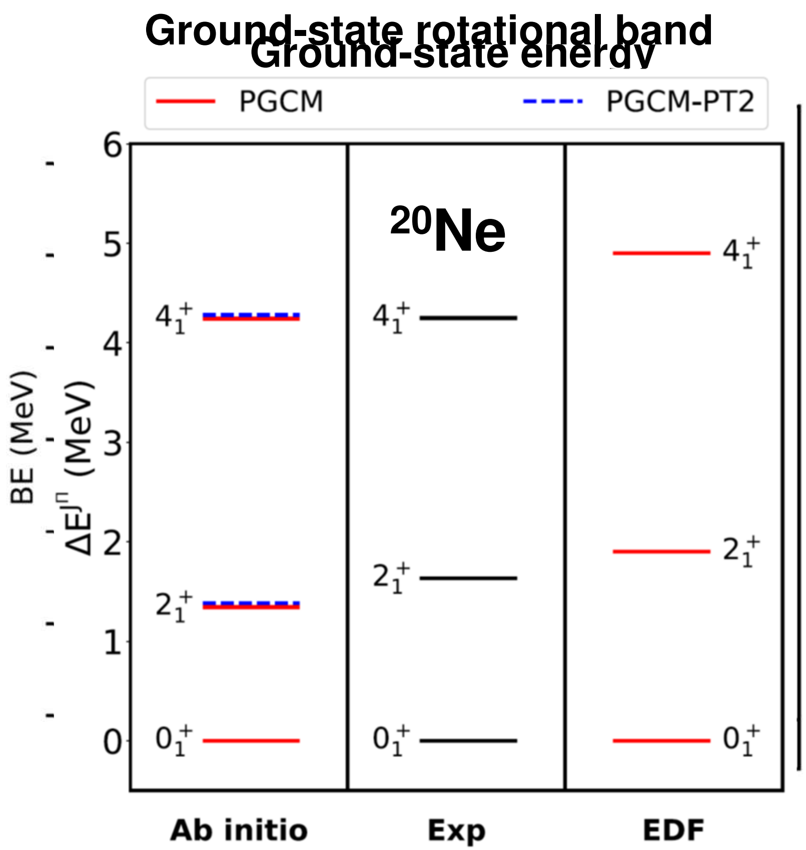
MR-EDF
- ► H^{gen} = DD-PC1

Numerical setting
- ► e_{max} = 6, hω = 20 MeV
- ► dHFB states with β_{20} in [0.3,0.8]
- ► Proj N, Z and J

Duguet *et al.* (2023)

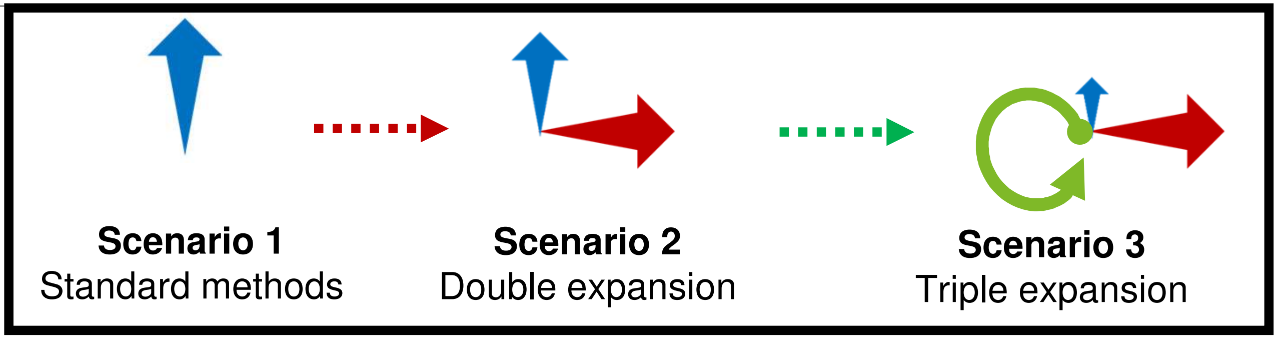
Ground-state energy
- ► **sHFB→dHFB→PGCM very different in absolute**
  - → Sequence rather consistent however
  - → PGCM ~45MeV unbound with H vs ok with $H^{\rm gen}$
- ► PGCM-PT(2) good via 42 MeV dynamical correlations
  - → PGCM ok with $H^{\rm eff}_{\rm MR} \approx (H + HRH_1)_{|\Theta^\sigma_k\rangle}$

Rotational excitations
- ► **PGCM and PGCM-PT(2) spectra identical**
  - → J^π = 0^+, 2^+ and 4^+ shifted down by same 42 MeV
- ► PGCM/PGCM-PT(2) close to Exp. and MR-EDF



Intermediate conclusions
- ► $H^{\rm eff}_{\rm MR} \approx (H + HRH_1)_{|\Theta^\sigma_k\rangle}$ good candidate for $H^{\rm gen}_{\rm MR}$
- ► Expensive $n^8_{\rm dim}$ dynamical correlations (key to BE)
- ► **Can one reduce the cost/obtain alternate $H^{\rm eff}_{\rm MR}$?**

Many-body expansion methods and pre-processing



$U(s)HU^{\dagger}(s)$

Dynamical Correlations

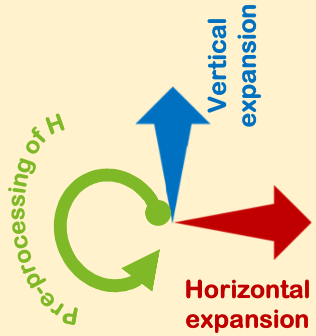
Pre-processing

$$H|\Psi_n^A\rangle = \mathrm{E}_n^A|\Psi_n^A\rangle$$

MR-IMSRG+PGCM-PT = Triple expansion for an optimal grasping of correlations

a. **Preprocessing of Hamiltonian** via MR-IMSRG with respect to PGCM state
b. PGCM to **capture static correlations** at low computational cost
c. PGCM-PT(2) to bring **remaining dynamical correlations**

Three non-orthogonal « auto-adapting » (no double counting) processes

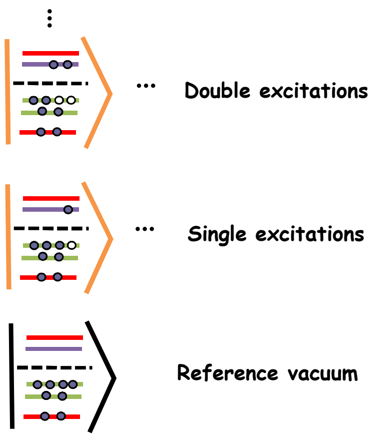


$$H_0|\Theta_k^{(0)}\rangle = E_k^{(0)}|\Theta_k^{(0)}\rangle$$

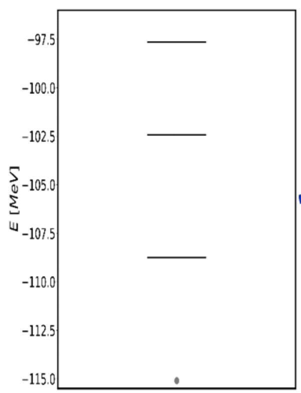
Vertical expansion

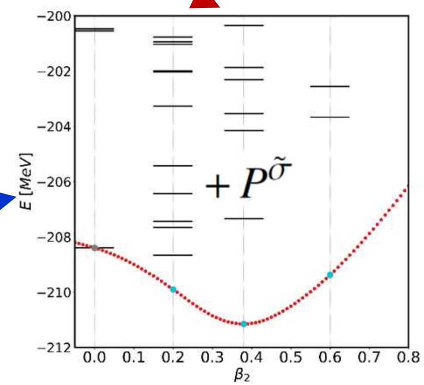
Dynamical Correlations

$$|\Psi_k^A\rangle \equiv \Omega_k|\Theta_k^{(0)}\rangle$$



SR expansion





PGCM-PT expansion

[Frosini et al., EPJA58 (2022) 64]

Ab initio versus EDF

Ab initio

$$H \equiv T + V + W$$

$$H(\lambda) \equiv U(\lambda) H U^{\dagger}(\lambda) = T + V(\lambda) + W(\lambda) + \cancel{\ldots}$$

$$H \equiv \bar{h}^{(0)}[\rho] + \bar{h}^{(1)}[\rho] + \bar{h}^{(2)}[\rho] + \cancel{\bar{h}^{(3)}}[\rho]$$

$$\left(|\Theta_k^{(0)}\rangle, H_0\right) \quad \text{by mininimizing} \quad \mathcal{E}_k = \langle \Theta_k^{(0)} | H | \Theta_k^{(0)} \rangle$$

$$E_k^{\tilde{\sigma}} \equiv \frac{\langle \Theta_k^{(0)} | H | \Psi_k^{\sigma} \rangle}{\langle \Theta_k^{(0)} | \Psi_k^{\sigma} \rangle} = \langle \Theta_k^{(0)} | H \Omega_k | \Theta_k^{(0)} \rangle = \sum_{q=0}^{\infty} \langle \Theta_k^{(0)} | H f_k^{(q)}(H_1) | \Theta_k^{(0)} \rangle$$

Unitarily transformed such that the expansion corrections are reduced… or even cancelled, i.e. $\Omega_k(\text{"}\infty\text{"}) \approx 1$

$$E_k^{\tilde{\sigma}} = \langle \Theta_k^{(0)}(s) | \boxed{H(s)} \boxed{\Omega_k(s)} | \Theta_k^{(0)}(s) \rangle$$

with $\quad H(s) \equiv U(s) H U^{\dagger}(s) \qquad |\Theta_k^{(0)}(s)\rangle \equiv U(s) |\Theta_k^{(0)}\rangle$

EDF

$$H^{\text{gen}} \equiv T + \sum_i c_i V_i^{\text{gen}} + \sum_j c_j W_j^{\text{gen}}$$

$$|\Theta_k^{(0)}\rangle \quad \text{by mininimizing} \quad E_k^{\tilde{\sigma}} = \langle \Theta_k^{(0)} | \boxed{H^{\text{gen}}} | \Theta_k^{(0)} \rangle$$

$$H(\text{"}\infty\text{"}) \approx H_{\text{MR}}^{\text{eff}}$$

becomes directly the P-space effective Hamiltonian

Connecting MR-EDF to ab initio in ^{20}Ne

Pre-processing H via MR-IMSRG with respect to the PGCM state $H(s) \equiv U(s) H U^{\dagger}(s)$ Duguet *et al.* (2023)

① **Initial condition** $H(0) \equiv H \approx h^{(0)} + h^{(1)} + h^{(2)}$

② **Flow equation** $\dfrac{dH(s)}{ds} = [\eta(s), H(s)]$

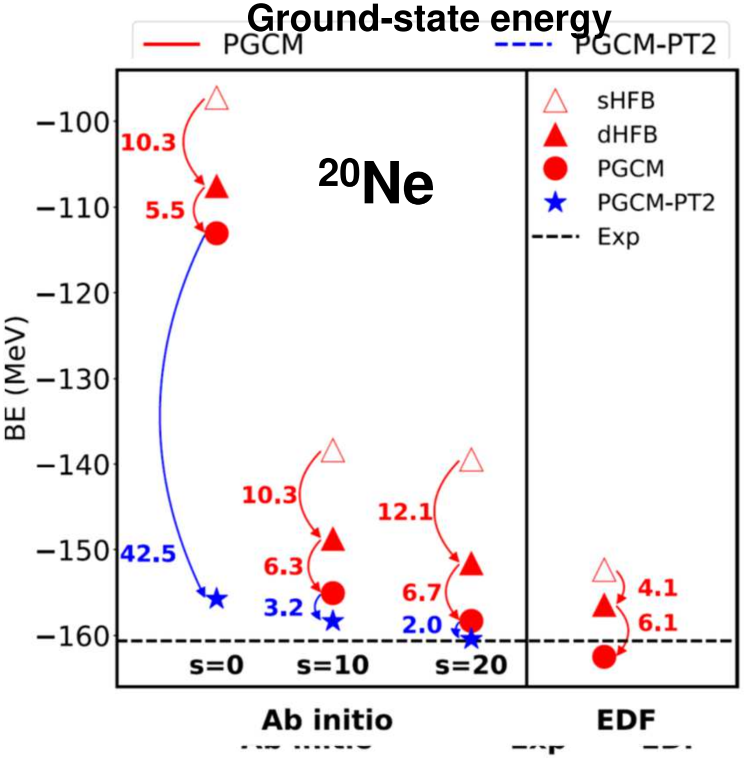
Generator parameterizes the unitary transformation
- ►Chosen to (quasi) decouple PGCM state from complementary Q space
- ►Reshuffles dynamical correlations into H(s)

Normal ordering with respect to PGCM state
- ►Kutzelnigg-Mukherjee generalized Wick Theorem
- ►Normal-ordered (NO) two-body approximation

Truncated up to 2-body NO operators = MR-IMSR(2)
- ►Unitarity violation as flow parameter s grows
- ► $n_{dim}{}^{6}$ cost

Hergert *et al.* (2016), ..., Yao et al. (2020)

Ground-state rotational band
Ground-state energy



Ground-state energy
- ►sHF reference point drastically lowered (45 MeV)
- ►Static correlations slightly enhanced (15 MeV → 18 MeV)
- ►**Dynamical PT correlations drastically reduced (42 MeV → 2 MeV)**
  - → Remaining not entirely negligible (~1.5%)
- ►**Hierarchy of correlations with $H(\text{''}\infty\text{''})$ consistent with MR-EDF**

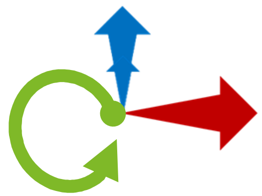
Ground-state rotational band
- ►PGCM spectrum slightly spread by MR-IMSRG pre-processing
- ►**PT effects on spectra consistently increased**
  - → Effect of dynamical correlations on spectrum non negligible

Conclusions
- ► $H(\text{''}\infty\text{''})$ ideal candidate for $H^{\text{gen}}_{\text{MR}}$
- ►**Must further reduce coupling to Q space**

Contents

Connecting MR-EDF to ab initio

Duguet *et al.* (2023)



① $H^{\mathrm{eff}}_{\mathrm{MR}} \approx (H + HRH_1)_{|\Theta^\sigma_k\rangle}$

- ►Very expensive n_{dim}^8
- ►Not a simple form

② $$H^{\mathrm{eff}}_{\mathrm{MR}} \approx H(\text{"}\infty\text{"}) \equiv h^{(0)}(\text{"}\infty\text{"}) + \frac{1}{(1!)^2}\sum_{\substack{a_1\\b_1}} h^{a_1}_{b_1}(\text{"}\infty\text{"})A^{a_1}_{b_1} + \frac{1}{(2!)^2}\sum_{\substack{a_1a_2\\b_1b_2}} h^{a_1a_2}_{b_1b_2}(\text{"}\infty\text{"})A^{a_1a_2}_{b_1b_2} + \ldots$$

- ►Expensive n_{dim}^6
- ► Straight Hamiltonian with same phenomenology (i.e. mean-field) EDF practitioners are used to
- ► Numerical access to 0-, 1- and 2-body ME $\left\{h^{(0)}(\text{"}\infty\text{"}), h^{a_1}_{b_1}(\text{"}\infty\text{"}), h^{a_1a_2}_{b_1b_2}(\text{"}\infty\text{"})\right\}$

Implicit (numerical) functionals of irreducible density matrices of PGCM state

$$\lambda^{a_1}_{b_1} \equiv \langle\Theta^\sigma_k|A^{a_1}_{b_1}|\Theta^\sigma_k\rangle$$

$$\lambda^{a_1a_2}_{b_1b_2} \equiv \langle\Theta^\sigma_k|A^{a_1a_2}_{b_1b_2}|\Theta^\sigma_k\rangle - \mathcal{A}\left(\lambda^{a_1}_{b_1}\lambda^{a_2}_{b_2}\right)$$

$$\lambda^{a_1a_2a_3}_{b_1b_2b_3} \equiv \langle\Theta^\sigma_\mu|A^{a_1a_2a_3}_{b_1b_2b_3}|\Theta^\sigma_k\rangle - \mathcal{A}\left(\lambda^{a_1}_{b_1}\lambda^{a_2}_{b_2}\right) - \mathcal{A}\left(\lambda^{a_1a_2}_{b_1b_2}\lambda^{a_3}_{b_3}\lambda^{a_3}_{b_3}\right)$$

$$\vdots$$

Potential research projects

- ►Improve decoupling for excited states: richer PGCM and Ensemble NO
- ►**Build ab initio-rooted MR-EDF generator** H^{gen}
  - → Generate ME of $H^{\mathrm{eff}}_{\mathrm{MR}} \approx H(\text{"}\infty\text{"})$ in selected set of nuclei
  - → Empirically investigate A-dependence of ME
  - → Test ansatz for H^{gen} with appropriate density dependences
  - → **Can this know-how eventually help to build a proper EFT for H^{gen}?**

Method	HFB	PGCM	PGCM-PT(2)	MR-IMSRG(2|3)	FCI
Runtime	$O(n^4_{\mathrm{dim}})$	$O(n_{\mathrm{proj}} n^2_{\mathrm{gcm}} n^4_{\mathrm{dim}})$	$O(n_{\mathrm{proj}} n^2_{\mathrm{gcm}} n^8_{\mathrm{dim}})$	$O(n^{6\|9}_{\mathrm{dim}})$	$O(n^A_{\mathrm{dim}})$
Storage	$O(n^4_{\mathrm{dim}})$	$O(n^4_{\mathrm{dim}})$	$O(n^2_{\mathrm{gcm}} n^8_{\mathrm{dim}})$	$O(n^{4\|6}_{\mathrm{dim}})$	$O(n^A_{\mathrm{dim}})$

Looking forward to ab initio PGCM-related projects

CALCULATIONS

Numerical optimization
- →Algorithmic improvements
- →Importance selections
- →Natural basis
- →Tensor factorization

Non-yrast states
- →Orthogonalization

Individual excitations
- →Extended PGCM ansatz

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

PGCM-PT & MR-IMSRG

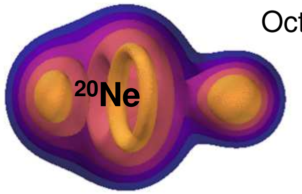
AB INITIO-BASED EDF

[Duguet *et al.* EPJA 2023]

H(s)+PGCM «=» MR-EDF

Cancel PT corrections
- →Ensemble MR-IMSRG evolution
- →Enriched PGCM ansatz

Ab initio rooted MR-EDF
- →Empirical H^{gen} «=» H(s)?
- →Invent EFT for H(s)?



Octupole vibration (^{16}O+α ↔ ^{12}C + 2α) at 7.2 MeV

[Beaujeault-Taudière, et al., PRC 2023]
[Frosini et al., unpublished]

Spectroscopy from PGCM

Excellent first account with H(0)
- →Low-lying states
- →Giant resonances

QRPA = harmonic limit of GCM Jancovici, Schiff (1964)
- →FT triaxial QRPA (QFAM) with NN+3N

Giant resonances with PQRPA
- →Development of «P»QRPA **See Talk by A. Porro on Thursday**
- →Development pf PQRPA Federschmidt, Ring (1985)

Statistical uncertainties from H
- →Development of PGCM-EC **See Talk by A. Roux on Friday**

Collaborators on ab initio many-body methods/calculations

B. Bally
J.-P. Ebran
M. Frosini
A. Porro
A. Roux
A. Scalesi
V. Somà
G. Stellin

P. Demol

C. Barbieri

G. Hagen
T. Papenbrock

H. Hergert

P. Navratil

A.Tichai
P. Arthuis
R. Roth

T. R. Rodriguez

J. M. Yao

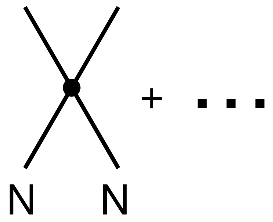
The « ab initio » theoretical scheme

[Weinberg, Gasser, Leutwyler, van Kolck, ..]

Ab initio = Chiral EFT = low-energy realization of QCD

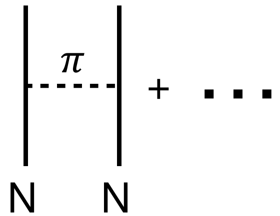
Effective degrees of freedom: Nucleons; Pions (m_π = 150MeV)

Manifestation of spontaneous chiral symmetry breaking at low energy

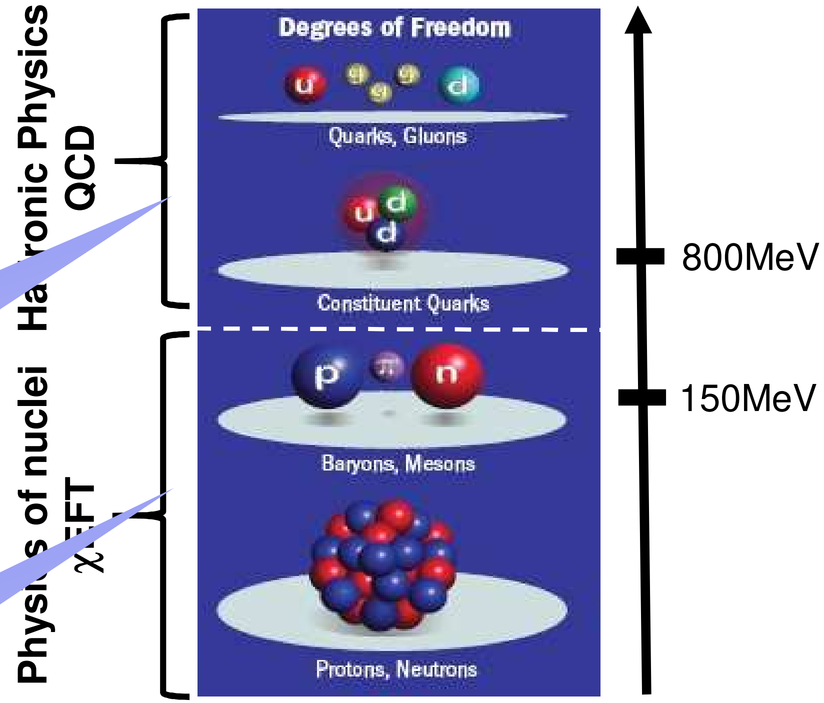


High-energy via contact interactions

∞ # operators compatible with symmetries of QCD



Pion-driven interactions explicit

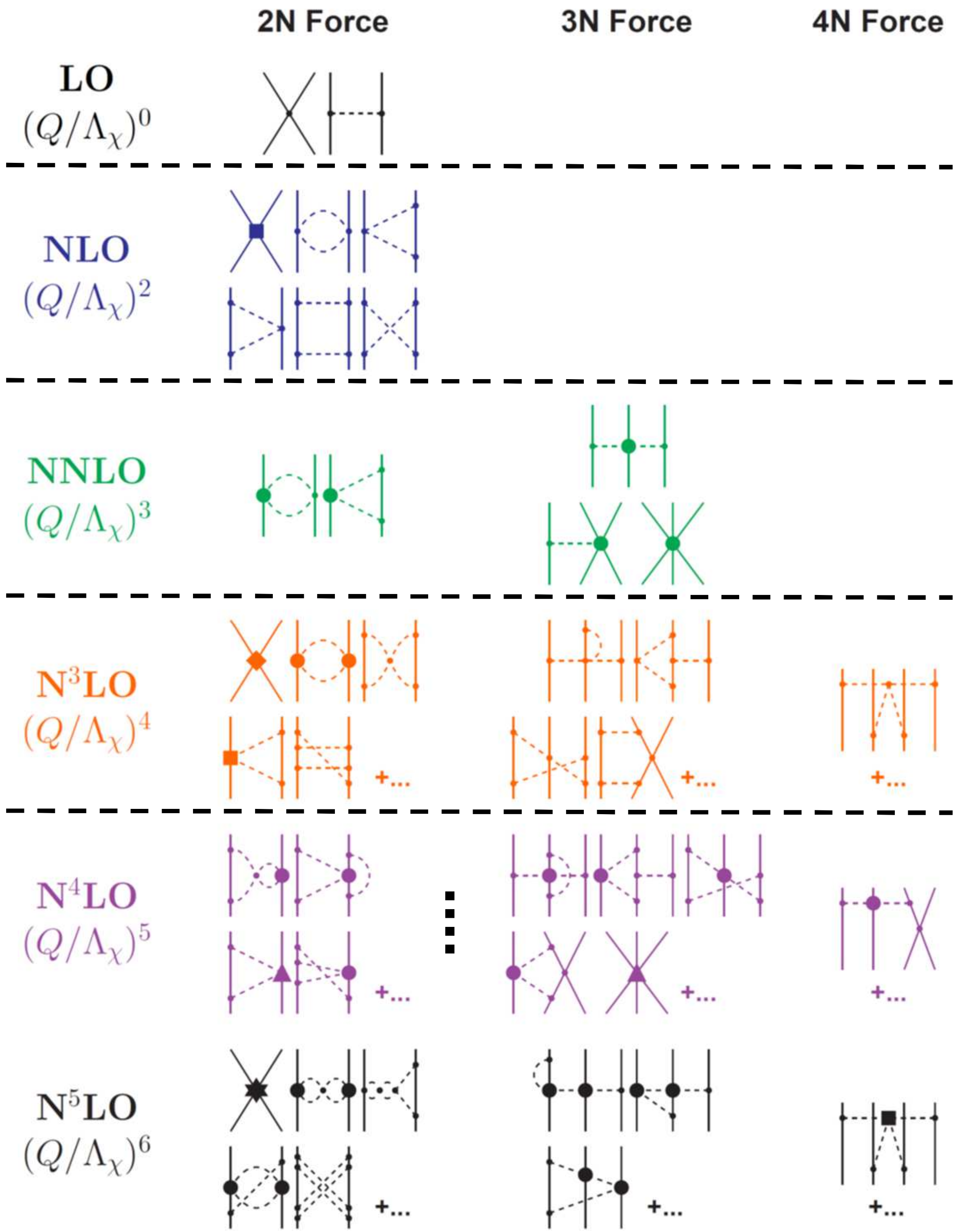


1) Organize according to expected importance = Power Counting

2) Truncate at working order k → Systematic uncertainty (1)

3) Adjust Low Energy Couplings → Statistical uncertainty (2)

Chiral effective field theory = interactions expansion



$$H_{\mathrm{LO}} \equiv T + V^{2\mathrm{N}}_{\mathrm{LO}}$$

$$H_{\mathrm{NLO}} \equiv T + V^{2\mathrm{N}}_{\mathrm{NLO}}$$

$$H_{\mathrm{N^2LO}} \equiv T + V^{2\mathrm{N}}_{\mathrm{N^2LO}} + V^{3\mathrm{N}}_{\mathrm{N^2LO}}$$

$$H_{\mathrm{N^3LO}} \equiv T + V^{2\mathrm{N}}_{\mathrm{N^3LO}} + V^{3\mathrm{N}}_{\mathrm{N^3LO}} + V^{4\mathrm{N}}_{\mathrm{N^3LO}}$$

$$\vdots$$

$$\boxed{H_{\mathrm{N^kLO}} \equiv T + V^{2\mathrm{N}}_{\mathrm{N^kLO}} + V^{3\mathrm{N}}_{\mathrm{N^kLO}} + \ldots}$$

Major challenges

- ►Can k-body, k>3, be omitted in A>>3?
- ►N$^{3/4}$LO 2N for high precision; 3N? 4N?
- ►More profound issues…

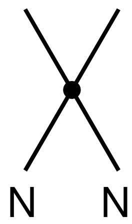
The « ab initio » theoretical scheme

[Weinberg, Gasser, Leutwyler, van Kolck, ..]

Chiral EFT = low-energy realization of QCD

Effective degrees of freedom: Nucleons; Pions ------ m_π = 150MeV

Manifestation of chiral symmetry breaking at low energy



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High-energy via contact interactions

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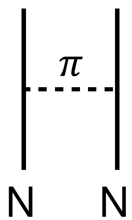

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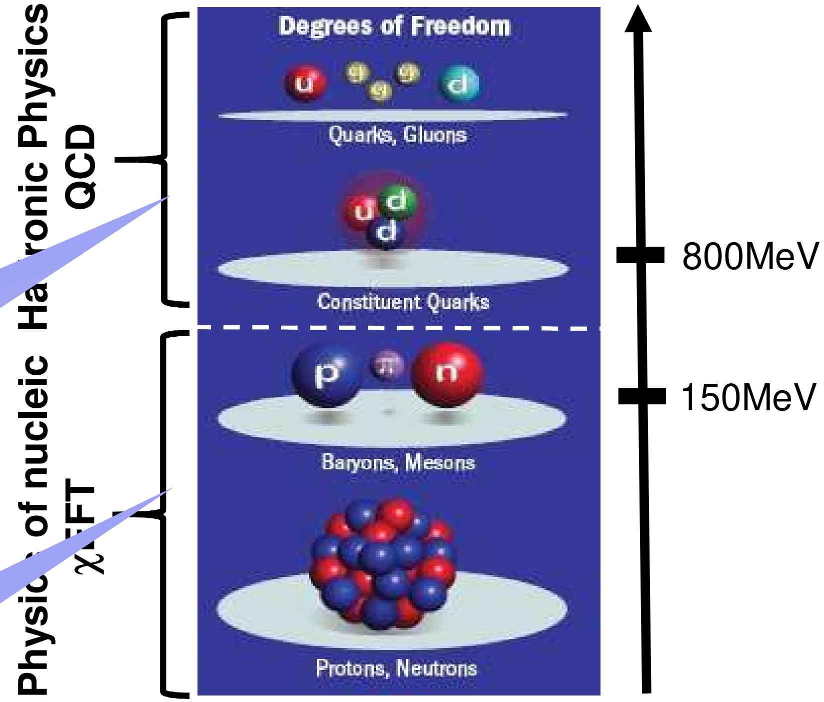
Pion-driven interactions explicit

1) Organize according to expected importance = Power Counting

2) Truncate at working order k → Systematic uncertainty (1)

3) Adjust Low Energy Couplings → Statistical uncertainty (2)



4) **Solve A-body Schrödinger Equation**

$$H_{\mathrm{N}^k\mathrm{LO}}|\Psi_n^A\rangle = E_n^A|\Psi_n^A\rangle$$

Quickly impossible to do exactly
→ **Systematic error (3)**

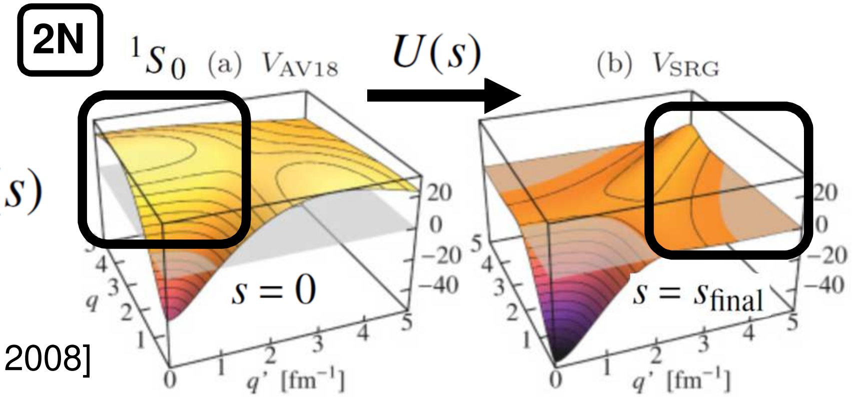
- ► What accuracy can be reached?
- ► **How does this evolve with A=N+Z?**
- ► **All types of nuclei equivalent?**

Similarity renormalization group transformation of H

►Need very large n_{dim} (e_{max}) due to **hard core of V^{2N}** → large ME between low and high basis states

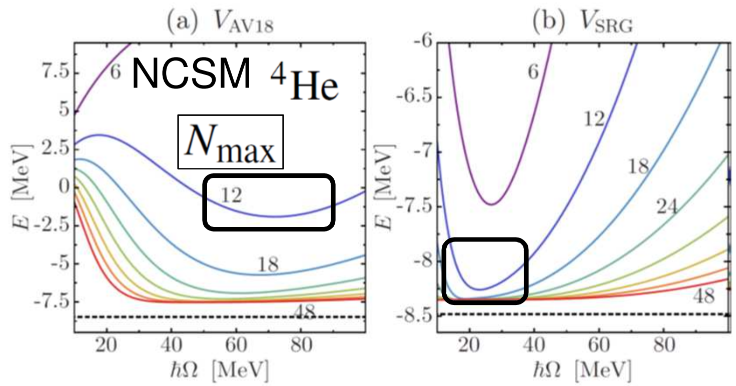
→ Unitary **Similarity Renormalization Group** (SRG) transformation of H to tame it down

$$H(s) = U(s)HU^{\dagger}(s)$$



[Roth, Reinhardt, Hergert 2008]

Relative momentum basis of $\mathcal{H}_2$



►Drastically accelerated convergence / n_{dim}

►Need

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

►Low to high off-diagonal matrix elements suppressed

►Needed: **JT-coupled SRG-evolved 3N** matrix elements

→ Mass A~50 (e_{1max} = 13 / e_{2max} = 26 / e_{3max} = 16)

2NF ~ 2GB 3NF ~ 25GB

SRG = huge help for ab initio calculations up to A~80

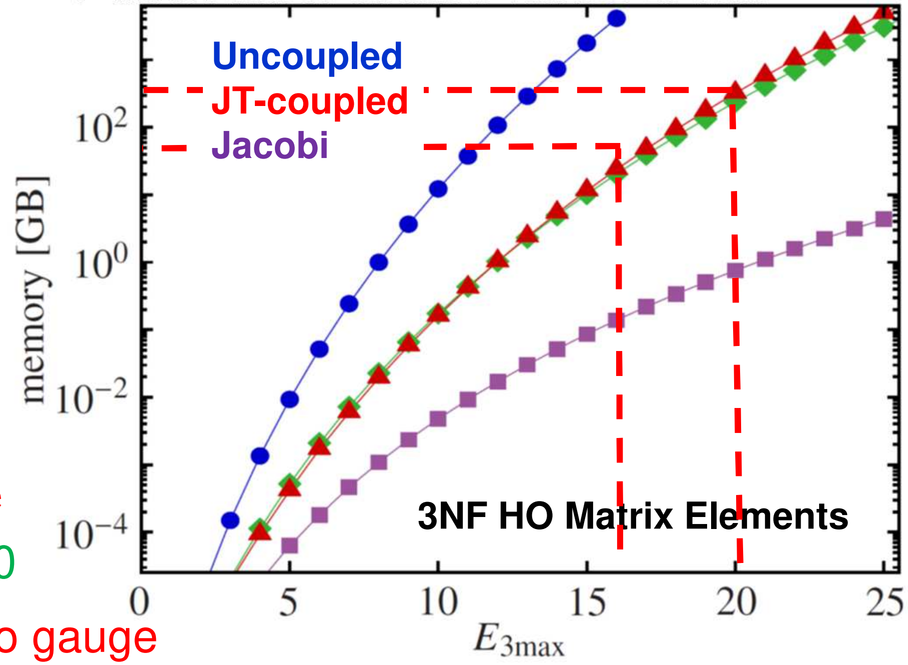
→ Mass A~100 (e_{1max} = 15 / e_{2max} = 30 / e_{3max} = 20)

2NF ~ 7GB 3NF ~ 350GB → **Too much to handle**

More tricks needed to reduce the load to go beyond A~100

Eventually truncating n_{dim} is always a source of error (3) to gauge

[R. Roth *et al.*, PRC90 (2014) 024325]

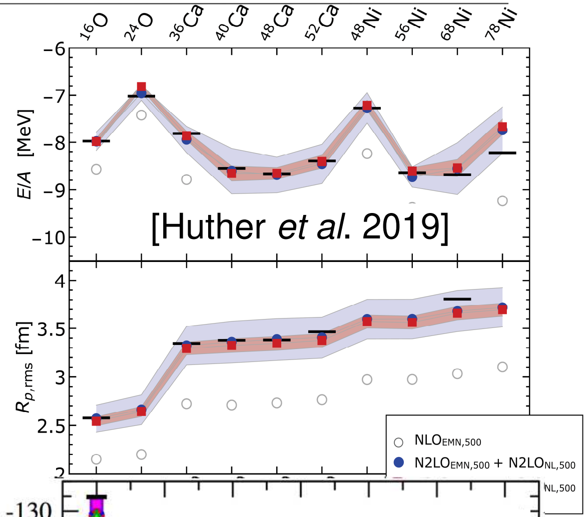


Systematic uncertainties

Truncated χEFT Hamiltonian expansion = Error (1)

$$H = T + \boxed{V_{\mathrm{LO}} + V_{\mathrm{NLO}} + V_{\mathrm{N^2LO}}} + \cdots$$

Order-by-order estimate [Binder et al. 2018]
BE and radii at N³LO: 5-6% up to A~80

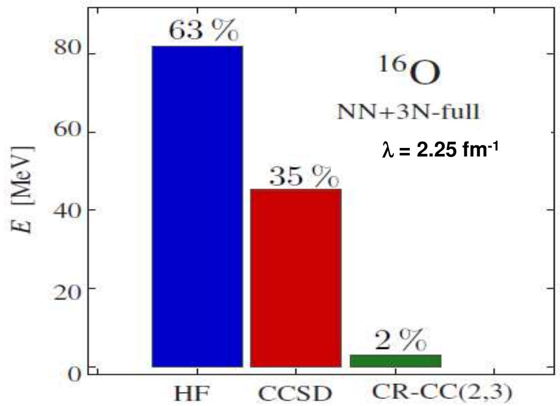


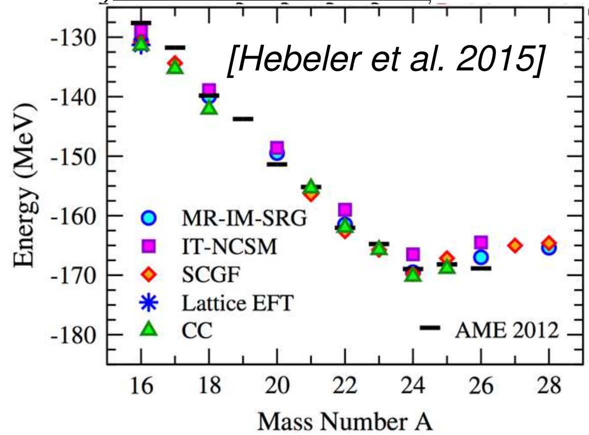
Truncated A-body expansion = Error (5)

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

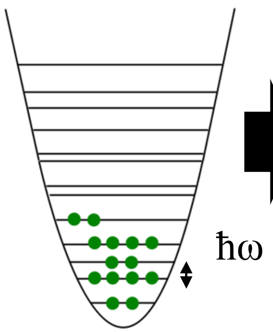
Work-horse methods = ~3%
Top-tier methods < 1%

[Binder et al. 2015]



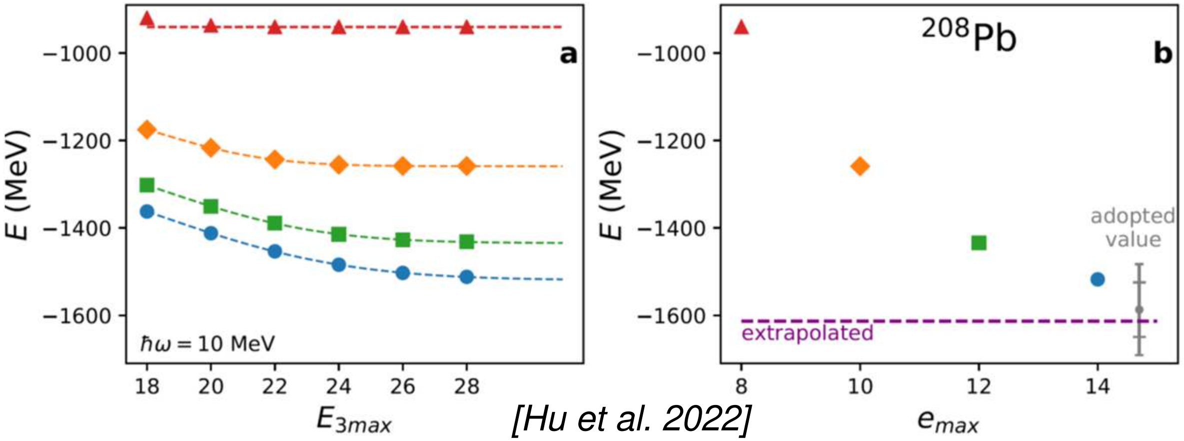


Truncated basis expansion = Error (3)



1-body: e_{1max}
2-body: e_{2max}
3-body: e_{3max}

A~50 < 0.1%
A~200 ~ 8%



[Hu et al. 2022]

Statistical uncertainties

Propagating parameter uncertainties of H = Error (2) + Global Sensitivity Analysis

N simulations = expensive

$$H|\Psi_n^A\rangle = \mathrm{E}_n^A|\Psi_n^A\rangle$$

Simulations = 20y of CPU

↕

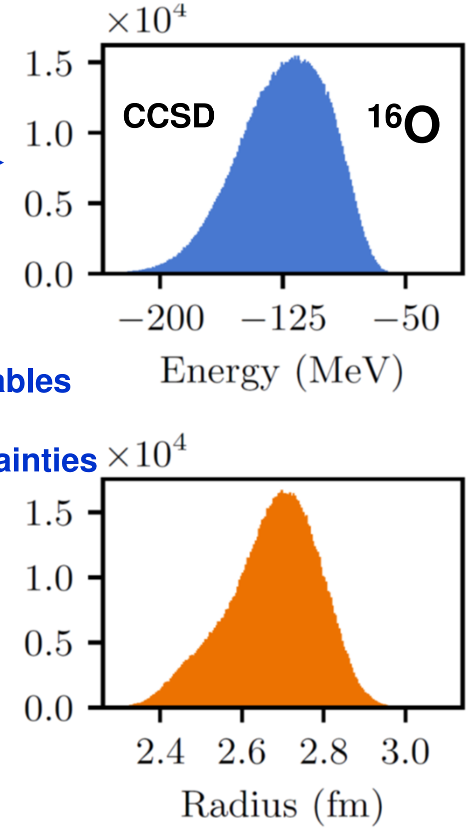
Emulations = 1h on a laptop

N sets

$$H \equiv H(\{\lambda_i\}) \xrightarrow{\text{fit}} \boxed{\lambda_i = \bar{\lambda}_i + \boxed{\delta\bar{\lambda}_i}} \; \pm 5\% \longrightarrow E^{\mathrm{A}} + \delta E^{\mathrm{A}}$$

1 114 112 samples

A-body observables with statistical uncertainties



Ekstrom, Hagen (2019)

◉ **Emulator based on the Eigenvector Continuation (EC) method**

Frame *et al.* (2018)
Duguet *et al.* (2023)

1) **Solve** $H|\Psi_n^A\rangle = \mathrm{E}_n^A|\Psi_n^A\rangle$ **for a small set (few 100s) of parameter values = moderate**

2) **Diagonalize the huge number of** $H(\{\lambda_i + \delta\lambda_i\})$ **in small basis generated in 1) = cheap**

→ **Implementation of a PGCM-EC emulator**

See Talk by A. Roux on Friday

◉ **Rule of the game**

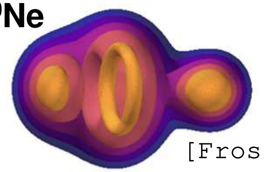
Evaluating any source of error = repeating several/many/very many times the ab initio calculation
➲ Enormous increase of the cost
Reducing systematic error = going to next order or larger n_{dim}
➲ Huge increase of the cost

Some ab initio frontiers

SPECTROSCOPY

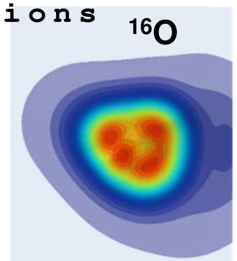
- Single-particle excitations
- Collective excitations
- Clustering

^{20}Ne



Tetrahedral ground state intrinsic density

^{16}O



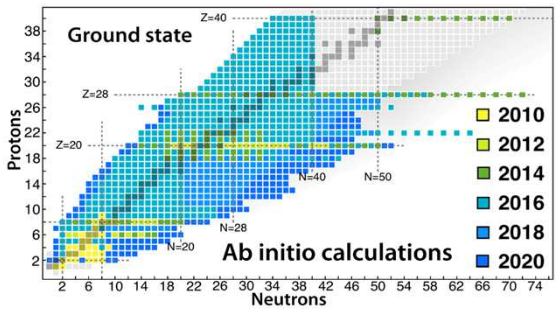
[Frosini et al., 2023]

[Bally et al., 2023]

$1^-/3^-$ vibration (^{16}O+α ↔ ^{12}C + 2α) at 7.2 MeV

OPEN-SHELL

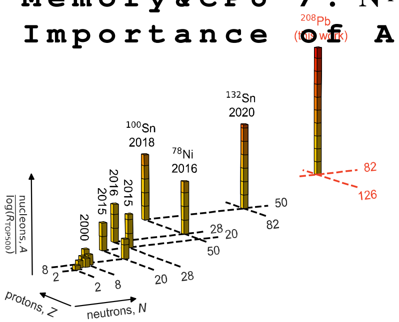
- Novel many-body methods
- Memory&CPU ↗: $\tilde{N}^p \rightarrow N^q$ ($\tilde{N} \ll N$)



[Hergert, 2020]

MASS

- Memory&CPU ↗: N^p with N ↗
- Importance of AN forces?



[Hu et al, 2022]

UNCERTAINTIES

- **Systematic**

Hamiltonian

$$H = T + V_{\mathrm{LO}} + V_{\mathrm{NLO}} + V_{\mathrm{N^2LO}} + \ldots$$

A-body solution

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

Basis representation

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

- **Statistical**

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

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

MANY-BODY METHODS

ACCURACY

- Algebra cost ↗

Difficult manually

- Numerical cost ↗

Memory&CPU: $N^p \rightarrow N^q$ (q>p)

HAMILTONIAN

- S=0/S≠0 interactions
- Power counting
- Currents
- Fit

REACTIONS

- Light nuclei
- Optical potential
- Transition densities