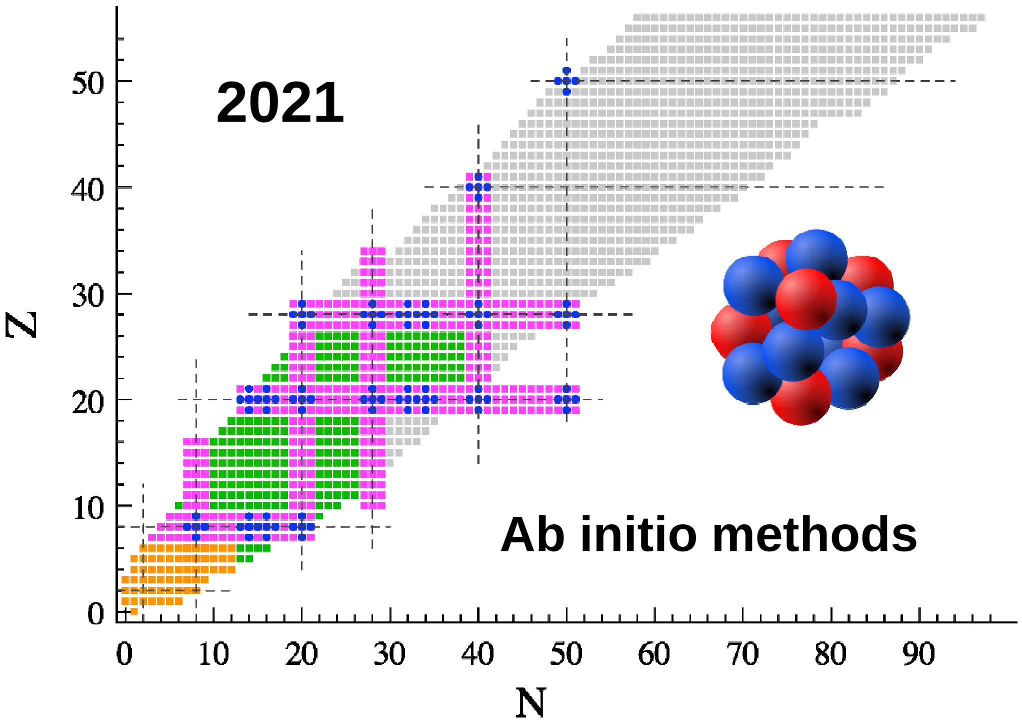
Panorama of the methods in each discipline

II. Low-energy Nuclear Physics



Thomas DUGUET

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

Workshop on wave-function methods in quantum chemistry and nuclear physics

February 8-12 2021, GDR NBODY&RESANET

Workshop Program

https://wiki.lct.jussieu.fr/gdrnbody/index.php/QC/NP_workshop_2021

Schedule

There will be five afternoons with two presentations (one from quantum chemisty, one from nuclear physics) per afternoon with a total of 1.5 hour (including discussions) for each presentation.

Times are in the Paris time zone (UTC+01:00)

Session: ***Panorama of the methods in each discipline***

- **Monday 8 February**
  - 2:00pm-3:30pm **Pierre-François Loos**
  - 4:00pm-5:30pm **Thomas Duguet**

Session: ***Specific computational aspects in each discipline***

- **Tuesday 9 February**
  - 2:00pm-3:30pm **Emmanuel Giner**
  - 4:00pm-5:30pm **Benjamin Bally** & **Alexander Tichai**

Session: ***Methods based on selection and/or stochastic sampling of parts of the Hilbert space***

- **Wednesday 10 February**
  - 2:00pm-3:30pm **Claudia Filippi**
  - 4:00pm-5:30pm **Robert Roth**
- **Thursday 11 February**
  - 2:00pm-3:30pm **Lorenzo Contessi** & **Denis Lacroix**
  - 4:00pm-5:30pm **Sandeep Sharma**

Session: ***Methods based on tensor decomposition approximations***

- **Friday 12 February**
  - 2:00pm-3:30pm **Stefan Knecht**
  - 4:00pm-5:30pm **Alexander Tichai**

Today
I. General background
II. Preparation and brief connection to days 2,3,5
III. Ab initio expansion methods for mid-mass nuclei

Leave entirely
I. CI and selected CI to Robert (wednesday)
II. Monte-Carlo to Denis&Lorenzo (thursday)
III. EDF, reaction theory to another meeting…

+ I benefit from Titou's talk regarding HF, MBPT, CC…

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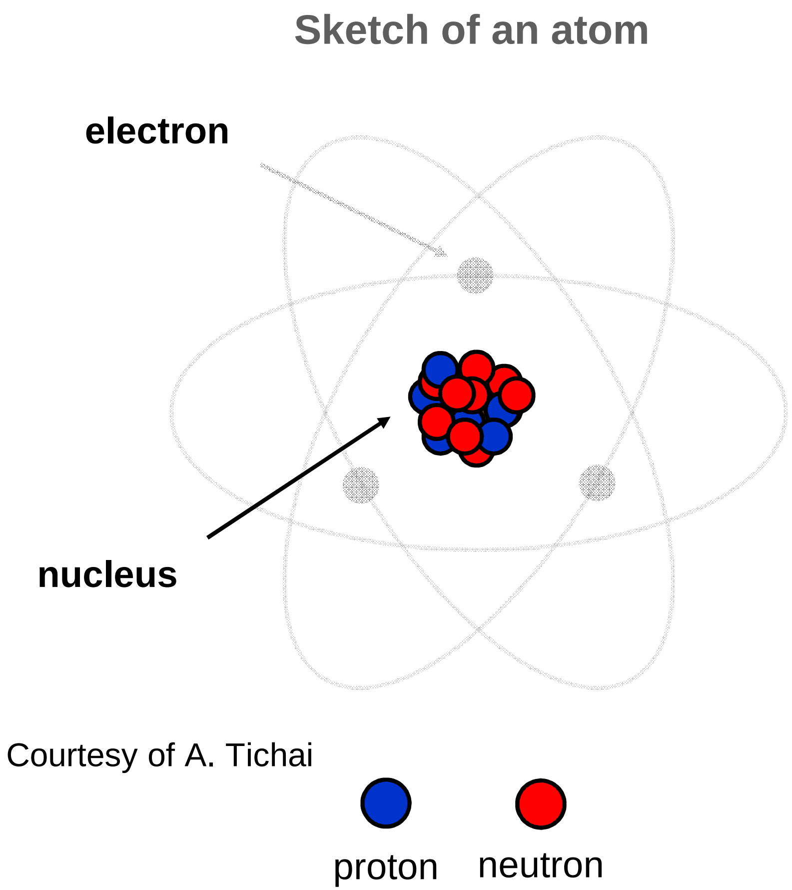
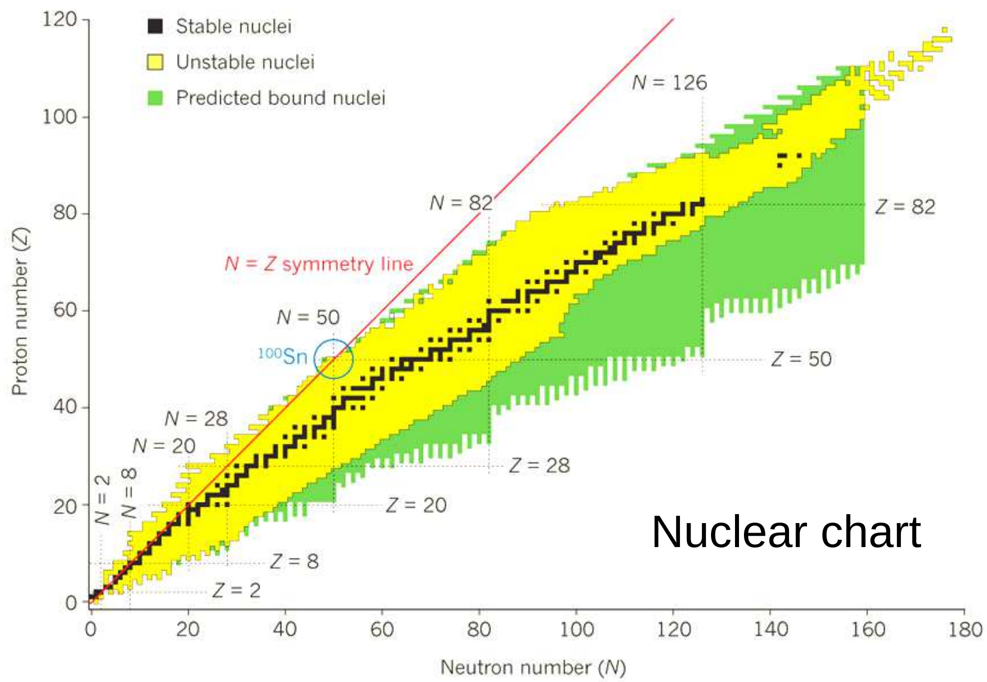
The simple of view of an atomic nucleus

❶ Self-bound (or resonant) state of ***Z* protons and *N* neutrons**

4-fermions system (spin up/down ⊗ isospin up/down)

❷Residual strong force between color-less objects





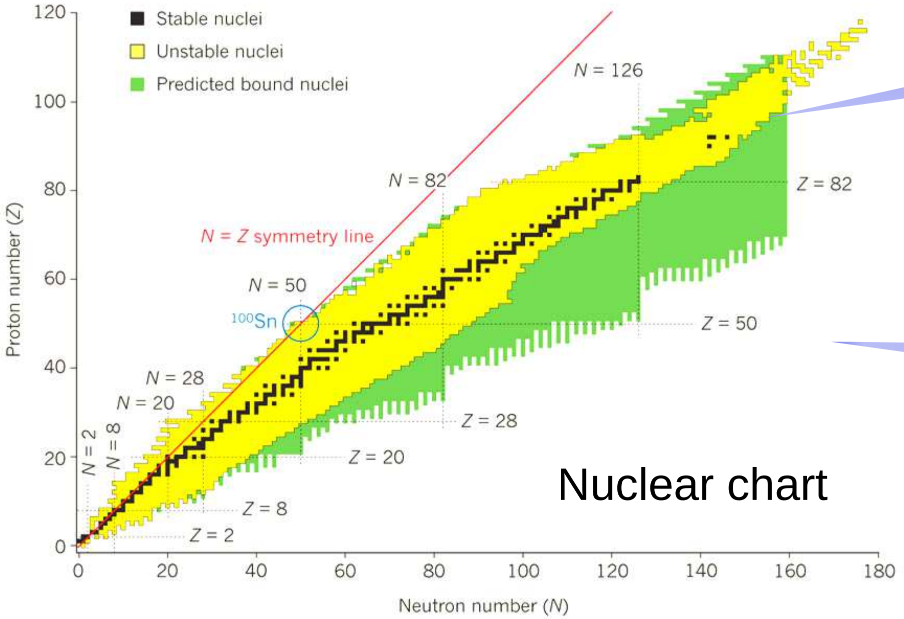
Elementary questions driving the field and our activity

○ **How many** nuclei are bound by the strong force; 6000-9000?

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

○ Where are **magic numbers** over the nuclear chart?

N=20/28 shown to disappear away from stability in 1975/1993



○ **What is the heaviest** possible element?

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

○ What are the various radioactive decay modes?

2p decay identified beyond the proton dripline in ^{45}Fe in 2002

○ Where is the neutron drip-line?

Extended from Z=8 (^{24}O) to Z=10 (^{34}Ne) in 2019

○ How have heavier elements than Fe been produced?

Gravitational wave + kilonova from neutron stars merger in 2017

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

Several scales at play:

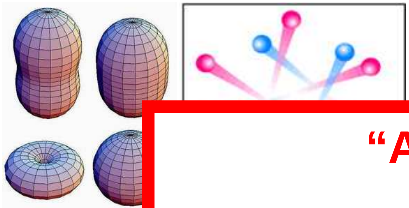
p & n momenta ~ **10^8** eV

Separation energies ~ **10^7** eV

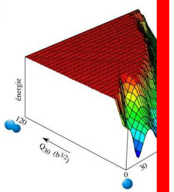
Vibrational excitations~ **10^6** eV

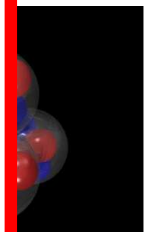
0^4 eV

Ground state
Mass, size, superfluidity, e.m. moments…



Radioa
β, 2β, (



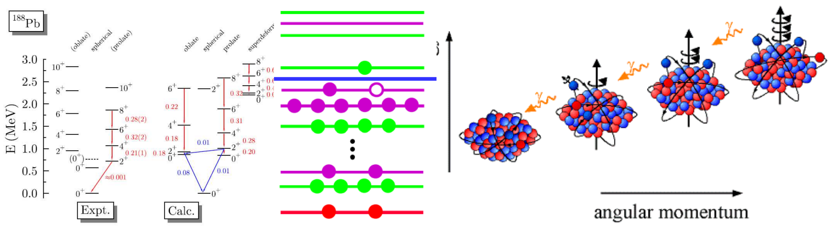


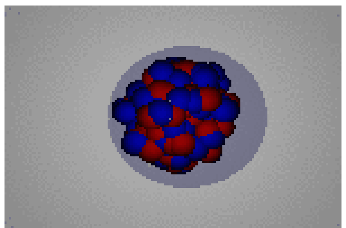
"Ab initio", i.e. Chiral-EFT in A-body sector, long-term endeavor

Can nuclear systems be described

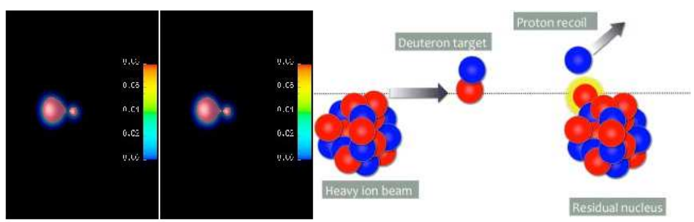
1) Consistently (from a single theoretical rationale?)
2) Systematically (complete phenomenology?)
3) Accurately enough (relevant to experimental uncertainty?)
4) From inter-nucleon interactions (right balance between reductionism/emergence?)
5) Rooted in QCD (sound connection to underlying EFT?)

Spectroscopy
Excitation modes





Reaction processes
Fusion, transfer, knockout, …



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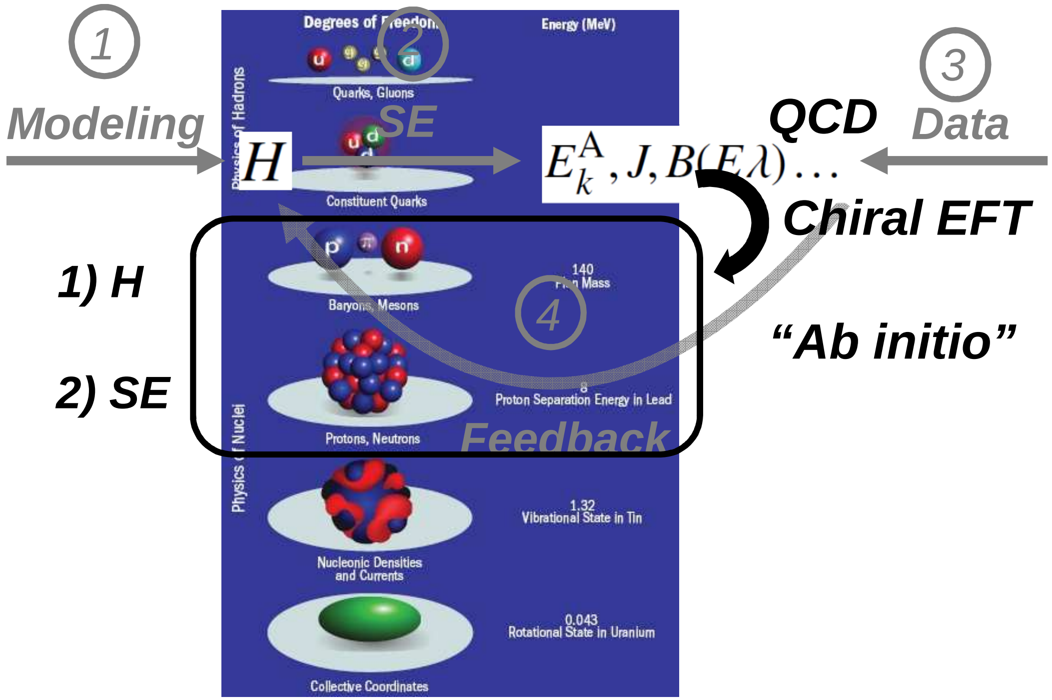
Ab initio (i.e. In medias res) quantum many-body problem

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

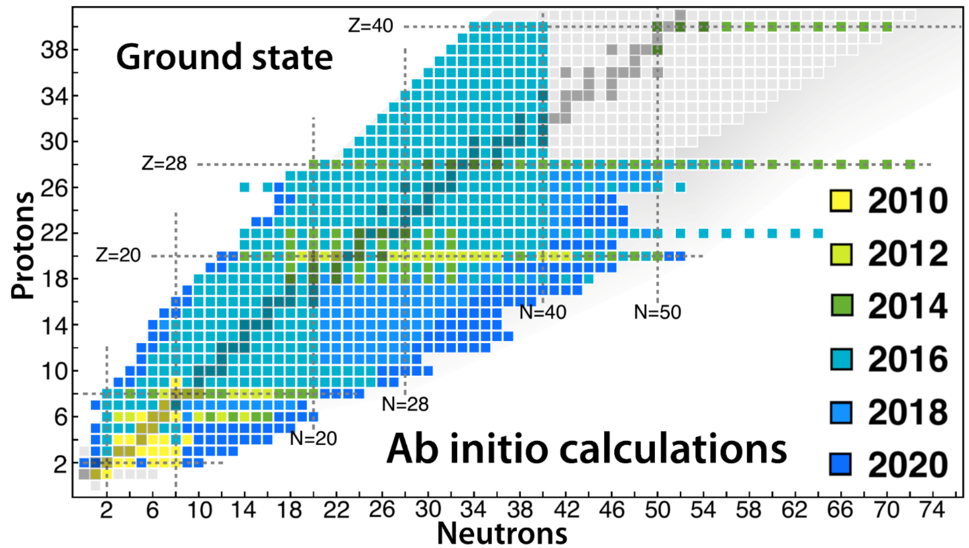
1) *A* structure-less nucleons as degrees of freedom at low energy
2) Interactions mediated by pions and contact operators based on, e.g., Weinberg, power counting
3) **Solve A-body Schrödinger equation to relevant accuracy**

A-body Schrödinger Equation

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



Rapidly evolving field in the last 15 years



H. Hergert, Front. in Phys. 8 (2020) 379

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The nuclear Hamiltonian

Build H (and other operators) with χEFT 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 tensor to experimental data (or lattice QCD) in A = k-body systems

Organization = power counting
Importance of interaction terms

A-body Schrödinger Equation

$$H|\Psi_k^{\mathrm{A}}\rangle = E_k^{\mathrm{A}}|\Psi_k^{\mathrm{A}}\rangle$$

Effective description = *A*-body operator in principle

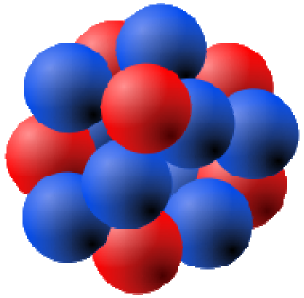
$$H = T + V^{2\mathrm{N}} + V^{3\mathrm{N}} + V^{4\mathrm{N}} + \ldots + V^{A\mathrm{N}}$$

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

For the actual construction of V^{kN} operators via χEFT

- See my talk at the GDR NBODY kickoff meeting, Lille, January 2020
- Not recalled here

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)**

$[H,P_i] = 0$ ➲ $| \Phi^{P}_{cm} > | \Psi_{im} >$

❷ **Rotationally invariant: SU(2)**

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

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

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

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

$$H \equiv \sum_{i=1}^{A} \frac{\vec{p}_i^{\,2}}{2m} + \frac{1}{2}\sum_{i\neq j}^{A} V^{2N}(i,j) + \frac{1}{6}\sum_{i\neq j\neq k}^{A} V^{3N}(i,j,k) + \dots$$

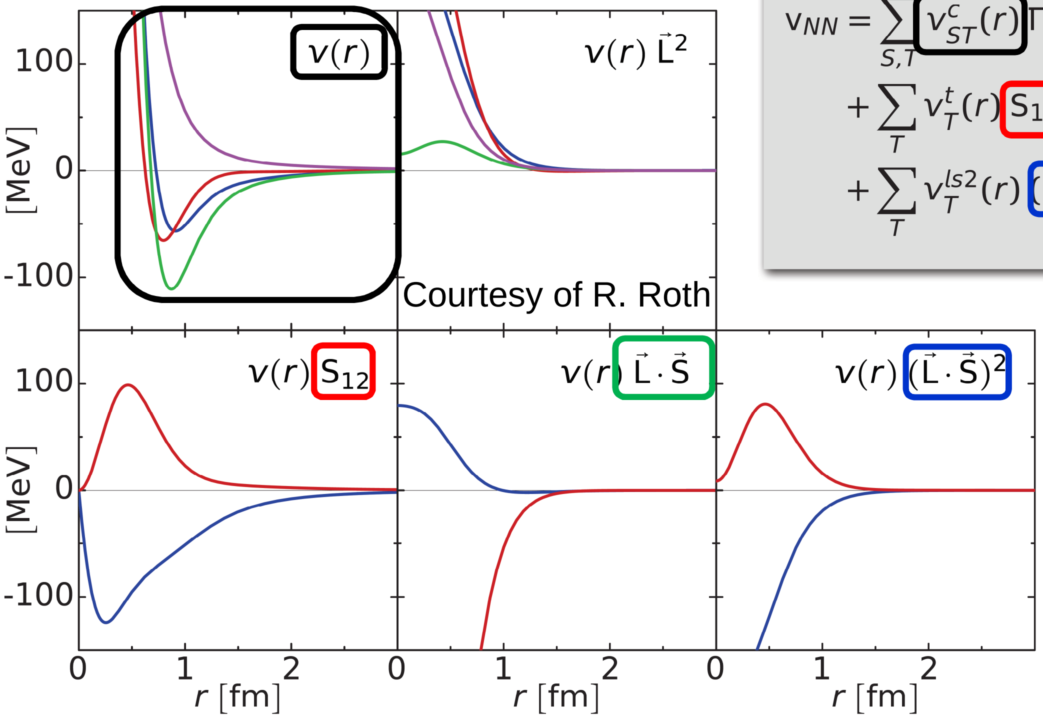
$$= \sum_{\alpha\beta} t_{\alpha\beta} a_\alpha^\dagger a_\beta + \left(\frac{1}{2!}\right)^2 \sum_{\alpha\beta\gamma\delta} \bar{v}^{2N}_{\alpha\beta\gamma\delta} a_\alpha^\dagger a_\beta^\dagger a_\delta a_\gamma + \left(\frac{1}{3!}\right)^2 \sum_{\alpha\beta\gamma\delta\zeta\epsilon} \bar{v}^{3N}_{\alpha\beta\gamma\delta\zeta\epsilon} a_\alpha^\dagger a_\beta^\dagger a_\gamma^\dagger a_\epsilon a_\zeta a_\delta + \cdots$$

Interactions between effective 4-components point fermions

➲ nucleons = ±½ isospin & ±½ spin projections

1. **Complex operator structure in r⊗σ⊗τ spaces (constrained by symmetries)**

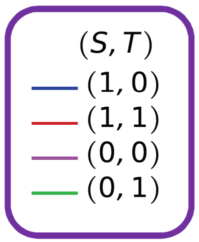
AV18 2N interaction



$$v_{NN} = \sum_{S,T} v^{c}_{ST}(r)\,\Pi_{ST} + \sum_{S,T} v^{l2}_{ST}(r)\,\vec{L}^2\,\Pi_{ST} + \sum_{T} v^{t}_{T}(r)\,S_{12}\,\Pi_{1T} + \sum_{T} v^{ls}_{T}(r)\,(\vec{L}\cdot\vec{S})\,\Pi_{1T} + \sum_{T} v^{ls2}_{T}(r)\,(\vec{L}\cdot\vec{S})^2\,\Pi_{1T} + \dots$$

✶Central operator
~Lennard-Jones
Short-range repulsion
✶Tensor operator
✶Spin-orbit
✶Spin-orbit²

[Wiringa et al. 1995]



4 two-body spin-isospin channels

[See talks by A. Tichai & R. Roth for further discussions]

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

Phenomenology of inter-nucleon interactions

$$H \equiv \sum_{i=1}^{A} \frac{\vec{p}_i^{\,2}}{2m} + \frac{1}{2}\sum_{i\neq j}^{A} V^{2N}(i,j) + \frac{1}{6}\sum_{i\neq j\neq k}^{A} V^{3N}(i,j,k) + \ldots$$

$$= \sum_{\alpha\beta} t_{\alpha\beta} a^\dagger_\alpha a_\beta + \left(\frac{1}{2!}\right)^2 \sum_{\alpha\beta\gamma\delta} \bar{v}^{2N}_{\alpha\beta\gamma\delta} a^\dagger_\alpha a^\dagger_\beta a_\delta a_\gamma + \left(\frac{1}{3!}\right)^2 \sum_{\alpha\beta\gamma\delta\zeta\epsilon} \bar{v}^{3N}_{\alpha\beta\gamma\delta\zeta\epsilon} a^\dagger_\alpha a^\dagger_\beta a^\dagger_\gamma a_\epsilon a_\zeta a_\delta + \cdots$$

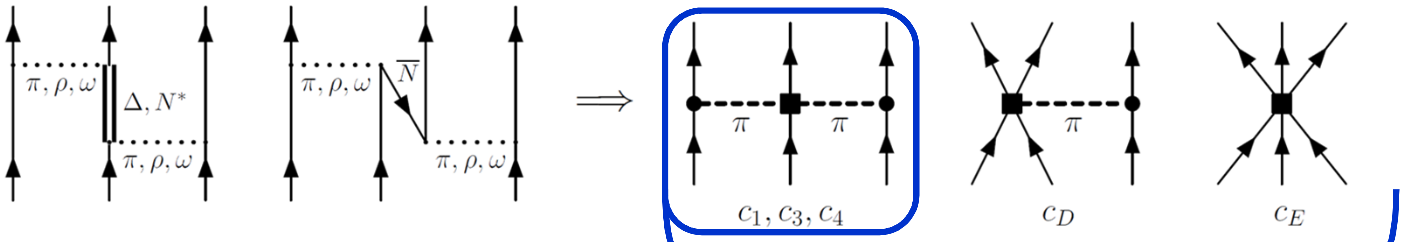
Interactions between effective 4-components point fermions

➲ nucleons = ±½ isospin & ±½ 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

Example 3N



2π-exchange diagram

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

Example of analytical expression

Tensor operator

$$\langle \vec{p}_1'\vec{p}_2'\vec{p}_3' | V^{3N}_{2\pi N^2LO} | \vec{p}_1\vec{p}_2\vec{p}_3 \rangle = \frac{g_A^2}{8F_\pi^4} \frac{\vec{\sigma}_1\cdot\vec{q}_1\,\vec{\sigma}_3\cdot\vec{q}_3}{[q_1^2+m_\pi^2][q_3^2+m_\pi^2]} \Big[\vec{\tau}_1\cdot\vec{\tau}_3\left(2c_3\,\vec{q}_1\cdot\vec{q}_3 - 4c_1 m_\pi^2\right)$$

Spin-orbit-like operator

$$+ c_4\,\vec{\tau}_1\times\vec{\tau}_3\cdot\vec{\tau}_2\,\vec{q}_1\times\vec{q}_3\cdot\vec{\sigma}_2\Big]\delta(\vec{P}'-\vec{P})$$

$$+ \text{all permutations of } (1,2,3)$$

ME in plane-wave basis of $\mathcal{H}_3$

$$\vec{q}_i = \vec{p}_i' - \vec{p}_i \qquad \vec{P} = \sum_{i=1}^{3} \vec{p}_i$$

Low-Energy Constants (LECs)

Fixed on π-nucleon scatt. exp.

Contents

Nuclear many-body problem

A-body Schrödinger Equation

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

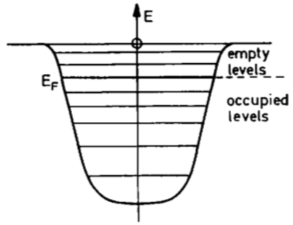
Ex: $H_{\mathrm{N^2LO}} = T + V^{\mathrm{2N}}_{\mathrm{N^2LO}} + V^{\mathrm{3N}}_{\mathrm{N^2LO}}$ **+ ∅ because of the truncation of χEFT expansion of the operator**

Contents

Specificities of atomic nuclei: mean field

1) **Self-bound system**
2) **Neutrons & protons**
3) **SU(2) sym. + strong L.S**

RHF mean-field approximation

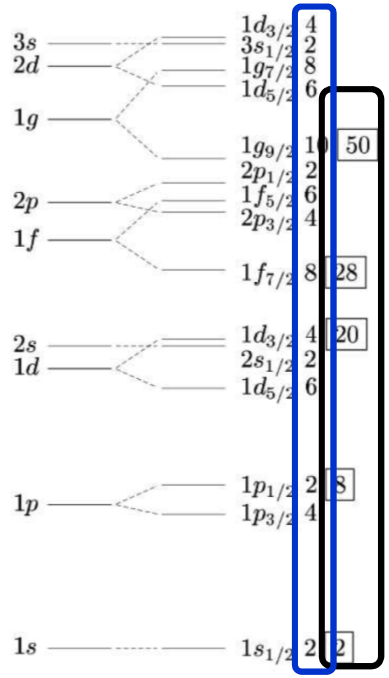


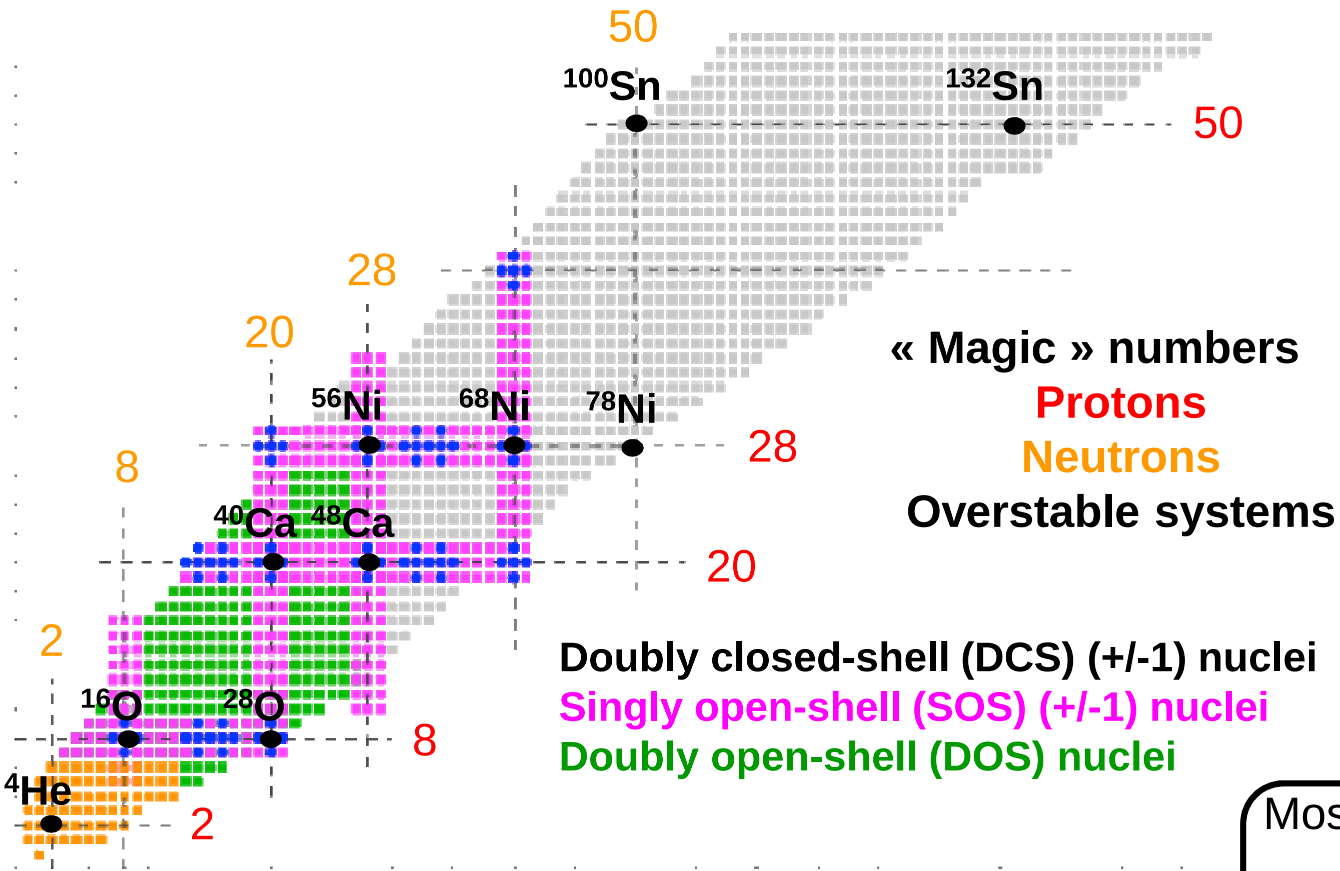
Average potential

Specificities

1) **Self created/centered**
2) **One for each species**
3) **j=l+s → 2j+1 degeneracy**

Filling of nuclear shells





Mostly *open-shell* ground-states

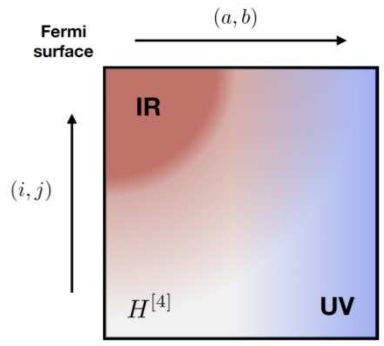
Strong (« static ») correlations

Contents

Pre-processing of short-range correlations

1) **Short-r repulsion**
2) **Bound np/Virtual nn**

Beyond mean-field ➡ expansion



Residual interaction

Many-body ➡ correlations

1) **Dynamic corr. in UV**
2) **Strong static corr. in IR**
   2a) **Pairing in SOS**
   2b) **Collect. Quad. in DOS**

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

$$H(s) \equiv U(s) H U^{\dagger}(s)$$

➡ Unitary **Similarity Renormalization Group** (SRG) transformation $= T + V^{2N}(s) + V^{3N}(s) + \ldots$

- Paramaterize the *change* of the Hamiltonian $\dfrac{dH(s)}{ds} = [\eta(s), H(s)]$

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

$H \equiv H_{\mathrm{D}} + H_{\mathrm{OD}}$ ➡ $\eta(s) \equiv [H_{\mathrm{D}}, H(s)]$ ➡ $\dfrac{d}{ds} H(s) = 0$ when $[H_{\mathrm{D}}, H(s)] = 0$

Trivial fixed point — H(s) diagonal

- To tame short-range choose $H_{\mathrm{D}} \equiv T$ = diagonal in momentum space basis

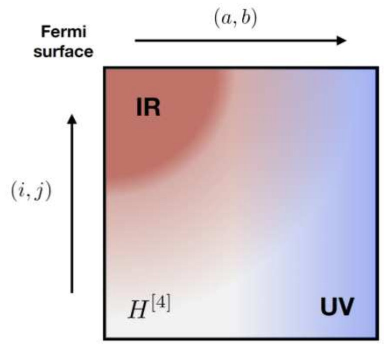
- Do not go all the way to fixed point because $[\eta(s), H(s)]$ ***induces multi-body operators in H(s)***

➡ Run until appropriate s_{final} = pre-diagonalization

Pre-processing of short-range correlations

1) Short-r repulsion
2) Bound np/Virtual nn

Beyond mean-field expansion



Many-body correlations

1) Dynamic corr. in UV
2) Strong static corr. in IR
  2a) Pairing in SOS
  2b) Collect. Quad. in DOS

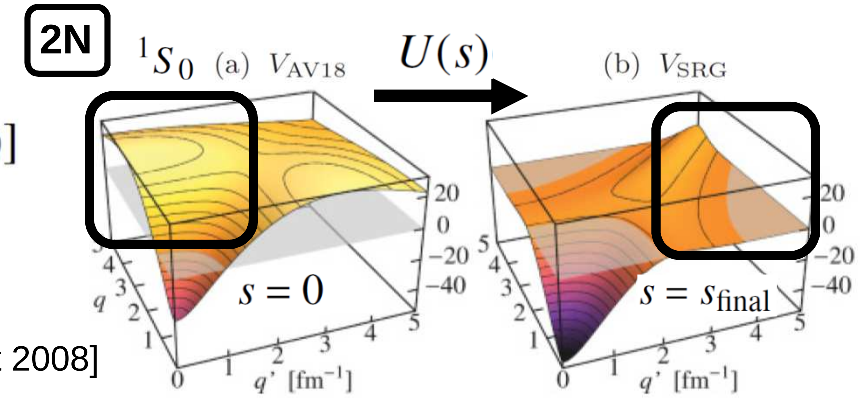
1) Taming down the short-range/coupling to UV in the Hamiltonian

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

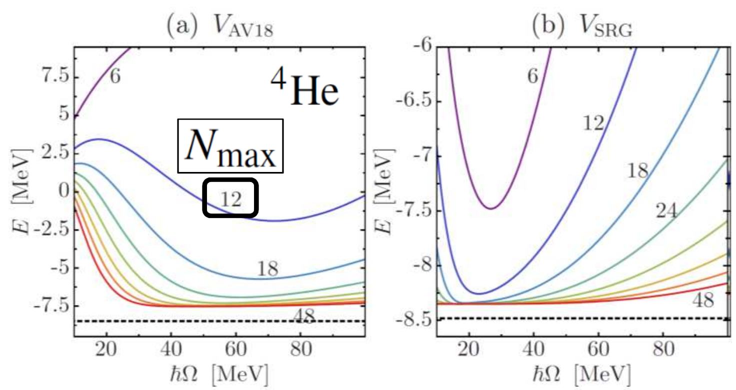
$$\frac{dH(s)}{ds} = [\eta(s), H(s)]$$

$$\eta(s) \equiv [T, H(s)]$$

[Roth, Reinhardt, Hergert 2008]



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



Remaining dynamical/static correlations
Drastically accelerated convergence
➲ **Still ~2000 basis states needed in mid-mass**
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** $\mathscr{H}_3$ [See talks by A. Tichai & R. Roth for further details]

Limit to DCS&SOS to utilize AMC → 200 states [See talk by A. Tichai]
Limit to « low » orders (CCSD(T), IMSRG(2), MBPT(3))
Limit to mid-mass (A~100)

Pre-processed nuclear many-body problem

$U(s)$ ➡ **SRG**

A-body Schrödinger Equation

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

Rather strong coupling to UV

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

Pre-processed nuclear many-body problem

« Soft » Hamiltonian
=
much reduced coupling to UV

A-body observables independent of s

A-body Schrödinger Equation

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

Ex: $H_{\mathrm{N^2LO}}(s) = T + V^{\mathrm{2N}}_{\mathrm{N^2LO}}(s) + V^{\mathrm{3N}}_{\mathrm{N^2LO}}(s) + \ldots$ **to be tractable** ⇒ $\frac{d}{ds}E_k^{\mathrm{JNZ}} \neq 0$ **violate unitarity**

Induced k-body forces (k≤ A)

Choose truncation & s

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

SRG transformation is a compromised between

- Reduction of coupling to UV
- Size of induced k-body interactions that cannot be handled

Contents

Expansion many-body methods

2) Include remaining dynamical and static correlations

Cost of solving SE scales as N^A = limited to A < 12

- Introduce **importance sampling/selection** — Wednesday/Thursday
- Design **expansion methods scaling as** N^p — **Today**/Tuesday/Friday

I. Mean-field reference state

Symmetry-conserving partitioning

$$H = H_0 + H_1 \text{ such that } [H_0, J^2] = [H_0, J_z] = [H_0, A] = 0$$

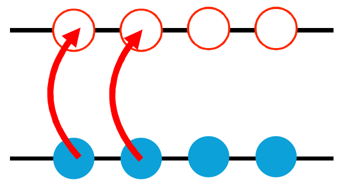
Stands for N&Z

➡ $H_0|\Phi_0\rangle = \mathcal{E}_0|\Phi_0\rangle$

Exactly solvable

Spherical Slater determinant (« RHF »)

Closed-shell



Non-degenerate
Good starting point for expansion

II. Many-body expansion

$$H = H_0 + H_1$$

$$|\Psi_0^{J=0\,A}\rangle = \Omega_0|\Phi_0\rangle$$

Wave operator   Reference state

► Expand in terms of elementary (np-nh) excitations of $|\Phi_0>$
► Accounts for « weak/dynamical » correlations
► Expand as a series (MBPT, CC…) + truncate = N^p cost

III. Examples in nuclear physics

SCGF	Self-Consistent Green's Function [ADC(2,3)]
MBPT	Many-Body Perturbation theory [(2,3)]
CC	Coupled Cluster [Λ-CCSD(T), CR-CC(2,3)]
IM-SRG	In-Medium Similarity Renormalization Group

In-medium similarity renormalization group method

Goal: Solve SRG flow equation $\frac{dH(s)}{ds} = [\eta(s), H(s)]$ **in** $\mathcal{H}_A$ **such that** $|\Phi_0\rangle$ **is the GS of H(∞)**

1. Normal order H with respect to $|\Phi_0\rangle$ **(instead of** $|0\rangle$ **for standard SRG)**

Working basis of $\mathcal{H}_1$ & MEs calculation [see Talk by A. Tichai]

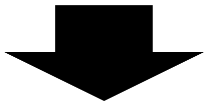
Hamiltonian $$H = \sum_{pq} t_{pq} c^\dagger_p c_q + \frac{1}{(2!)^2} \sum_{pqrs} v_{pqrs} c^\dagger_p c^\dagger_q c_s c_r + \frac{1}{(3!)^2} \sum_{pqrstu} w_{pqrstu} c^\dagger_p c^\dagger_q c^\dagger_r c_u c_t c_s$$

Reference state (« RHF ») $$|\Phi_0\rangle \equiv \prod_{i=1}^{A} a^\dagger_i |0\rangle \quad \text{with} \quad \rho_{qp} \equiv \frac{\langle \Phi_0 | a^\dagger_p a_q | \Phi_0 \rangle}{\langle \Phi_0 | \Phi_0 \rangle} = n_p \delta_{pq}$$

$n_i = 1$ holes

$n_a = 0$ particles

Standard Wick's theorem



Normal-ordered (NO) with respect to $|\Phi_0\rangle$

$$H = h^{(0)} + \sum_{pq} h^{(1)}_{pq} : a^\dagger_p a_q : + \frac{1}{2!} \sum_{pqrs} h^{(2)}_{pqrs} : a^\dagger_p a^\dagger_q a_s a_r : + \frac{1}{6!} \sum_{pqrstu} h^{(3)}_{pqrstu} : a^\dagger_p a^\dagger_q a^\dagger_r a_u a_t a_s :$$

HF basis & MEs transformation [see Talk by A. Tichai]

[Hergert *et*. al, Phys. Rep. 2016]

In-medium similarity renormalization group method

Matrix elements of nomal-ordered operators

$$h^{(0)} = \sum_i t_{ii} n_i + \frac{1}{2}\sum_{ij} v_{ijij} n_i n_j + \frac{1}{6}\sum_{ijk} w_{ijkijk} n_i n_j n_k = \mathcal{E}_0$$

$$h^{(1)}_{pq} = t_{pq} + \sum_i v_{piqi} n_i + \frac{1}{2}\sum_{ij} w_{pijqij} n_i n_j$$

$$h^{(2)}_{pqrs} = t_{pqrs} + \sum_i w_{pqirsi} n_i$$

$$h^{(3)}_{pqrstu} = w_{pqrstu}$$

✶Large part of the original 3N transfered into *effective* lower-rank tensors/NO operators

⌦Neglect residual NO 3N operator = NO2B approx

⌦Many-body machinery with 2N operators only (1-3% error benchmarked up ^{16}O via IT-NCSM)

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

In-medium similarity renormalization group method

2. Flow equation for normal-ordered form of H(s)

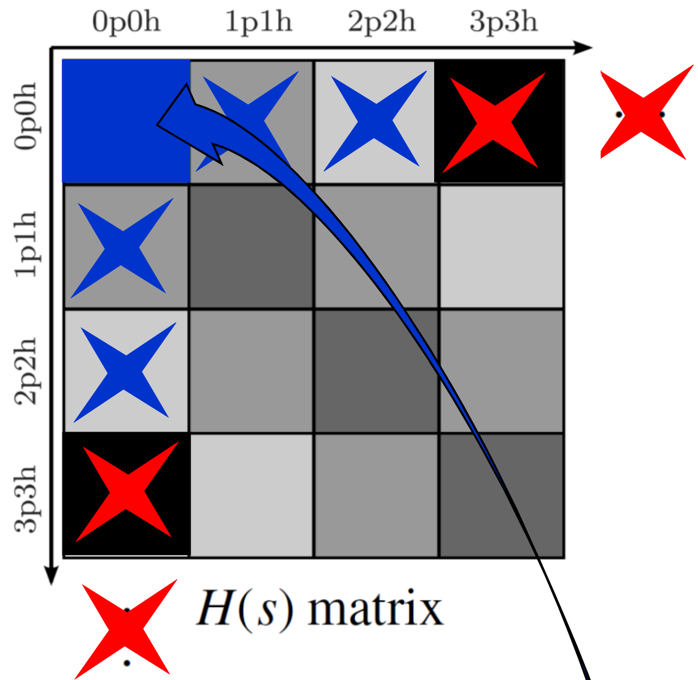
Basis of $\mathcal{H}_A$ = elementary (npnh) excitations of $| \Phi_0 >$

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

$s = 0$

$s \neq 0$

$s \longrightarrow \infty$



n **m**

Flow equation $\frac{dH(s)}{ds} = [\eta(s), H(s)]$ **each step**

$$H(s) = h^{(0)}(s) + h^{(1)}(s) + h^{(2)}(s) + h^{(3)}(s) + \ldots$$ **up to n+m-1**

$$\eta(s) = \eta^{(1)}(s) + \eta^{(2)}(s) + \eta^{(3)}(s) + \ldots$$ Induced k-body terms

⌦Neglect flowing k-body operators with n ≤ k ≤ A = IMSRG(n) approx → violates unitarity (small?)

⌦IMSRG(2) workhorse of current ab initio calculations

Pursued decoupling

$$\lim_{s\to\infty} \langle \Phi_0 | H(s) : a^\dagger_a a_i : | \Phi_0 \rangle = \lim_{s\to\infty} h^{(1)}_{ai}(s) = 0$$

$$\lim_{s\to\infty} \langle \Phi_0 | H(s) : a^\dagger_a a^\dagger_b a_i a_j : | \Phi_0 \rangle = \lim_{s\to\infty} h^{(2)}_{abij}(s) = 0$$

ph&pphh matrix elements

Associated « off-diagonal » Hamiltonian defining η(s)

$$H_{OD}(s) = \sum_{ai} h^{(1)}_{ai}(s) : a^\dagger_a a_i : + \frac{1}{4} \sum_{abij} h^{(2)}_{abij}(s) : a^\dagger_a a^\dagger_b a_i a_j : + \text{H.c.}$$

$$H(\infty)|\Phi_0\rangle = \mathcal{E}_0(\infty)|\Phi_0\rangle$$ with $\mathcal{E}_0(\infty) = (\approx) E_0^{\text{JNZ}}$

In-medium similarity renormalization group method

2. Agebraic form of the coupled flow equations in the IMSRG(2) approximation

Evaluate $[\eta(s), H(s)]$ through Wick's theorem

$$\frac{dh^{(0)}}{ds} = \sum_{ij}(n_i - n_j)\eta^{(1)}_{ij} h^{(1)}_{ji} + \frac{1}{2}\sum_{ijab}\eta^{(2)}_{ijab} h^{(2)}_{abij} n_i n_j \bar{n}_a \bar{n}_b$$

Size extensive
Connected diagrams only

$$\frac{dh^{(1)}_{pq}}{ds} = \sum_{r}(1 + P_{pq})\eta^{(1)}_{pr} h^{(1)}_{rq} + \sum_{ij}(n_i - n_j)(\eta^{(1)}_{ij} h^{(2)}_{jpiq} - h^{(1)}_{ij}\eta^{(2)}_{jpiq})$$

$$+ \frac{1}{2}\sum_{ija} n_i n_j \bar{n}_a (1 + P_{pq})\eta^{(2)}_{apij} h^{(2)}_{ijaq} + \frac{1}{2}\sum_{abi}\bar{n}_a \bar{n}_b n_i (1 + P_{pq})\eta^{((2)}_{ipab} h^{(2)}_{abiq}$$

$$\frac{dh^{(2)}_{pqrs}}{ds} = \sum_{t}\left\{(1 - P_{pq})(\eta^{(1)}_{pt} h^{(2)}_{tqrs} - h^{(1)}_{pt}\eta^{(2)}_{tqrs}) - (1 - P_{rs})(\eta^{(1)}_{tr} h^{(2)}_{prts} - h^{(1)}_{tr}\eta^{(2)}_{prts})\right\}$$

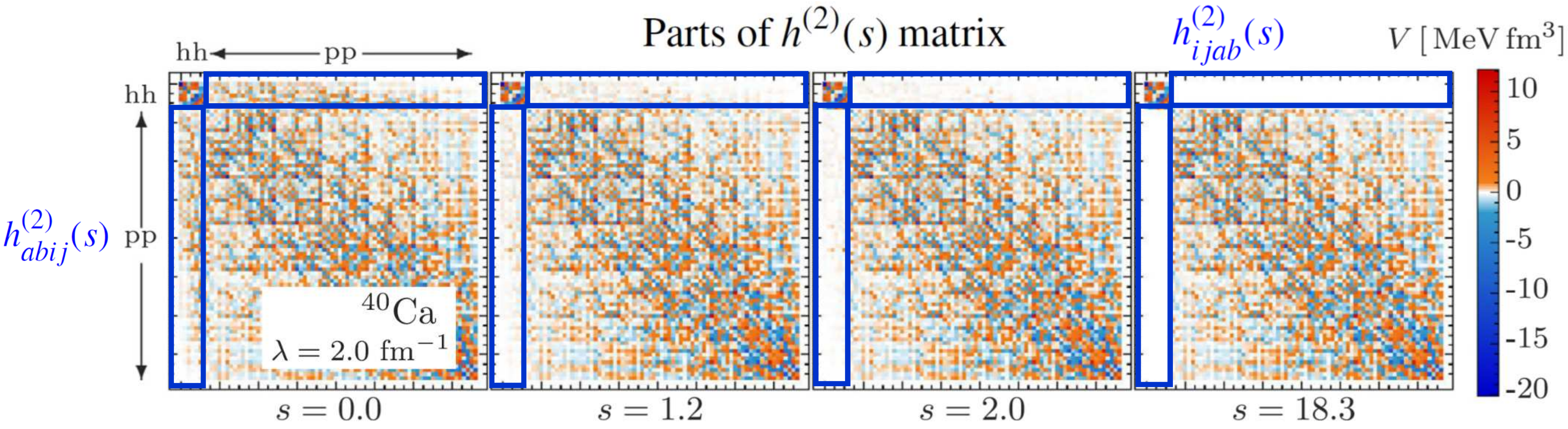
$$+ \frac{1}{2}\sum_{ij}(1 - n_i - n_j)(\eta^{(2)}_{pqij} h^{(2)}_{ijrs} - h^{(2)}_{pqij}\eta^{(2)}_{ijrs})$$ pp-hh ladders

$$- \sum_{ij}(n_i - n_j)(1 - P_{pq})(1 - P_{rs})\eta^{(2)}_{jqis} h^{(2)}_{ipjr}$$ p-h rings

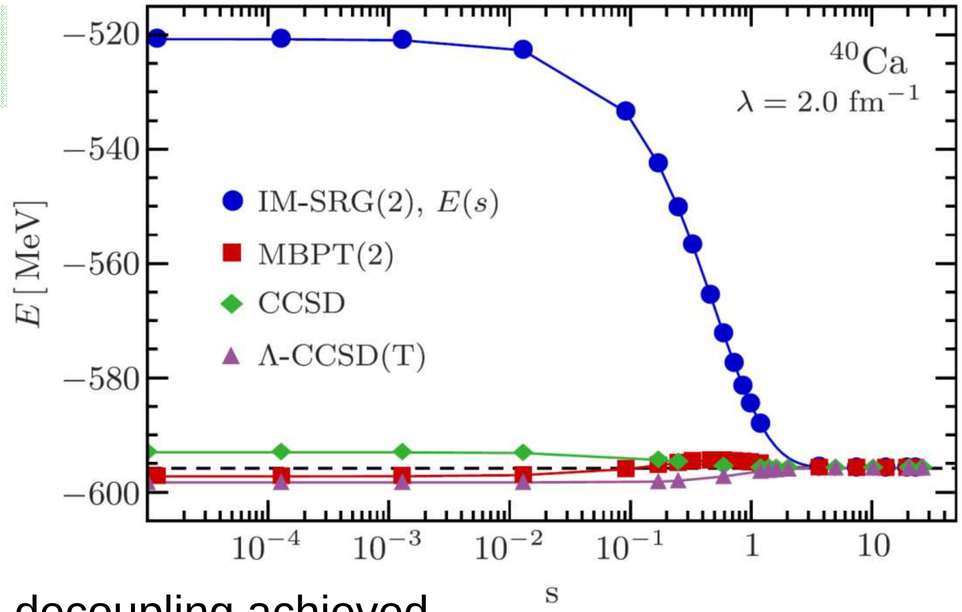
+ interferences as s → ∞

Scale as N^6 ⇔ CCSD

In-medium similarity renormalization group method



N^{3}LO chiral-EFT (no 3N here) SRG evolved λ = 2 fm^{-1}



Decoupling

❖Well under way after 20 steps (s=2.0)

❖Numerically achieved at s=18.3

Convergence

❖MBPT(2)/CCSD/Λ-CCSD(T) with evolving H(s)

❖Beyond s=2.0 $\mathcal{E}_0(\infty) \approx E_{\Lambda\text{−CCSD(T)}}(\infty)$ ⇔ full decoupling achieved

❖ $E_{\Lambda\text{−CCSD(T)}} \leq \mathcal{E}_0(\infty) \leq E_{\text{CCSD}}$ ⇔ understood from MBPT(n) analysis

➲ Current challenge is to go to IMSRG(3) truncation order

[Hergert *et*. al, Phys. Rep. 2016]

Expansion many-body methods

2) Include remaining dynamical correlations and static correlations in the IR

Cost of solving SE scales as N^A = limited to A < 12

- Introduce **importance sampling**
  Wednesday/Thursday
- Design **expansion methods scaling as** N^p
  Today/Tuesday/Friday

I. Mean-field reference state

Symmetry-conserving partitioning

$$H = H_0 + H_1 \text{ such that } [H_0, J^2] = [H_0, J_z] = [H_0, A] = 0$$

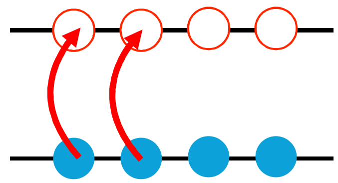
Stands for N&Z

$$\Rightarrow H_0|\Phi_0\rangle = \mathcal{E}_0|\Phi_0\rangle$$

Exactly solvable

Spherical Slater determinant (« RHF »)

Closed-shell



Non-degenerate
Good starting point for expansion

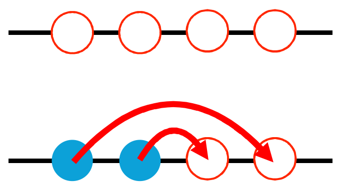
II. Many-body expansion

$$H = H_0 + H_1$$

$$|\Psi_0^{J=0\,A}\rangle = \Omega_0|\Phi_0\rangle$$

Wave operator — Reference state

Open-shell



Degenerate
Improper starting point for expansion
Most of nuclear GS are open-shell…

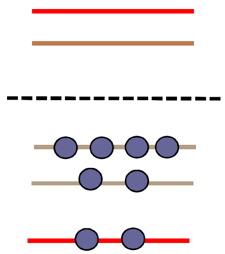
- ► Expand in terms of elementary (np-nh) excitations of $|\Phi_0\rangle$
- ► Accounts for « weak/dynamical » correlations
- ► Expand as a specific series (MBPT, CC…) + truncate = N^p cost

Contents

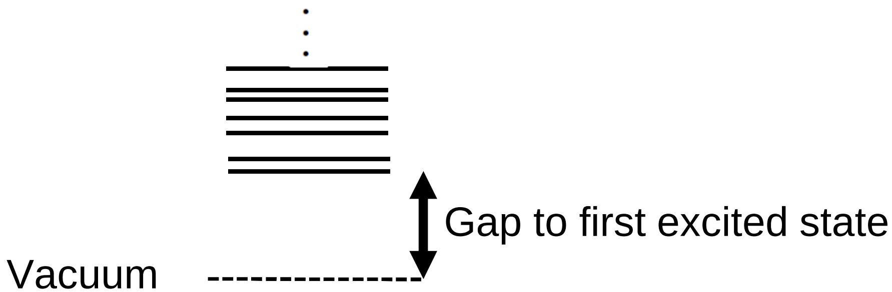
Static correlations and (near) degenerate systems

I. The basic facts

Closed-shell RHF reference vacuum



Gap-full elementary excitation (EE) spectrum

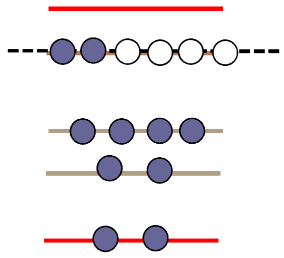


Controlled expansions

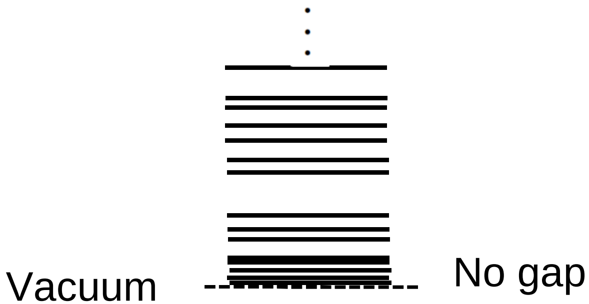
Ex:

$$\Delta E^{(2)}_{\mathrm{MBPT}} = -\frac{1}{4}\sum_{ijab}\frac{|h^{(2)}_{ijab}|^2}{e_a+e_b-e_i-e_j} \quad > 0$$

Open-shell RHF reference vacuum



Gap-less EE spectrum



Singular expansions

Ignite static correlations
Nature&Strength
➲ $h^{(2)}$ in IR

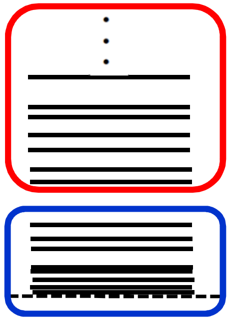
Ex:

$$\Delta E^{(2)}_{\mathrm{MBPT}} = -\frac{1}{4}\sum_{ijab}\frac{|h^{(2)}_{ijab}|^2}{e_a+e_b-e_i-e_j} \quad = 0$$

Static correlations and (near) degenerate systems

II. Possible remedies

Multi-reference (MR) state from **orthonormal EE** in IR



From diago

$$|\Theta^{J=0\,A}_{0\ IR}\rangle = \sum_{\mu\in IR} c_\mu |\Phi_\mu\rangle$$

Re-opens a gap in EE spectrum

Controlled expansions on top of MR state

$$|\Psi^{J=0\,A}_0\rangle = \Omega^{UV}_0 |\Theta^{J=0\,A}_{0\ IR}\rangle$$

Typical of QC

MR-MBPT, MR-CC…

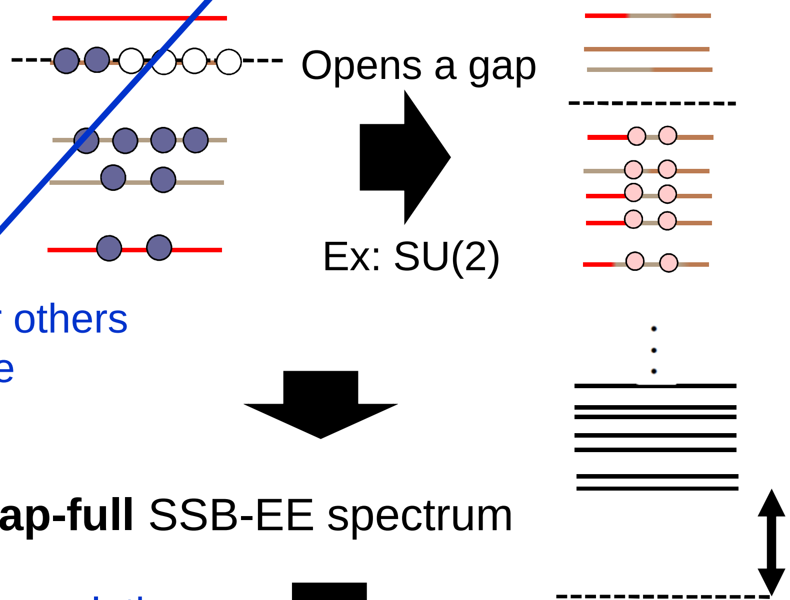
Capture static correlations

Depends on SOS vs DOS

[See talk by B. Bally]

Spontaneous symmetry-breaking (SSB)

1) Break SU(2)
UHF state
2) Break U(1)
HFB state
3) Break both or others
UHFB state



Gap-full SSB-EE spectrum

Controlled expansions on top of **single-reference** SSB state

$$H = H_0 + H_1 \text{ with } [H_0, J^2] \neq 0$$

$$|\Psi^{J=0\,A}_0\rangle = \Omega^{SB}_0 |\Phi^{SB}_0\rangle$$

Ex:

$$\Delta E^{(2)} = -\frac{1}{4!}\sum \frac{|\Omega^{40}_{k_1k_2k_3k_4}|^2}{E_{k_1}+E_{k_2}+E_{k_3}+E_{k_4}}$$

Breaking of U(1) $\;E_{k_1}+E_{k_2}+E_{k_3}+E_{k_4} > 0$

Typical of NP

- ✶ Truncated series breaks symmetry
- ✶ Symmetry must eventually be restored
- ✶ **PBMBPT, PCC** [Duguet 2015, Qiu *et al.* 2017, 2020]

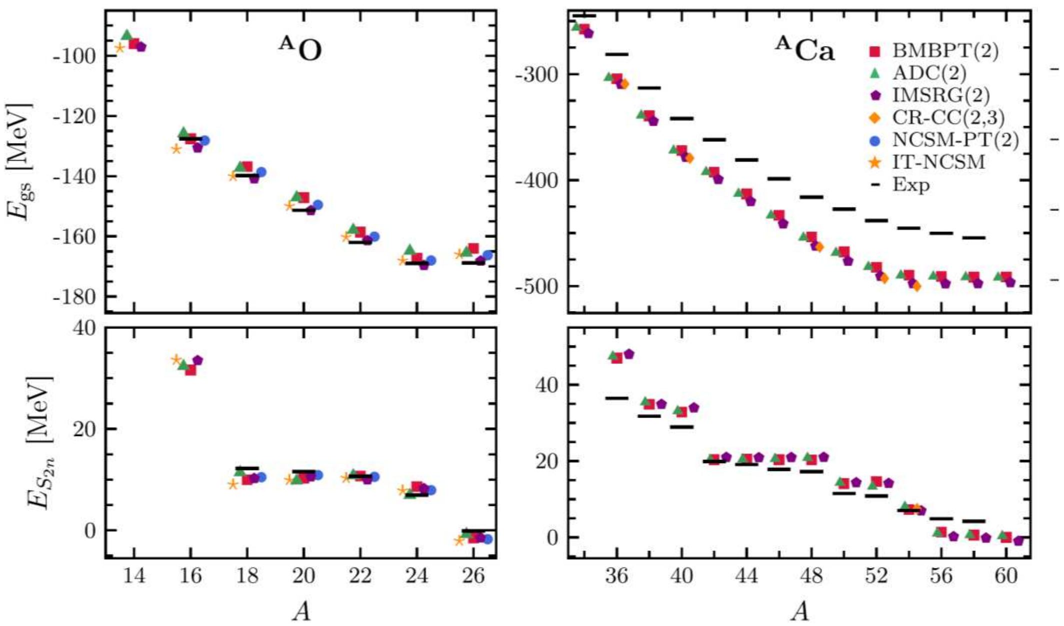
Ex. Bogoliubov many-body perturbation theory

◉ Perturbative reduction of BCC *[Duguet, Signoracci 2016]*

→ Code for automated generation&evaluation of many-body diagrams to arbitrary order *[Arthuis et al. 2018]*

→ Convergence properties at high orders and resummation methods *[Demol et al. 2020]*

◉ **Validation of BMBPT(2,3)** in mid-mass SOS nuclei *[Tichai et al. 2018]*



Calculation details

Chiral NN+3N Hamiltonian
SRG α = 0.08 fm^4
13 major shells (1820 s.p. states)
Canonical HFB reference

Runtime

NCSM:	20.000 hours
MCPT:	2.000 hours
IMSRG(2):	1.500 hours
SCGF(2):	400 hours
BMBPT(2):	**< 1min !**

→ 2-3% agreement of all methods with exact results (IT-NCSM)
→ Consistent with non-perturbative methods for basic ground-state properties

→ Optimal for first (i) test of novel χEFT Hamiltonians (ii) exploration of large A *[Tichai et al. 2020]*
→ Refined observables require non-perturbative methods (at high order)

Static correlations and (near) degenerate systems

Order parameter of broken symmetry

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

II. Towards an optimal combination of SSB and MR

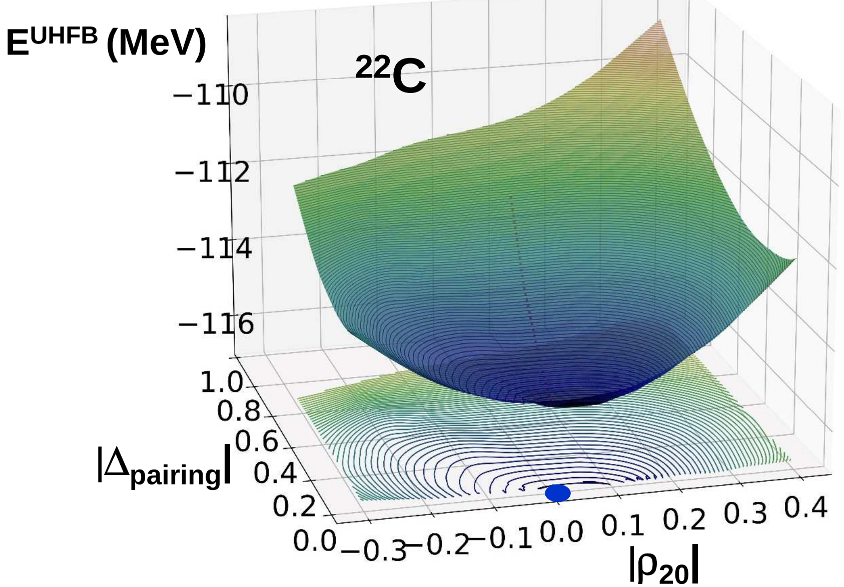
➪Mean-field energy as a function of broken symmetry(ies)

➪Use of symmetry-breaking operator Q to constrain symmetry breaking to |q|

➪Ex: **SU(2) ($q=\rho_{20}$)** and **U(1) ($q=\Delta_{pairing}$)** ➧ doubled-constrained UHFB calculations

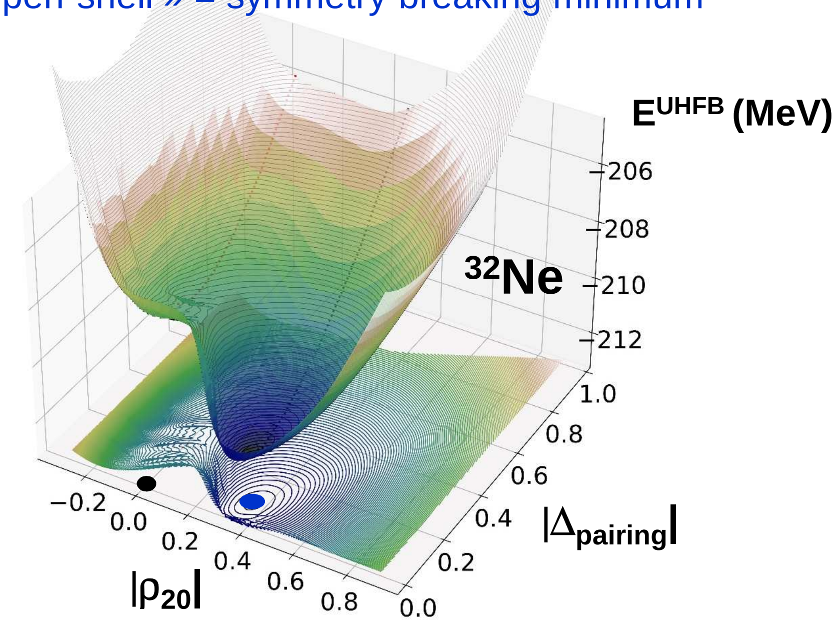
Vacuum total energy surface (TES)

« Closed-shell » = symmetry-conserving minimum



[Ebran, Duguet, unpublished]

« Open-shell » = symmetry-breaking minimum



✶Symmetry conserving = just one particular point when viewed from general perspective of vacuum TES

✶Vacuum TES contains physics beyond the minimum (symmetry conserving or not)

➲ softness around it indicates further collective/static correlations even for “closed-shell” system

Static correlations and (near) degenerate systems

II. Towards an optimal combination of SSB and MR

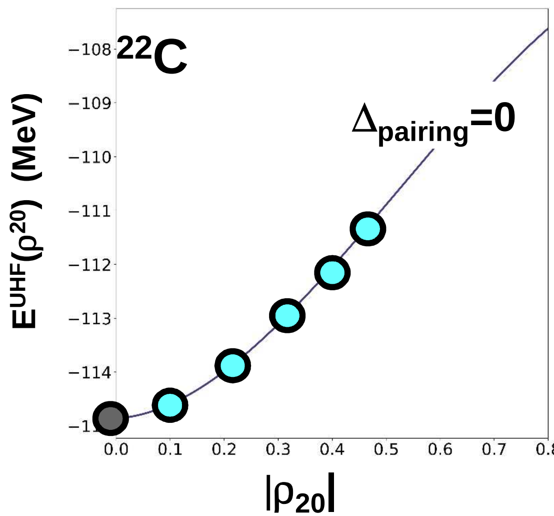
➪1D projection along ρ_{20} ($\geq$ 0) at Δ_{pairing} = 0

Order parameter of broken symmetry

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

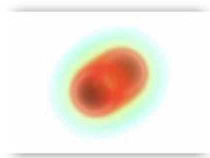
« Closed-shell » = symmetry-conserving minimum

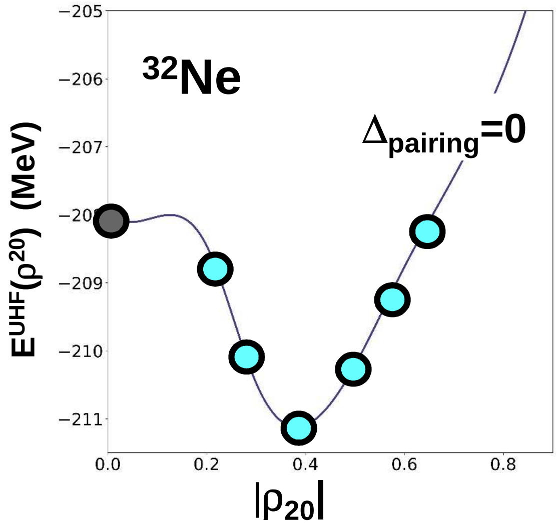
« Open-shell » = symmetry-breaking minimum



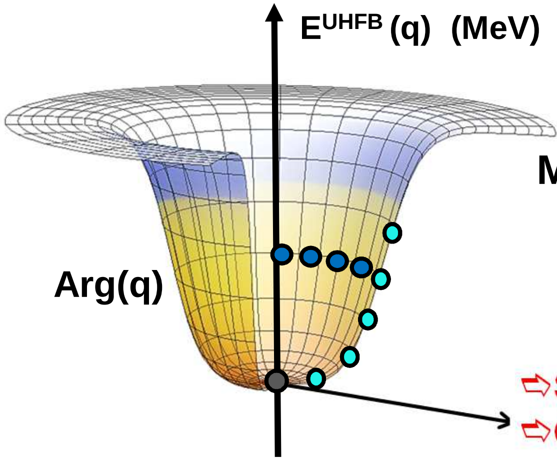
Vacuum total energy curve (TEC)

Add Arg(q)





[Ebran, Duguet, unpublished]



From (small) diago [see talk by B. Bally]

1) Change of |q| = quadrupole fluctuations

2) Change of Arg(q) = angular rotation

MR state from **non-orthogonal vacua (NOV)** in IR

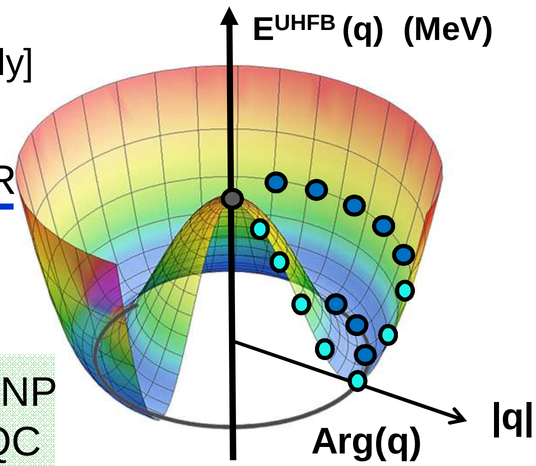
$$|\Theta_{0\ \text{NOV}}^{J=0\ A}\rangle = \sum_{q \in \text{NOV}} c_q |\Phi_q\rangle$$

➪Symmetry-projected state

➪Capture collective static correlations

1) PGCM in NP

2) NOCI in QC

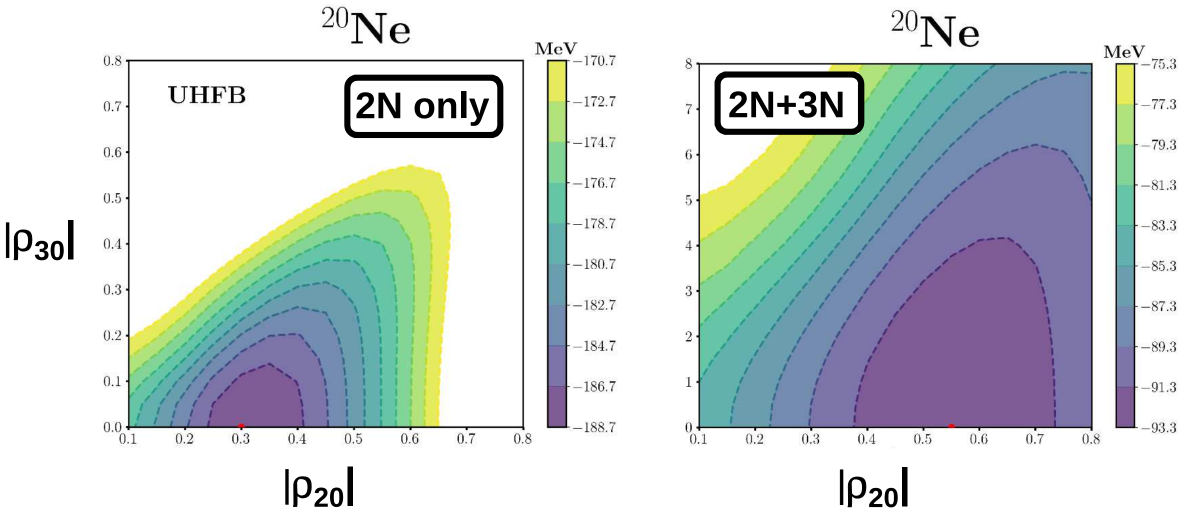


Ex. 2D-PGCM (i.e. NOCI) of ^{20}Ne

➪ **2D TES**: SU(2) breaking constrained along **both q = ρ_{20} and** ρ_{30} (free U(1) breaking)

➧ doubled-constrained UHFB calculations

↳ Breaks parity



◉ **Significative impact of 3N force**

Minima pushed towards larger $|\rho_{20}|$-$|\rho_{30}|$
Softer PES

[Frosini *et al.* unpublished (2021)]

➪: **PGCM** mix along a) |q| with q = ρ_{20} and ρ_{30}

b) Arg(q) = **projections on J, π, N and Z**

◉ **Good reproduction of collective spectroscopy**

Static collective correlations captured

◉ **Significant impact of 3N force**

Improved moment of inertia of rotational bands
Very improved 1^- band-head position

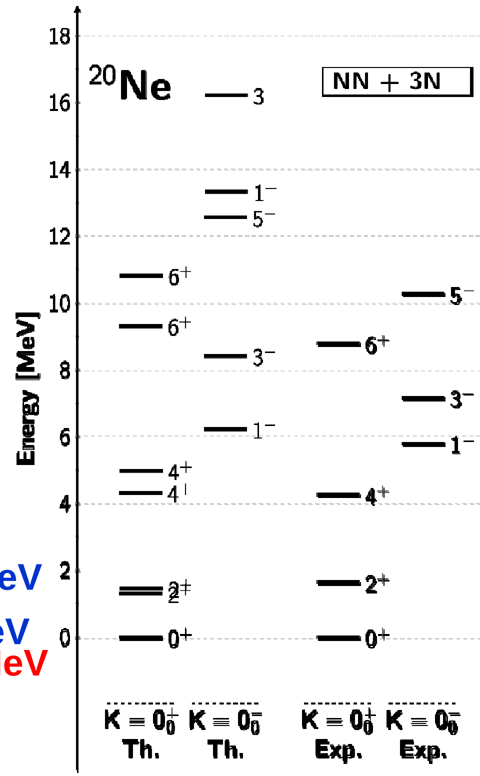
RHFB	**54%**	
Correlations	**46%**	
Static		23%
Dynamical		77%

◉ **Dynamical correlations missing**

Absolute binding energy entirely missed
Elementary excitations not accessed

1) RHFB	**-82 MeV**
2) UHFB	**-93 MeV**
3a) PGCM	**-100 MeV**
3b) UBMBPT(3)	**-153 MeV**
4) Exp	**-160 MeV**

11MeV
7MeV
60MeV



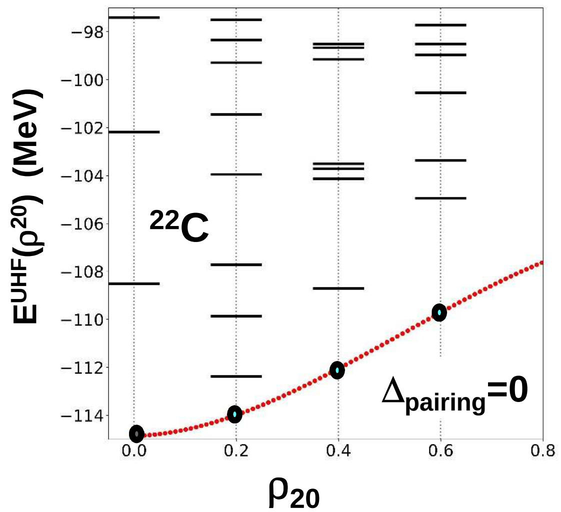
Static correlations and (near) degenerate systems

II. Towards an optimal combination of SSB and MR

➪**Elementary excitations on top of NOV:** $\{|\Phi_q^{k_q}\rangle ; q \in \mathrm{NOV}\ \text{and}\ k_q \in \mathrm{EE}_q\}$

« Closed-shell » = symmetry-conserving minimum

« Open-shell » = symmetry-breaking minimum



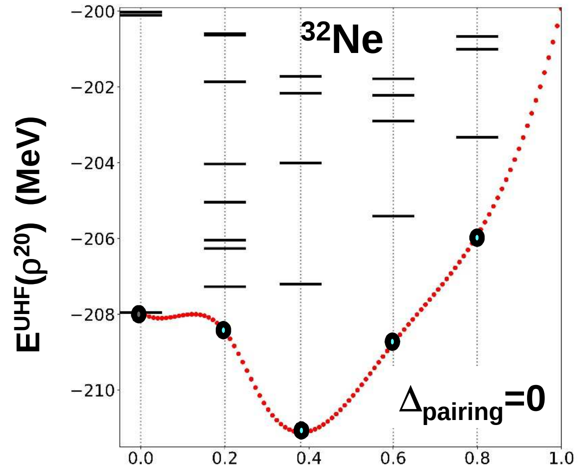
♦Dynamical correlations minimized via SSB

♦NOV mixing pertinent even in closed-shell

♦Dynamical correlations through EE_q

Expansions on top of MR-NOV state

$$|\Psi_0^{J=0\ A}\rangle = \Omega_0^{EE} |\Theta_{0\ NOV}^{J=0\ A}\rangle$$



[Ebran, Duguet, unpublished]

➪**This idea to consistently capture static and dynamical correlations should be pushed in the future**

➪**Two recent examples/proposals**

♦**MR-IMSRG in NP** [Hergert et al. (2013); Yao et al. (2020)]

♦**NOCI-PT in QC** [Burton, Thom (2020)]

Contents

Many-body tensor networks and basis representation

◉ **Many-body calculations employ mode-n tensors and compute tensor networks**

1) Input

$$H_{\rm nucl} = T + V + W + \ldots$$
$$\equiv \frac{1}{(1!)^2}\sum_{pq} t_{pq} c_p^\dagger c_q$$
$$+ \frac{1}{(2!)^2}\sum_{pqrs} \boxed{\bar{v}_{pqrs}} c_p^\dagger c_q^\dagger c_s c_r$$
$$+ \frac{1}{(3!)^2}\sum_{pqrstu} \boxed{\bar{w}_{pqrstu}} c_p^\dagger c_q^\dagger c_r^\dagger c_u c_t c_s$$

k-body force
↕
Mode-2k tensor
↕
Basis representation dim N
↕
Storage cost N[2k]

2) Output

$$E_0 = E_0^{\rm HF} + \frac{1}{2}\boxed{\sum_{ijab} \bar{v}_{ijab}\, t_i^a\, t_j^b} + \frac{1}{4}\sum_{ijab} \bar{v}_{ijab}\, \boxed{t_{ij}^{ab}}$$

Evaluated quantities (here energy)
↕
Tensor network of N[p] cost (here p=4)
↕
Unknown tensors evaluation N[q] cost (e.g. q=6)

◉ **Basis to represent operators/associated tensors**

Oscillator frequency

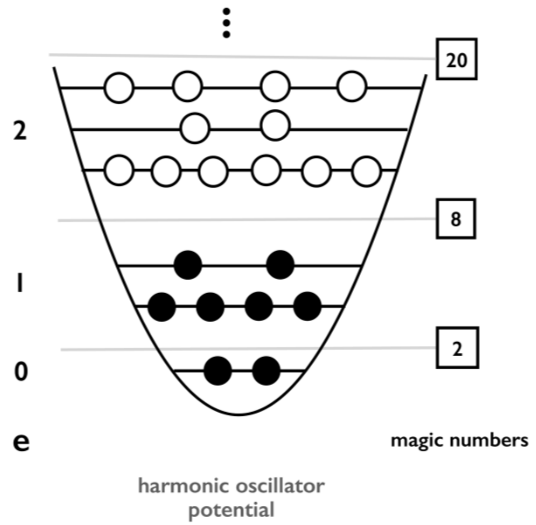
$$H_{\rm sHO} = \frac{\vec{p}^{\,2}}{2m} + \frac{1}{2} m \boxed{\omega^2} \vec{r}^{\,2}$$

○ Spherical harmonic oscillator (sHO) basis of $\mathcal{H}_1$

Finite basis set by maximum excitation $e_{\max} \equiv (2n_k + l_k)_{\max}$

○ Tensor-product basis of $\mathcal{H}_n$ used to represent $T_{i_1 \ldots i_n i_{n+1} \ldots i_{2n}}$

Maximum excitation of the n-body basis state set by $e_{n\max} \equiv n e_{\max}$



$$|k\rangle \equiv |n_k l_k j_k m_{j_k} m_{t_k}\rangle$$

Generalized Laguerre polynomials

$$e_{n_k l_k} = \hbar\omega\left(2n_k + l_k + \frac{3}{2}\right)$$

Many-body tensor networks and basis representation

◉ **Many-body calculations employ mode-n tensors and compute tensor networks**

1) Input

$$H_{\text{nucl}} = T + V + W + \dots$$
$$\equiv \frac{1}{(1!)^2} \sum_{pq} t_{pq} c_p^\dagger c_q + \frac{1}{(2!)^2} \sum_{pqrs} \bar{v}_{pqrs} c_p^\dagger c_q^\dagger c_s c_r + \frac{1}{(3!)^2} \sum_{pqrstu} \bar{w}_{pqrstu} c_p^\dagger c_q^\dagger c_r^\dagger c_u c_t c_s$$

k-body force
↕
Mode-2k tensor
↕
Basis representation dim N
↕
Storage cost N^{2k}

2) Output

$$E_0 = E_0^{\text{HF}} + \frac{1}{2} \sum_{ijab} \bar{v}_{ijab}\, t_i^a\, t_i^b + \frac{1}{4} \sum_{ijab} \bar{v}_{ijab}\, t_{ij}^{ab}$$

Evaluated quantities (here energy)
↕
Tensor network of N^p cost (here p=4)
↕
Unknown tensors evaluation N^q cost (e.g. q=6)

◉ **Challenge to store mode-6 tensors, e.g. 3N force, in large enough basis**

○ Storage/handling of full tensor impossible in Hilbert space initially considered

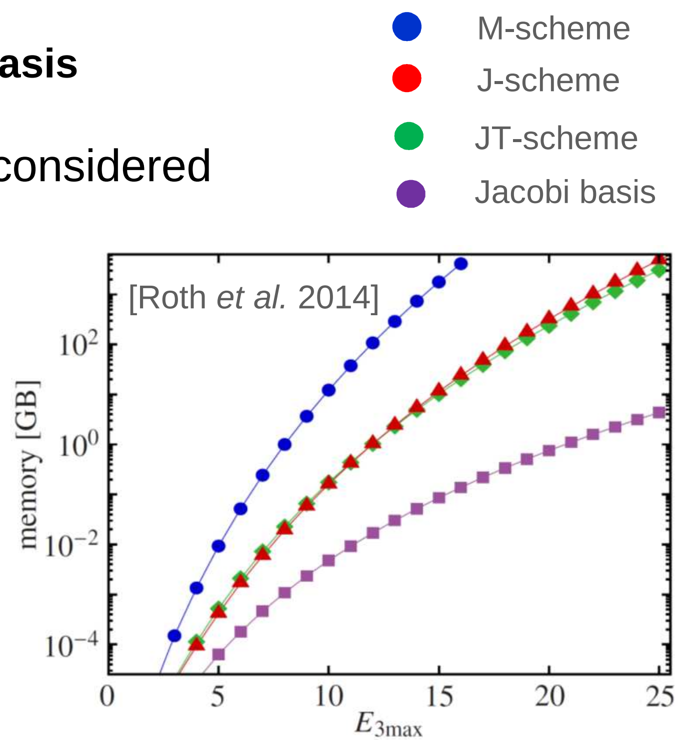
→ Need e_{1max} ~ 13 (N~2000)/ e_{3max} = 3*E_{1max} ~ 40 in mid-mass systems

→ Impossible! → Further truncation on e_{3max} mandatory

○ 3N matrix elements files can easily be 100Gb in size

○ CI benchmarks : 4N force quite small (~100keV in ^{4}He)

→ Size of 4N forces in medium-mass systems unknown!



Ex. Pre-processing tools: TF and IT

◉ **Many-body calculations employ mode-n tensors and compute tensor networks**

1) Input

$$H_{\rm nucl} = T + V + W + \dots$$
$$\equiv \frac{1}{(1!)^2}\sum_{pq} t_{pq} c_p^\dagger c_q + \frac{1}{(2!)^2}\sum_{pqrs} \boxed{\bar{v}_{pqrs}} c_p^\dagger c_q^\dagger c_s c_r + \frac{1}{(3!)^2}\sum_{pqrstu} \boxed{\bar{w}_{pqrstu}} c_p^\dagger c_q^\dagger c_r^\dagger c_u c_t c_s$$

k-body force
↕
Mode-2k tensor
↕
Basis representation dim N
↕
Storage cost N^{2k}

2) Output

$$E_0 = E_0^{\rm HF} + \frac{1}{2}\boxed{\sum_{ijab} \bar{v}_{ijab}\, t_i^a\, t_i^b} + \frac{1}{4}\sum_{ijab} \bar{v}_{ijab}\, \boxed{t_{ij}^{ab}}$$

Evaluated quantities (here energy)
↕
Tensor network of N^p cost (here p=4)
↕
Unknown tensors evaluation N^q cost (e.g. q=6)

◉ **Push ab initio calculations to (i) doubly open-shell (ii) heavier (A>130) (iii) better accuracy (<1%)**

→ **Storage/CPU** of ab initio calculations scale as $\mathbf{N^n}$

→ N = 1-body basis dimension

→ n = characteristic of accuracy/AN force

→ Systematic **data compression** techniques

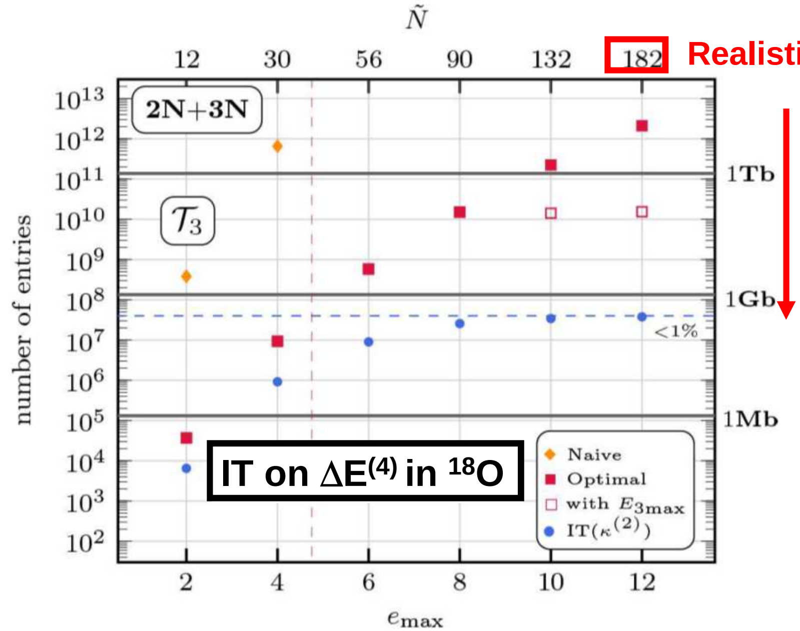
→ **Tensor Factorization** (TF) = **acts on n**

[Tichai et al. 2018] [see Talk by A. Tichai]

→ **Importance Truncation** (IT) = **acts on N**

[Tichai, Ripoche, Duguet 2019]

[Porro et al. unpublished 2021]



Realistic basis dimension

10^5 compression
1% error on $\Delta E^{(4)}$

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