Effective theory for deformed nuclei

Thomas Papenbrock

and OAK RIDGE NATIONAL LABORATORY

Aim: Example of an effective theory with spontaneous symmetry breaking relevant for atomic nuclei. Pedagogical treatment to a model-independent theory of nuclear rotation. Introduction to [TP, Nucl. Phys. 852, 36 (2011), TP and Weidenmüller, Phys. Rev. C 89, 014334 (2014)].

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Energy scales and relevant degrees of freedom

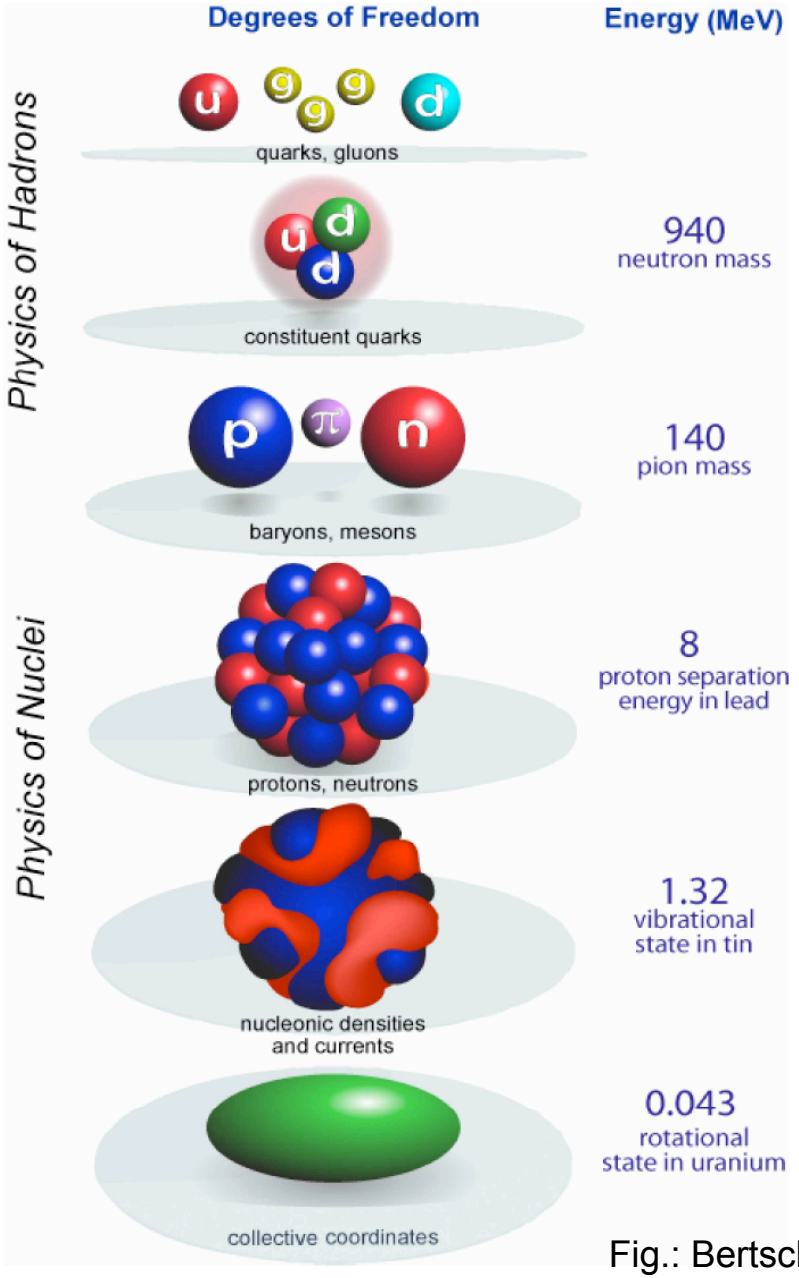

Fig.: Bertsch, Dean, Nazarewicz, SciDAC review (2007)

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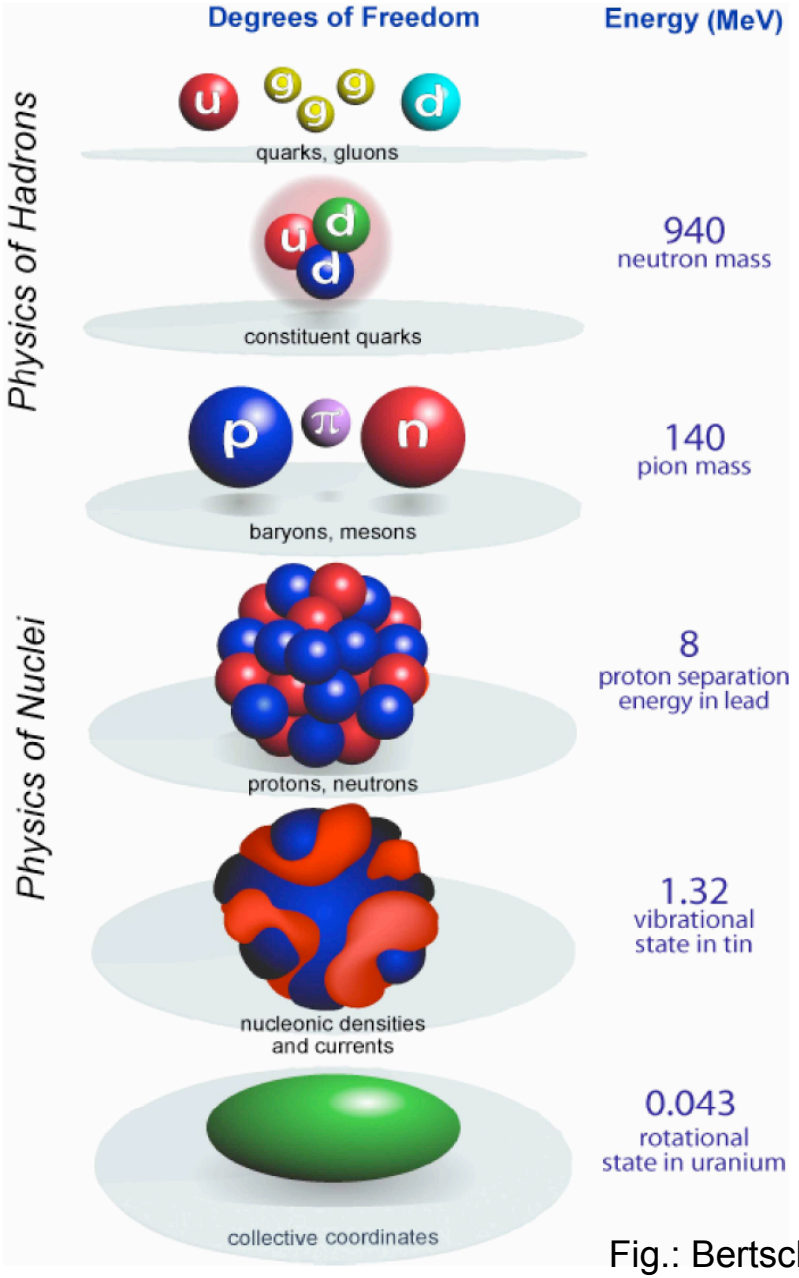

Chiral effective field theory

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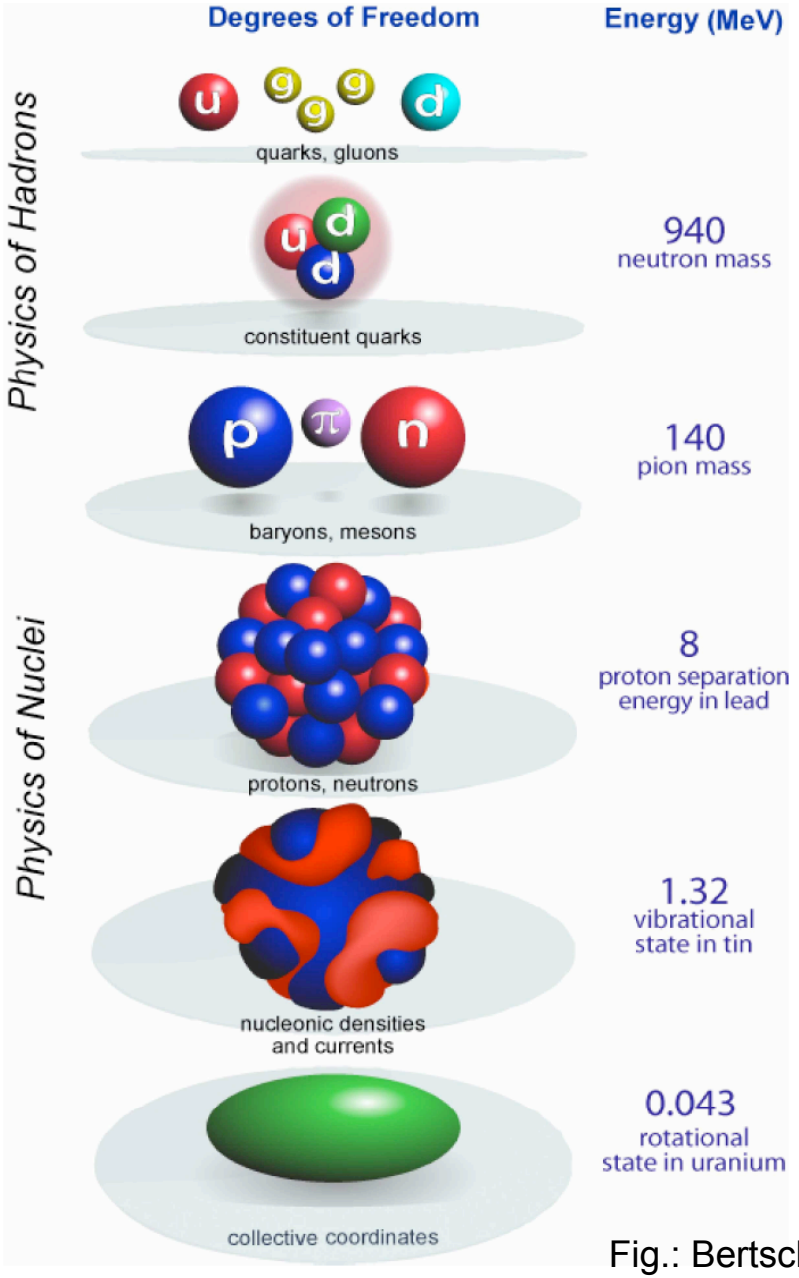

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Effective Theory for intrinsically deformed nuclei

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Comment: Strictly speaking, this can only happen in a macroscopic system.

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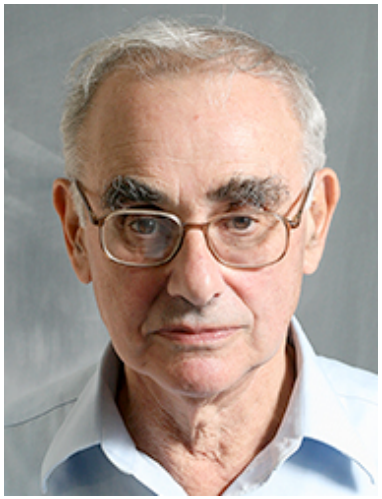
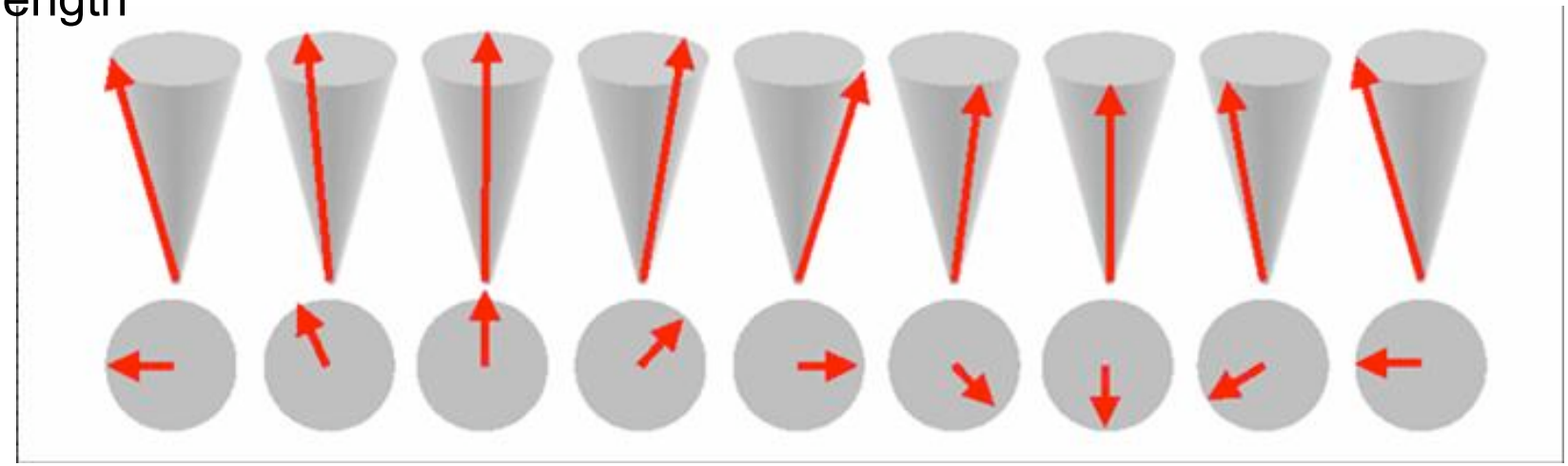
Nambu-Goldstone modes are low-lying excitations in the presence of spontaneous symmetry breaking



Spontaneous symmetry breaking of rotational symmetry: ferromagnet

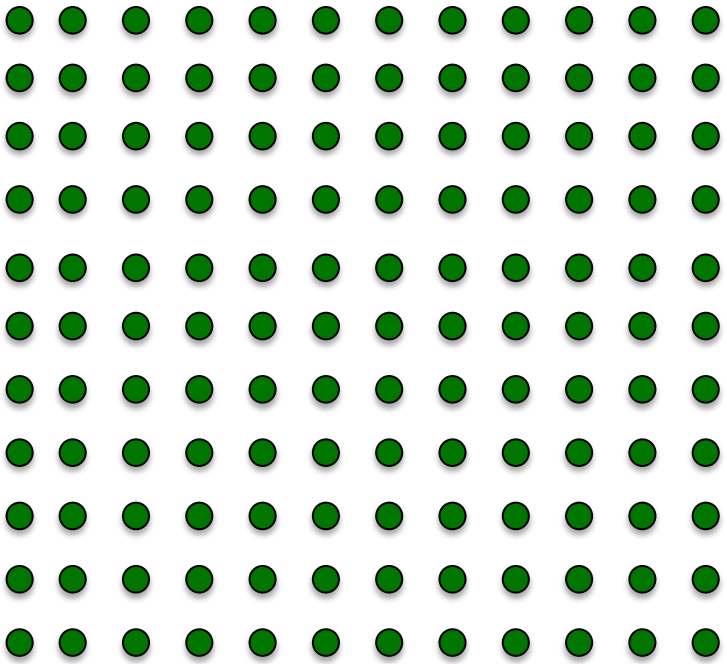
- Axially symmetric ground state breaks SO(3) rotational symmetry.
- Nambu-Goldstone modes generate local (i.e. position and time dependent) rotations of the spins.
- **$\exp(-i\,\psi_x(x,y,z,t)\,J_x - i\,\psi_y(x,y,z,t)\,J_y)$** with Nambu-Goldstone fields **(ψ_x, ψ_y)** and angular momentum operators **(J_x, J_y)**
- Spin waves (or magnons) are low-energy excitations with long wave length

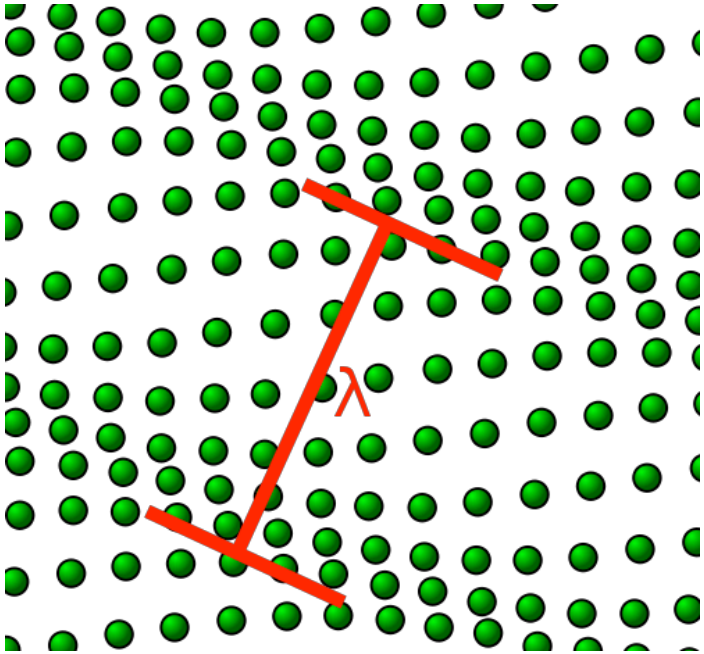


Picture: www-llb.cea.fr

Spontaneous breaking of translational symmetry: crystal

- Crystal lattice breaks translational symmetry.
- Nambu-Goldstone modes generate local (i.e. position and time dependent) translations of the lattice points (ions).
- **$\exp(-i\,\psi_x(x,y,z,t)\,P_x - i\,\psi_y(x,y,z,t)\,P_y - i\,\psi_z(x,y,z,t)\,P_z)$** with Nambu-Goldstone fields **(ψ_x, ψ_y, ψ_z)** and momentum operators **(P_x, P_y, P_z)**
- Phonons are low-energy excitations (wave length λ much larger than lattice spacing)





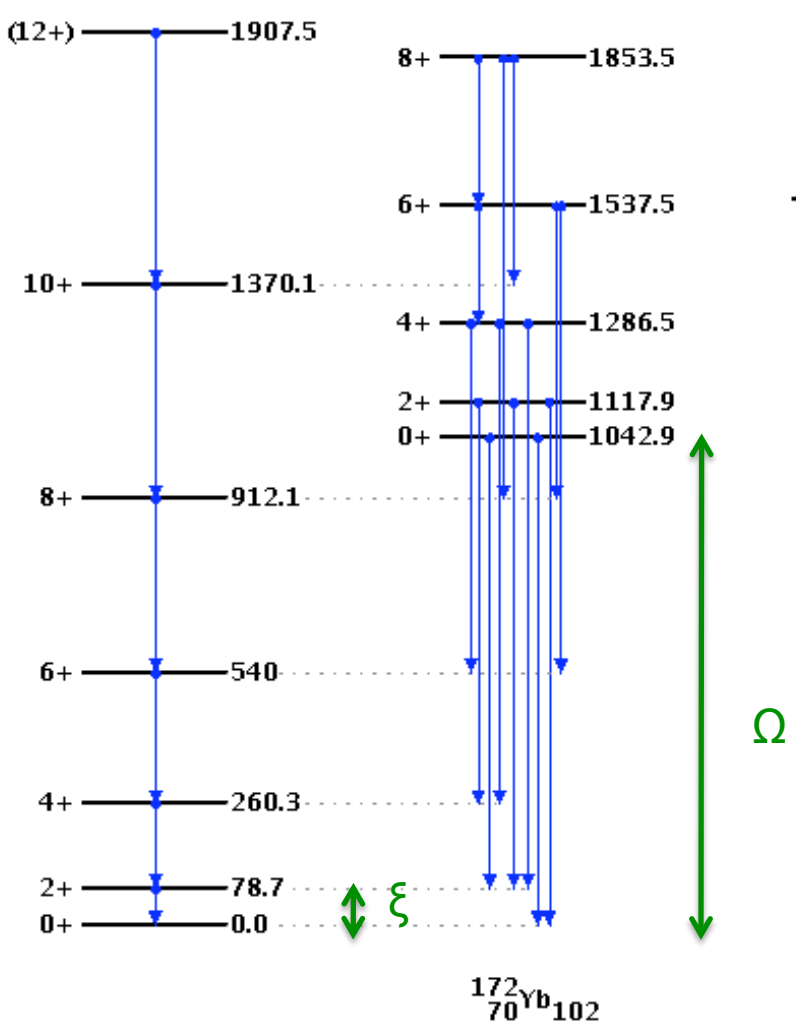
Source: wikipedia (Florian Marquard)

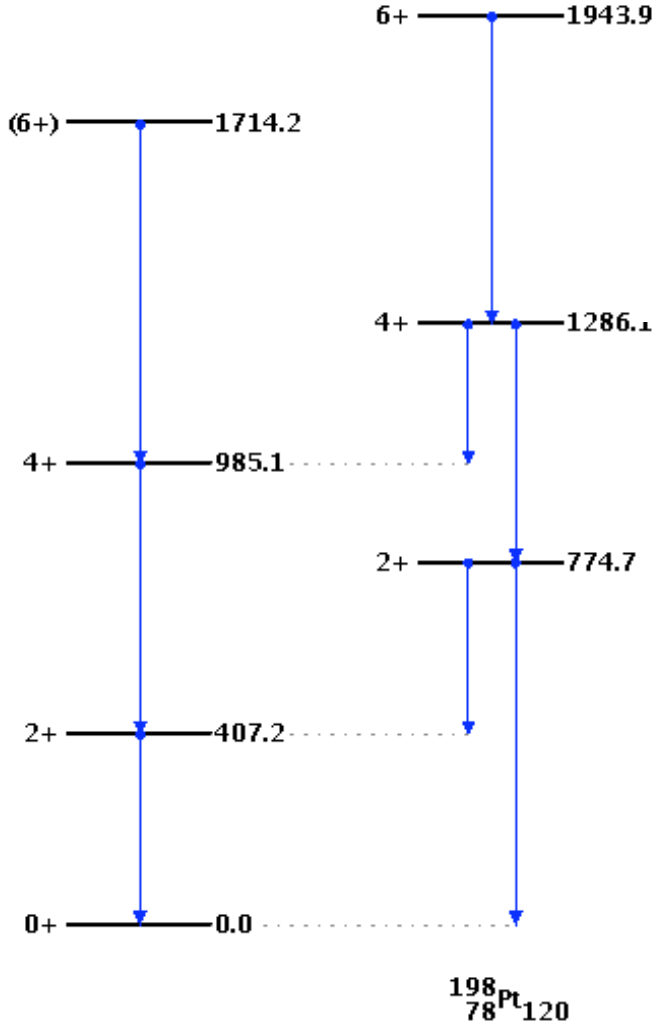
Atomic nuclei are (small) finite systems. There can not be spontaneous symmetry breaking

- **In infinite deformed systems**, different orientations correspond to inequivalent Hilbert spaces.
- The overlap between states in inequivalent Hilbert spaces is zero.
- Rotations of the whole system are not considered.
- Such rotations are “zero modes”: “Nambu-Goldstone” modes that depend only on time but not on position.

- **In finite systems**, states corresponding to different orientations have finite overlap.
- Nevertheless, in systems with “emergent symmetry breaking” exhibit low-lying excitations.
- Quantized rotations (“zero modes”) are the low lying excitations.

Spectra of two heavy nuclei





Rotor: Separation of scale: ξ << Ω
"almost" spontaneously broken rotational symmetry

"vibrational" exitations

Which of the following is correct?

1. Nuclei with rotational spectrum (such as ^{172}Yb) are deformed, i.e. rotational symmetry is spontaneously broken. They literally have an oblate or a prolate shape.
2. There is no spontaneous symmetry breaking in finite systems, and there are no deformed nuclei. States of atomic nuclei have good spin, and thus cannot be deformed.

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What do we mean by (intrinsically) “deformed” nuclei?

1. Nuclei with much enhanced strength in electric quadrupole transitions and (if they are even-Z, even-N) low-lying 2^+ states.
2. Nuclei that exhibit rotational bands and a separation of scale ($\xi << \Omega$) that reflects the precursors of spontaneous symmetry breaking in a finite system.
3. Mean-field computations of such nuclei would yield a deformed density of the single-particle ground state.
4. Intrinsic deformation: In the co-rotating (body-fixed) coordinate system, the nucleus is deformed
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Q: How can we economically solve a physical problem (by employing appropriate degrees of freedom)?

A: Exploit a separation of scales.

Examples:

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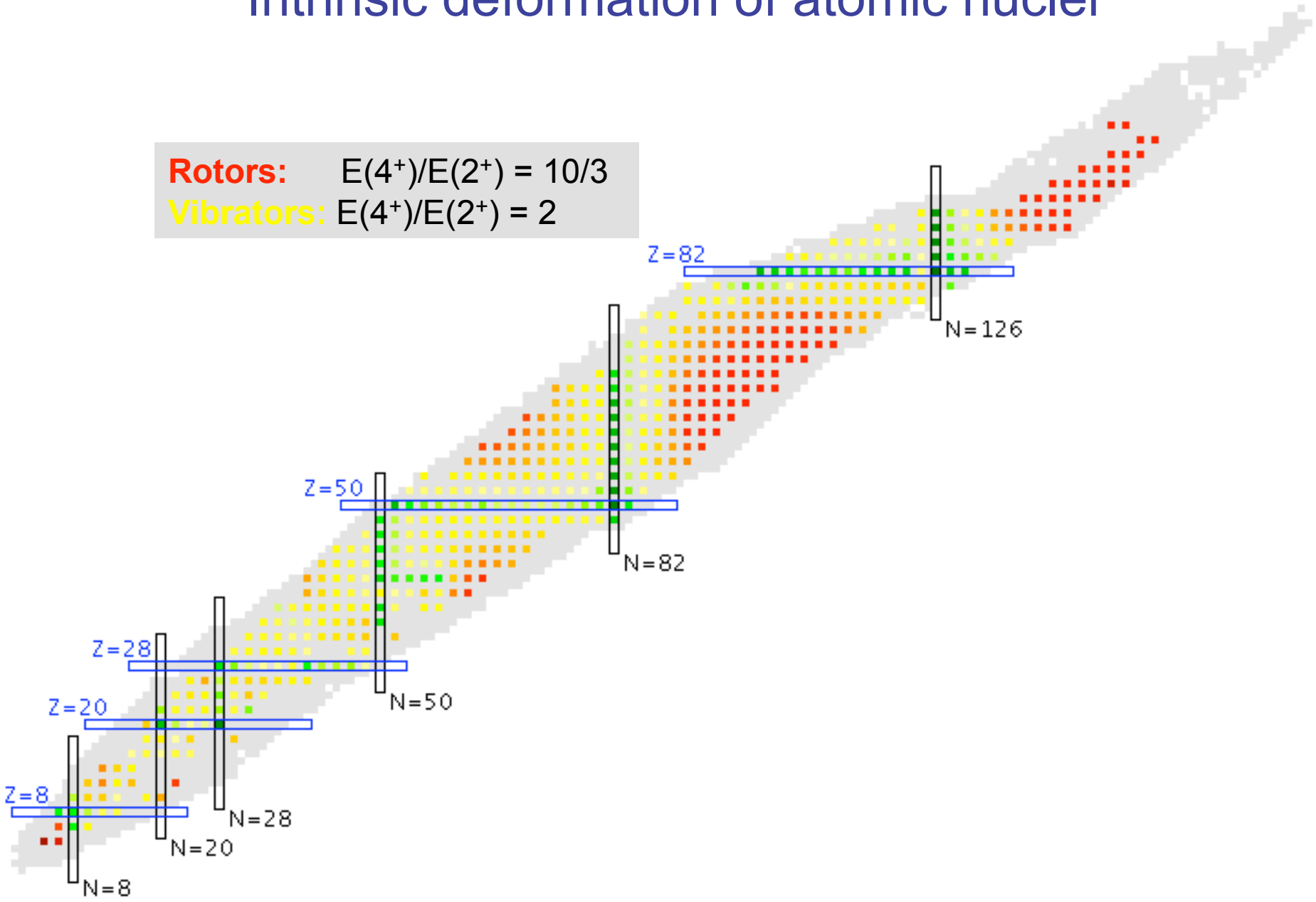
   Q: Why does it work?

   A: Excitation of nucleon (~300 MeV) >> excitation energies of nuclei (~ 1MeV)

Intrinsic deformation of atomic nuclei

Rotors: $E(4^+)/E(2^+) = 10/3$
Vibrators: $E(4^+)/E(2^+) = 2$



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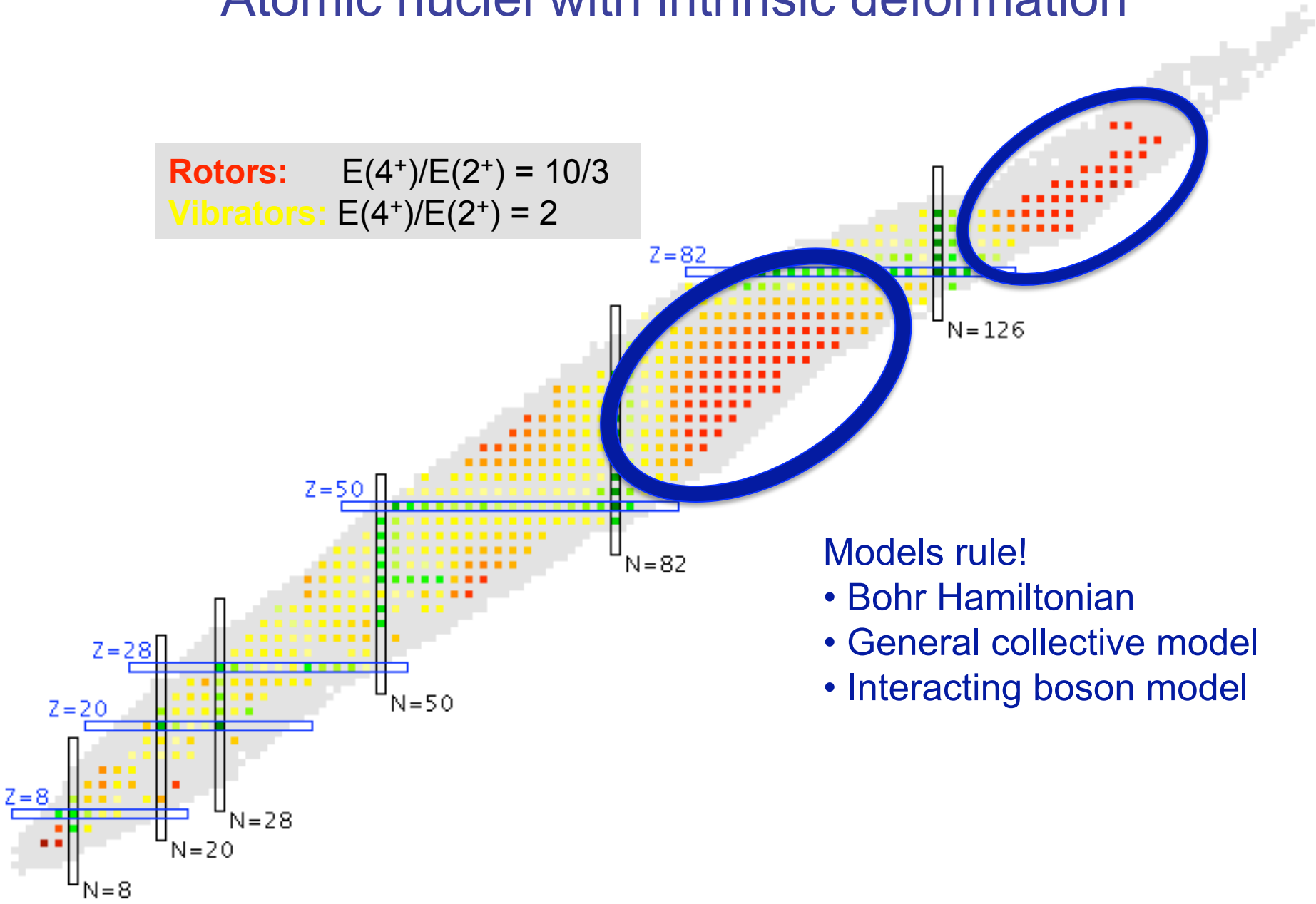

Models rule!

- Bohr Hamiltonian
- General collective model
- Interacting boson model

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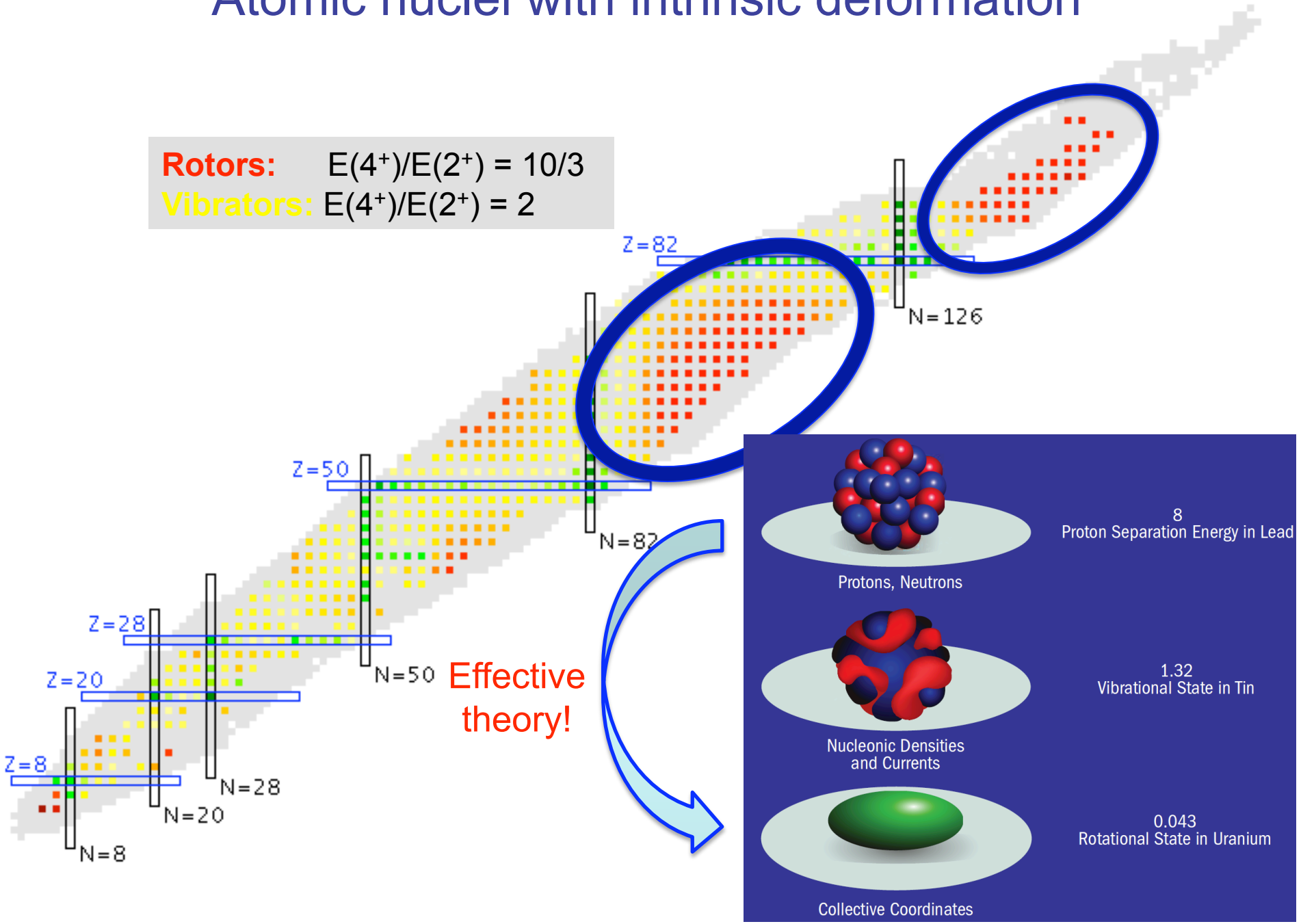


Construction of an EFT

1. Identify the **relevant degrees of freedom** for the resolution scale of interest

2. Identify the **relevant symmetries** of low-energy nuclear physics and investigate if and how they are broken

3. Construct the **most general Lagrangian** consistent with those symmetries and the symmetry breaking.

4. Design an **organizational scheme** (power counting) that can distinguish between more and less important contributions

Useful references:

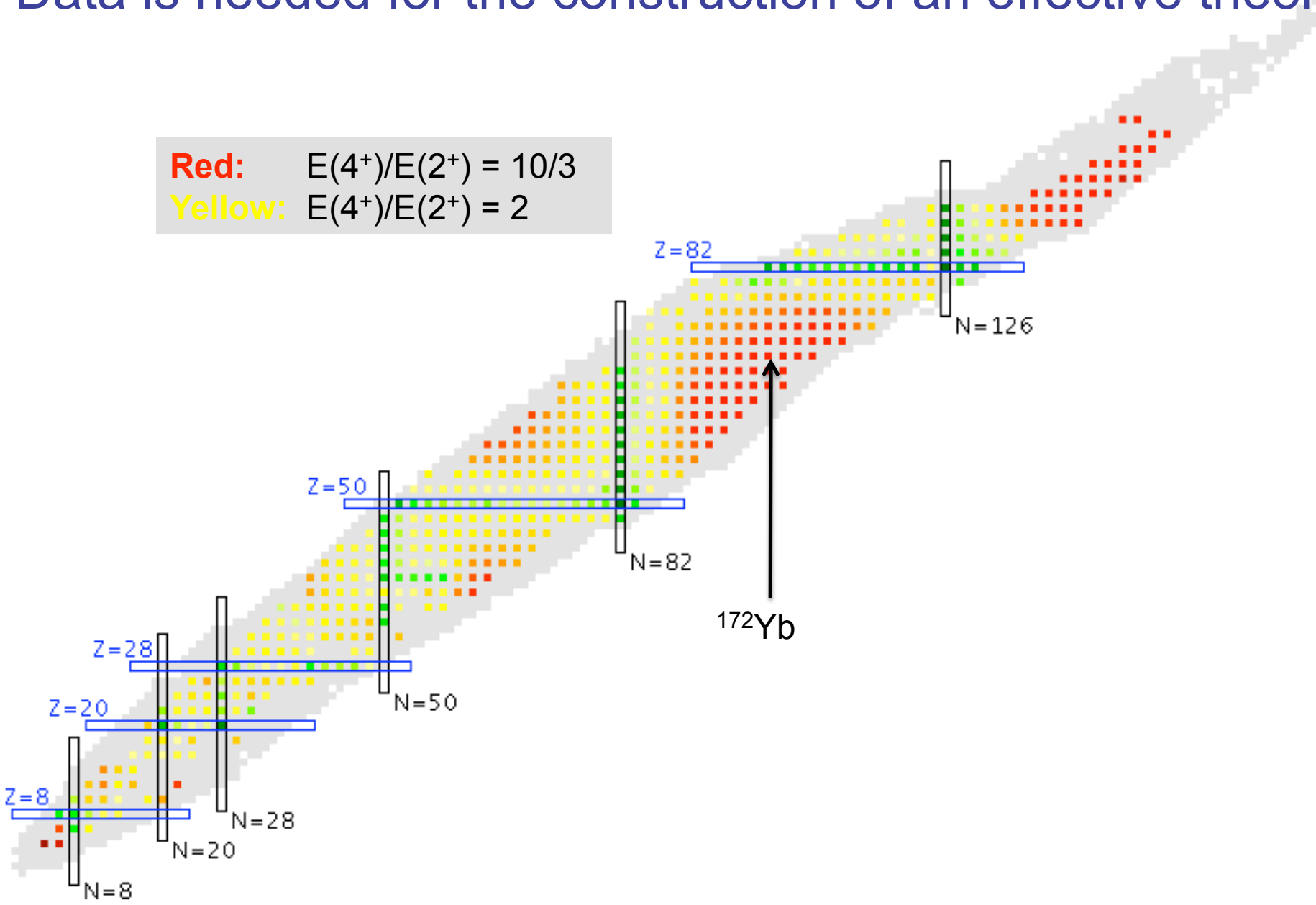
S. Weinberg, *The Quantum Theory of Fields,* Vol.II, chap. 19

H. Leutwyler, Phys. Rev. D **49** (1994) 3033, arXiv:hep-ph/9311264

C. P. Burgess, Physics Reports **330** (2000) 193

Data is needed for the construction of an effective theory

Red: $E(4^+)/E(2^+) = 10/3$
Yellow: $E(4^+)/E(2^+) = 2$



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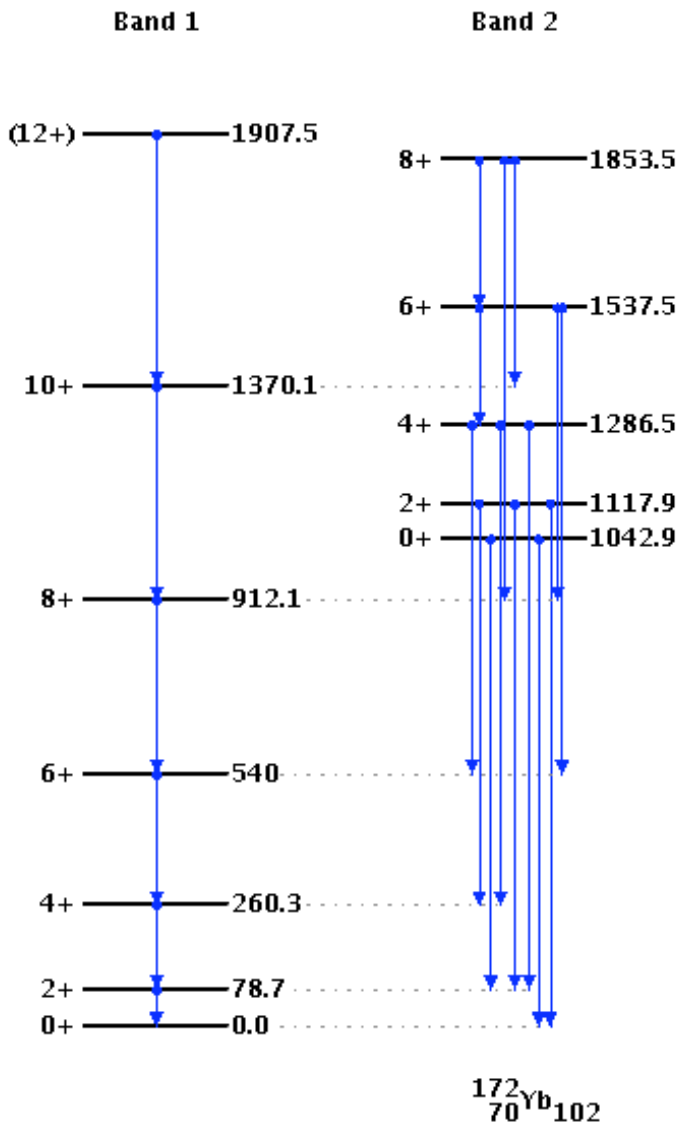

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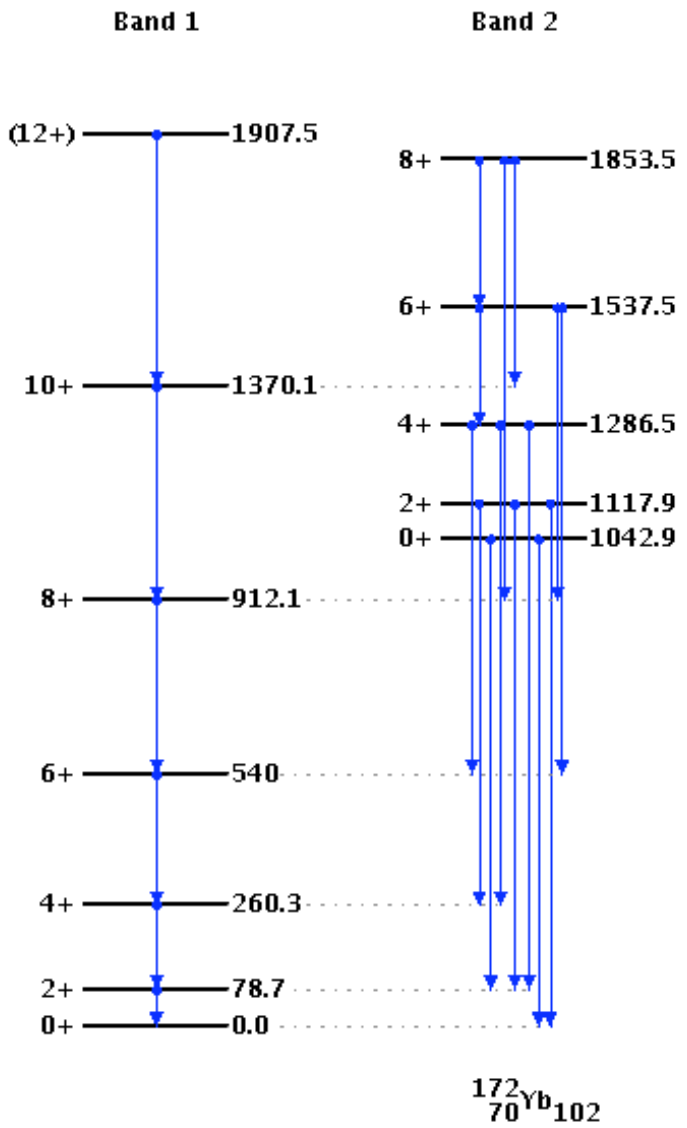

Quadrupole degrees of freedom describe spins and parity of low-energy spectra

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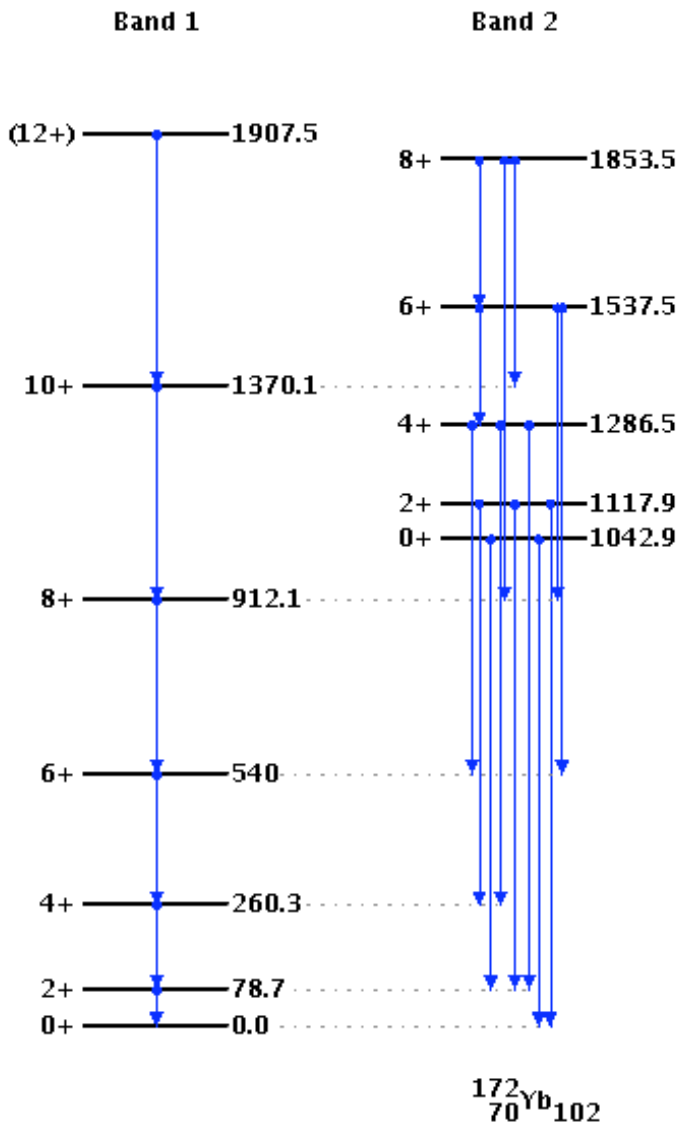
Q: What are the symmetries, and are they spontaneously broken?



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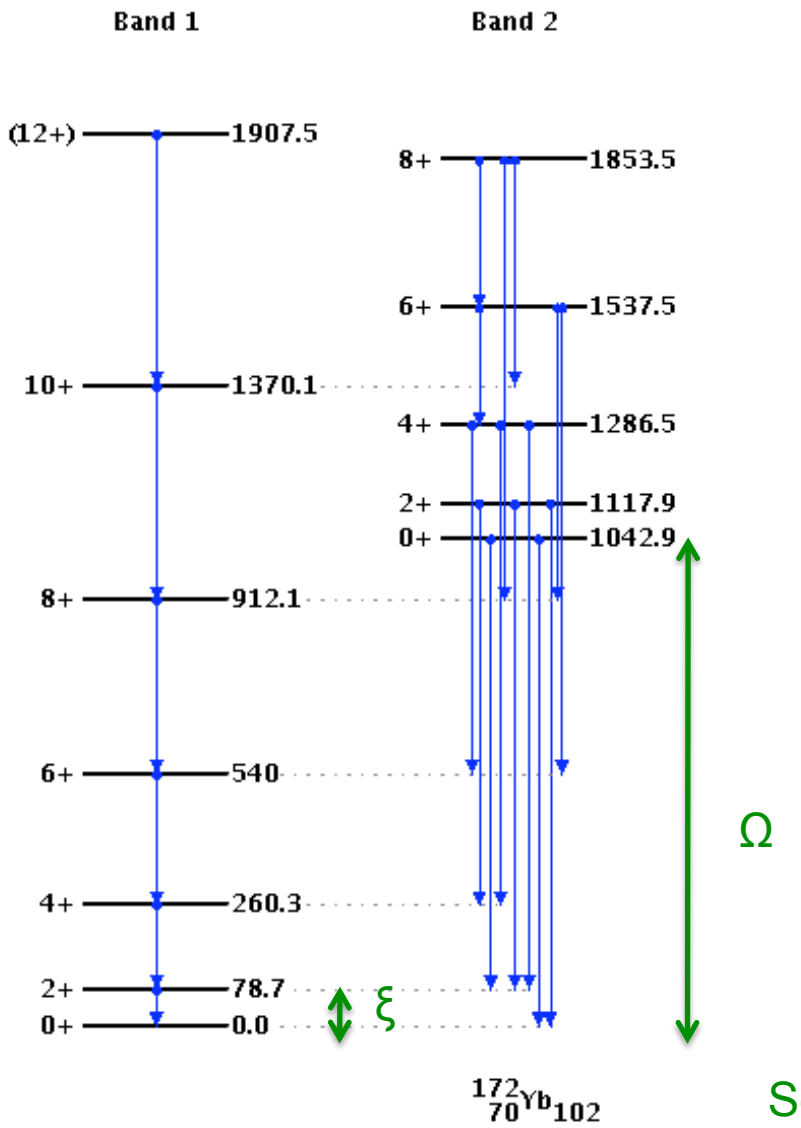

Separation of scale: $\xi \ll \Omega$

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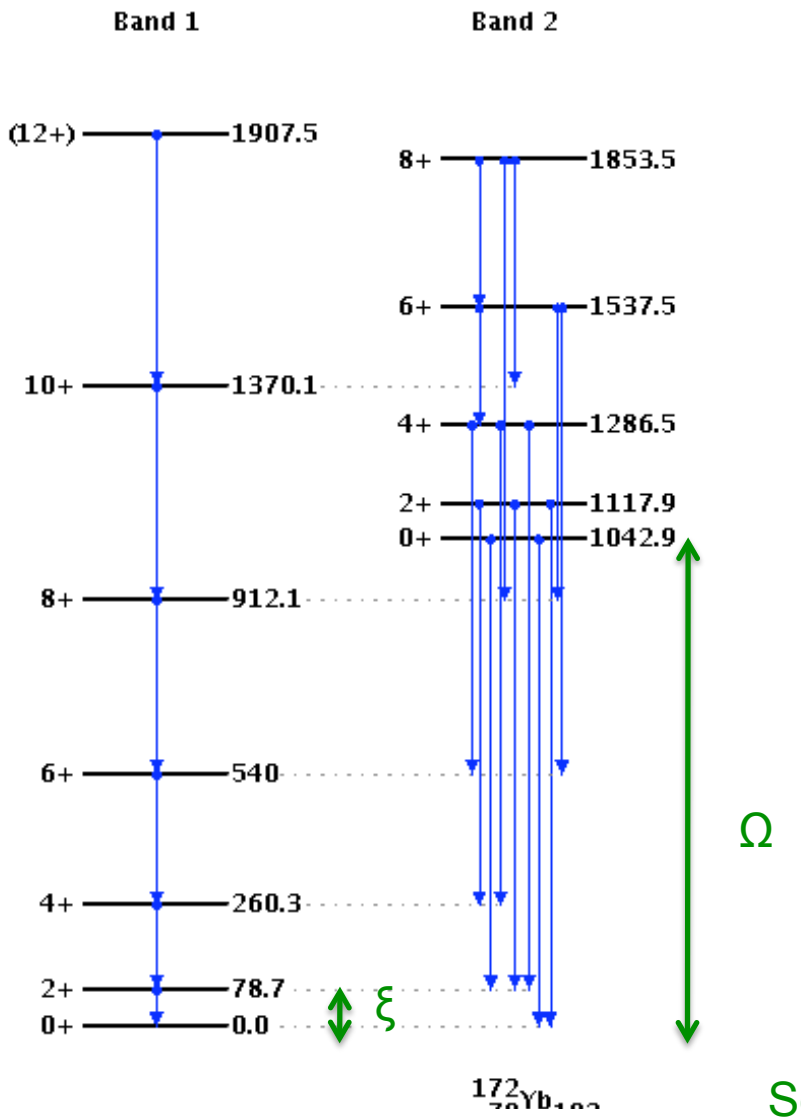
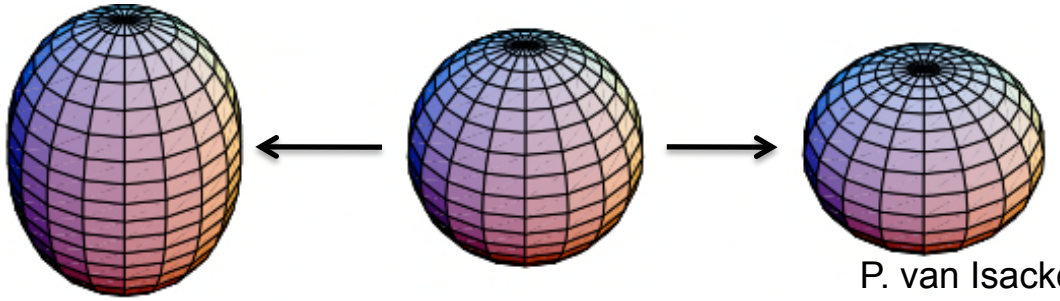


Separation of scale: ξ << Ω

Symmetry: Rotational invariance

Very low-energy (Nambu-Goldstone) modes precursors of spontaneous symmetry breaking

3. Construct the most general Hamiltonian consistent with the symmetry and the symmetry breaking



P. van Isacker 2008

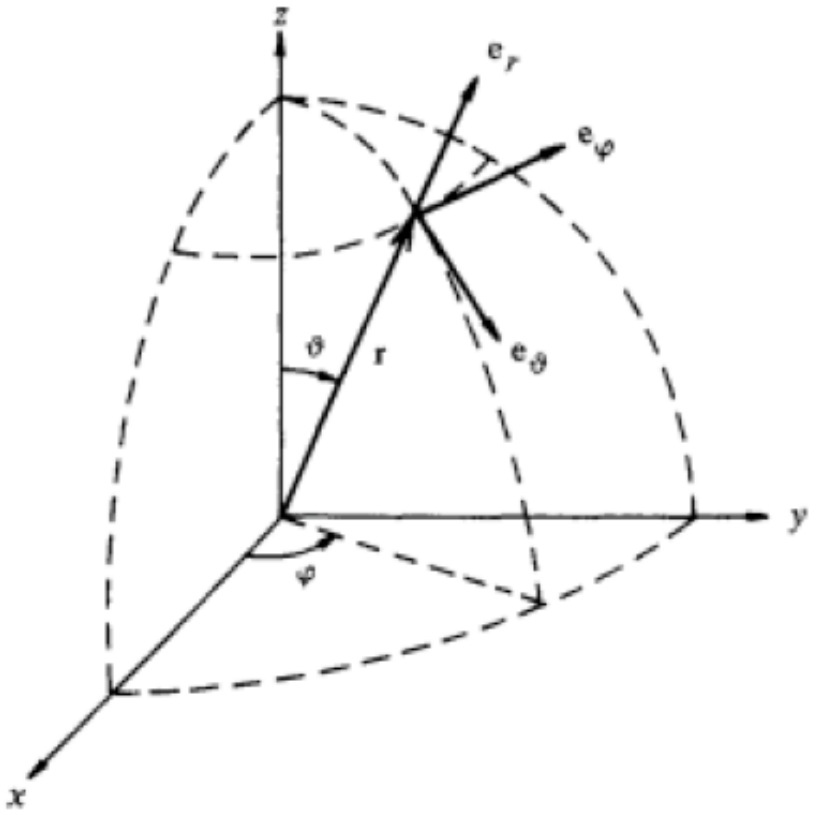
Rotational symmetry	→	Axial symmetry
SO(3)	→	SO(2)
3 generators		1 generator

There will be 3-1=2 Nambu-Goldstone bosons

Nambu-Goldstone modes parameterize the coset SO(3)/SO(2) ~ S^2, i.e. the two-sphere: [Weinberg 1967; Coleman, Callan, Wess & Zumino 1969; H. Leutwyler, Phys. Rev. D 49 (1994) 3033, arXiv:hep-ph/9311264

$$\vec{n}(\theta,\phi) = \begin{pmatrix} \cos\phi\sin\theta \\ \sin\phi\sin\theta \\ \cos\theta \end{pmatrix} = \vec{e}_r$$

Parameters of the sphere: coordinates ϑ and φ



velocity ("lives" in tangent plane):

$$\begin{aligned}\partial_t \vec{n} &= \dot{\phi}\sin\theta\vec{e}_\phi + \dot{\theta}\vec{e}_\theta \\ &= v_\phi\vec{e}_\phi + v_\theta\vec{e}_\theta\end{aligned}$$

velocity components

$$\begin{aligned}v_\phi &\equiv \dot{\phi}\sin\theta \\ v_\theta &\equiv \dot{\theta}\end{aligned}$$

$$\vec{n}(\theta,\phi) = \begin{pmatrix}\cos\phi\sin\theta \\ \sin\phi\sin\theta \\ \cos\theta\end{pmatrix} = \vec{e}_r$$

Question: How do the velocity components transform under a rotation?

Question: How does the vector n(ϑ,φ) transform under a rotation?

Transformation properties under rotations

Rotations do this

$$\delta\vec{n} = \delta\vec{\omega} \times \vec{n}$$

Change of vector n (in tangent plane!)

$$\delta\vec{n} = \delta\phi \sin\theta \vec{e}_\phi + \delta\theta\vec{e}_\theta$$

Result:

$$\begin{pmatrix} \delta\phi \\ \delta\theta \end{pmatrix} = \begin{pmatrix} -\cos\phi\cot\theta & -\sin\phi\cot\theta & 1 \\ \sin\phi & \cos\phi & 0 \end{pmatrix} \begin{pmatrix} \delta\omega_x \\ \delta\omega_y \\ \delta\omega_z \end{pmatrix}$$

Transformation of velocity components under rotations

$$\delta \begin{pmatrix} \dot{\phi} \sin\theta \\ \dot{\theta} \end{pmatrix} = \begin{pmatrix} \cos\gamma & -\sin\gamma \\ \sin\gamma & \cos\gamma \end{pmatrix} \begin{pmatrix} \dot{\phi} \sin\theta \\ \dot{\theta} \end{pmatrix}$$

with

$$\gamma \equiv -\frac{\cos\phi}{\sin\theta}\delta\omega_x - \frac{\sin\phi}{\sin\theta}\delta\omega_y$$

Key result: velocity components v_φ and v_ϑ transform as x- and y-components of a vector under SO(2) rotations, albeit with a complicated angle γ

→"Nonlinear realization" of rotational symmetry

Simplest invariant:

$$v_\theta^2 + v_\phi^2 = \dot{\theta}^2 + \dot{\phi}^2 \sin^2\theta$$

Question: I thought rotations do not commute, but the law above appears as axial symmetry [i. e. SO(2)] and not as from SO(3)

Physics of Nambu-Goldstone modes

Lagrangian $$L = \frac{C_0}{2}\left(\dot{\theta}^2 + \dot{\phi}^2 \sin^2\theta\right)$$

Hamiltonian $$H = \frac{1}{2C_0}\left(p_\theta^2 + \frac{p_\phi^2}{\sin^2\theta}\right)$$

Quantization $$p_\theta^2 \equiv \frac{1}{\sin\theta}\partial_\theta \sin\theta \partial_\theta$$
$$p_\phi \equiv -i\partial_\phi$$

Spectrum $$\hat{H}Y_{IM}(\theta,\phi) = \frac{I(I+1)}{2C_0}Y_{IM}(\theta,\phi)$$

Rotational bands are quantized Nambu-Goldstone modes (Superposition of differently oriented deformed nuclei).
Low-energy constant C_0 is moment of inertia and fit to data.

4. Power counting and next-to-leading order

Let us first understand dimensional analysis

1. Low-energy scale is ξ
2. Leading-order Lagrangian $L = \frac{C_0}{2}(\partial_t \vec{n}) \cdot (\partial_t \vec{n})$ must scale as: L~ξ
3. Energy-time uncertainty implies (ħ=1): $d_t \sim \xi$
4. Thus $C_0 \sim 1/\xi$

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Next-to-leading order term (scalar in NG modes that we can write down)

$$L = (C_2/4)\left((\partial_t \vec{n}) \cdot (\partial_t \vec{n}) \right)^2$$

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Q2: What is the dimension of C_2 in powers of energy?

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$$L = (C_2/4)\left((\partial_t \vec{n}) \cdot (\partial_t \vec{n}) \right)^2$$

Q2: What is the dimension of C_2 in powers of energy?

A2: It must have dimensions of energy^{-3} (We have two energy scales ξ << Ω)

4. Power counting and next-to-leading order

Let us first understand dimensional analysis

1. Low-energy scale is ξ
2. Leading-order Lagrangian $L = \frac{C_0}{2}(\partial_t \vec{n}) \cdot (\partial_t \vec{n})$ must scale as: L~ξ
3. Energy-time uncertainty implies (ħ=1): $d_t \sim \xi$
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Next-to-leading order term (scalar in NG modes that we can write down)

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A2: It must have dimensions of energy^{-3} (We have two energy scales ξ << Ω)

Q2: How should the term C_2 scale precisely? A2: ξ^{-3}, $\xi^{-2}\Omega^{-1}$, $\xi^{-1}\Omega^{-2}$, Ω^{-3} … ?

A2: $C_2/C_0 \sim$ energy^{-2} and is due to omitted physics at a high-energy scale Ω
Thus: $C_2/C_0 \sim \Omega^{-2}$ assuming ***naturalness***

4. Power counting and next-to-leading order

Lagrangian at next-to-leading

$$L = (C_0/2)(\partial_t \vec{n}) \cdot (\partial_t \vec{n}) + (C_2/4)\,(\,(\partial_t \vec{n}) \cdot (\partial_t \vec{n})\,)^2$$

Spectrum: $J(J+1)/(2C_0) - (J(J+1))^2\,(C_2/4C_0^4)$

→Bohr & Mottelson (of course!)

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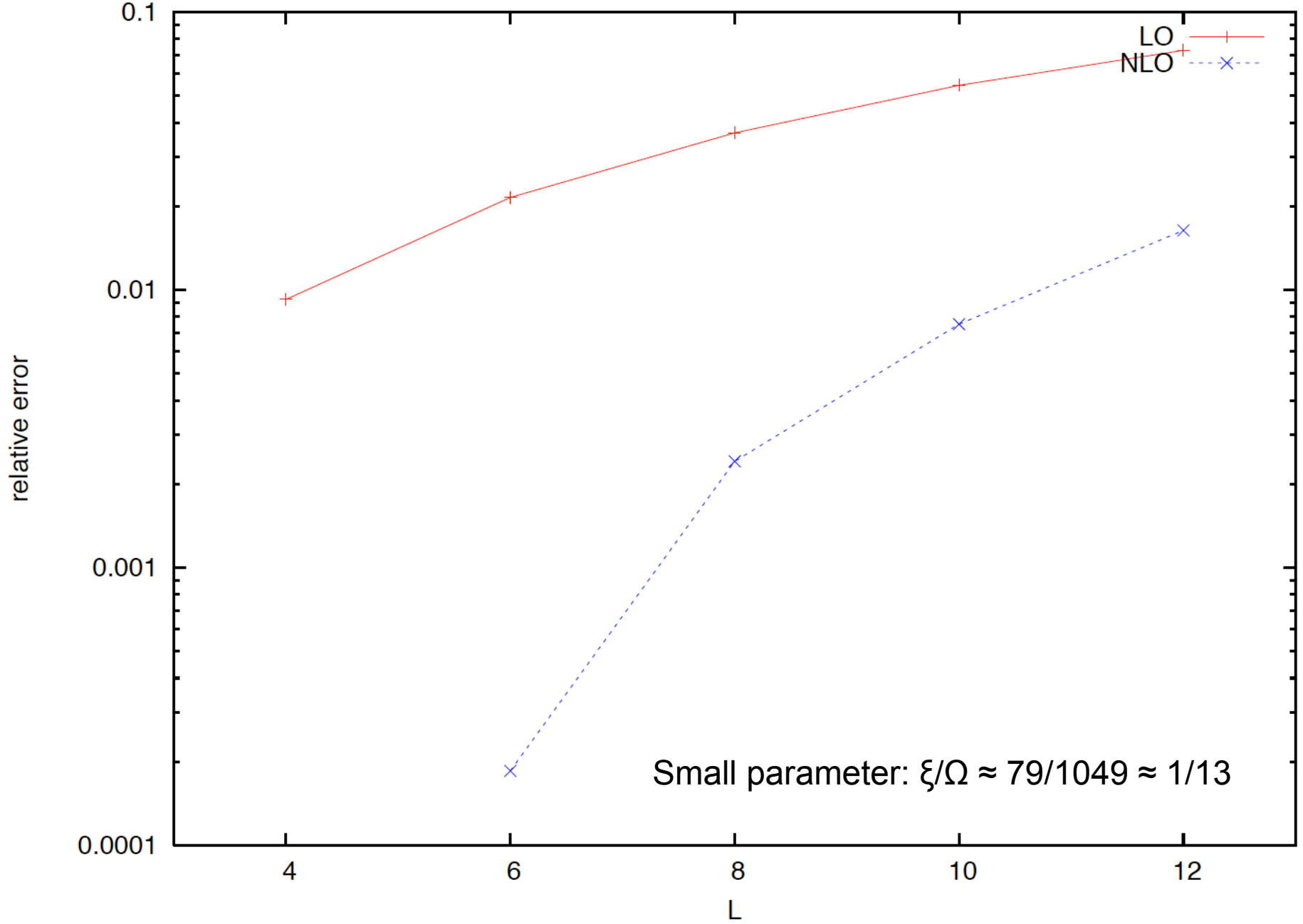
Q: When does the effective theory break down? How large can J be?

A1: energy correction << leading-order energy: $C_2/C_0^3\,J(J+1) << 1$
A2: Thus: $J << \Omega/\xi$

^{172}Yb: Relative error in LO and NLO



What about higher derivatives?

Vector in tangent plane

$$\vec{v} = v_\phi \vec{e}_\phi + v_\theta \vec{e}_\theta$$

Its time derivative…

$$\partial_t \vec{v} = \left(\dot{v}_\theta - v_\phi \dot{\phi} \cos\theta\right) \vec{e}_\theta + \left(\dot{v}_\phi + v_\theta \dot{\phi} \cos\theta\right) \vec{e}_\phi - \left(v_\phi \dot{\phi} \sin\theta + v_\theta \dot{\theta}\right) \vec{n}$$

… does not “live” in the tangent plane! ☹

Question: What does one do in this situation?

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… does not “live” in the tangent plane! ☹

Question: What does one do in this situation?

Answer: Introduce a “covariant” derivative (projection of derivative onto tangent plane)!

$$D_t v_\theta \equiv \dot{v}_\theta - v_\phi \dot{\phi} \cos\theta$$

$$D_t v_\phi \equiv \dot{v}_\phi + v_\theta \dot{\phi} \cos\theta$$

Odd-mass nuclei

Question: What's the key difference between ^{172}Yb and ^{173}Yb?

Answer:

1. We have to explicitly account for the odd neutron and add it as a degree of freedom (e.g. particle-rotor model)
2. At low energies, no one knows about the odd neutron, and we shall not add it.

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Question: Apart from the odd neutron, what's the key difference between ^{172}Yb and ^{173}Yb?

Answer: ^{173}Yb has a finite spin in its ground state. This breaks time reversal invariance and first-order derivatives enter the Lagrangian. Technically, we can add a monopole magnetic field inside the sphere.

Nuclei with finite ground-state spins: Wess Zumino terms

Notation on this slide: $\phi \rightarrow \alpha$, $\theta \rightarrow \beta$

Lagrangian
$$L_{\rm LO} = L_{\rm LO}^{(ee)} + L_{\rm WZ} = \frac{C_0}{2}\left(\dot\beta^2 + \dot\alpha^2 \sin^2\beta\right) - q\dot\alpha\cos\beta$$

Hamiltonian
$$H_{\rm LO} = \frac{p_\beta^2}{2C_0} + \frac{(p_\alpha + q\cos\beta)^2}{2C_0\sin^2\beta}$$

Eigenvalues and eigenfunctions (Identify q with ground-state spin!)

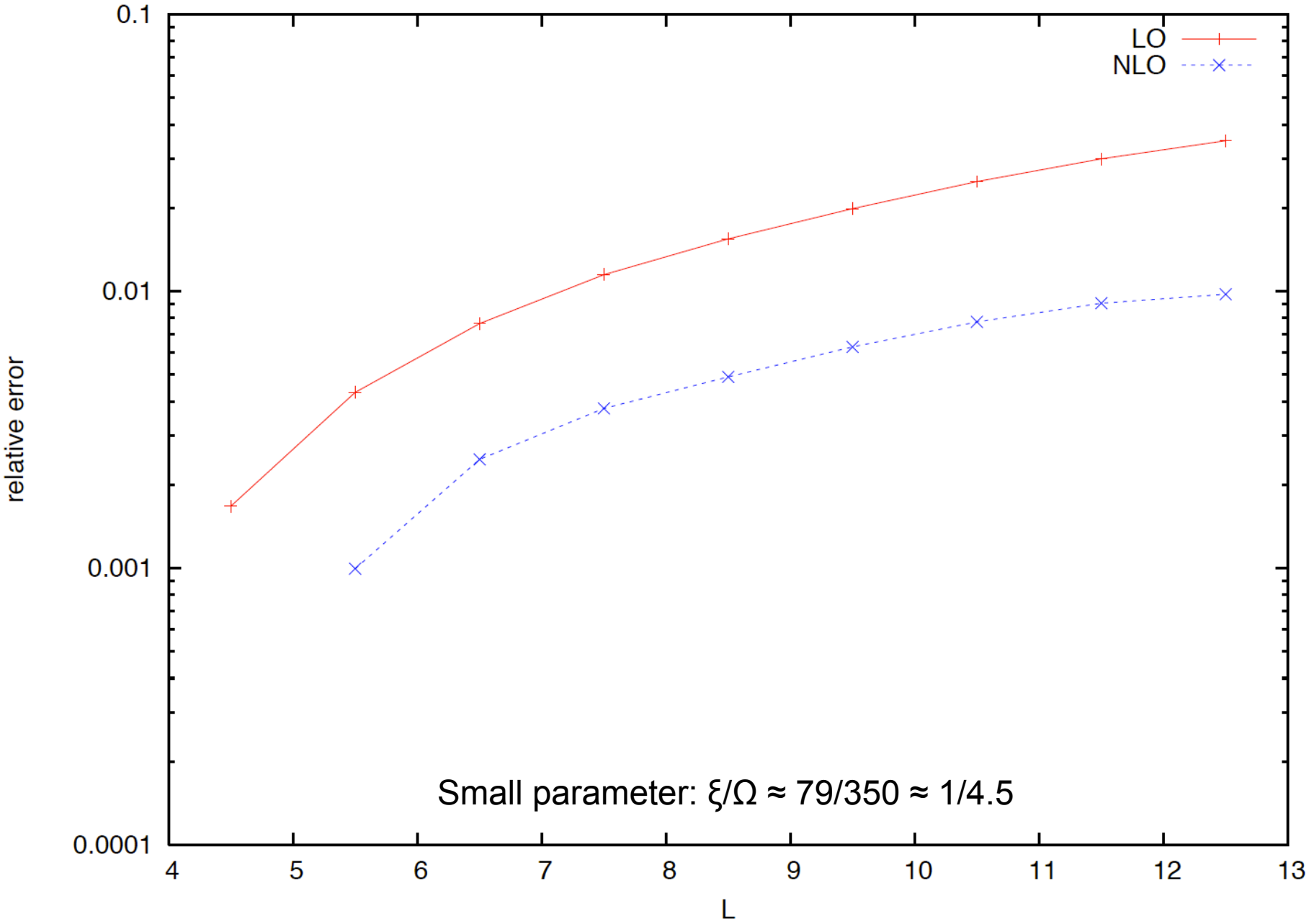
$$\hat H_{\rm LO}\, d^l_{mq}(\beta)e^{-i\alpha m} = E_{\rm LO}(q,l) d^l_{mq}(\beta)e^{-i\alpha m}$$

$$E_{\rm LO}(q,l) = \frac{l(l+1)-q^2}{2C_0}$$

$$l = |q|, |q|+1, |q|+2, \ldots$$

$$D^l_{mq}(\alpha,\beta,\gamma) \equiv e^{-im\alpha} d^l_{mq}(\beta) e^{-iq\gamma}$$ (Wigner D functions)

^{173}Yb: Relative error in LO and NLO



Summary

- Description of nuclear deformation within an effective theory
- Model-independent approach, treats odd-mass and even-even nuclei on equal footing
- Power counting: vibrational excitations >> rotational excitations

Interactions from chiral effective field theory and renormalization group transformations

Thomas Papenbrock

and OAK RIDGE NATIONAL LABORATORY

Aim of these lectures:

Give overview of nuclear forces from effective field theory, and renormalization group transformations

13th CNS Summer School

August 21–27, 2014 at Tokyo University, Wako Campus

Reading suggestions

More is different, P. W. Anderson, Science **177**, 393 (1972)

Elementary features of nuclear structure, B.R. Mottelson, in: H. Nifenecker, J.P. Blaizot, G. Bertsch, W. Weise, F. David (Eds.), *Trends in Nuclear Physics, 100 Years Later*, North-Holland, Amsterdam, 1998

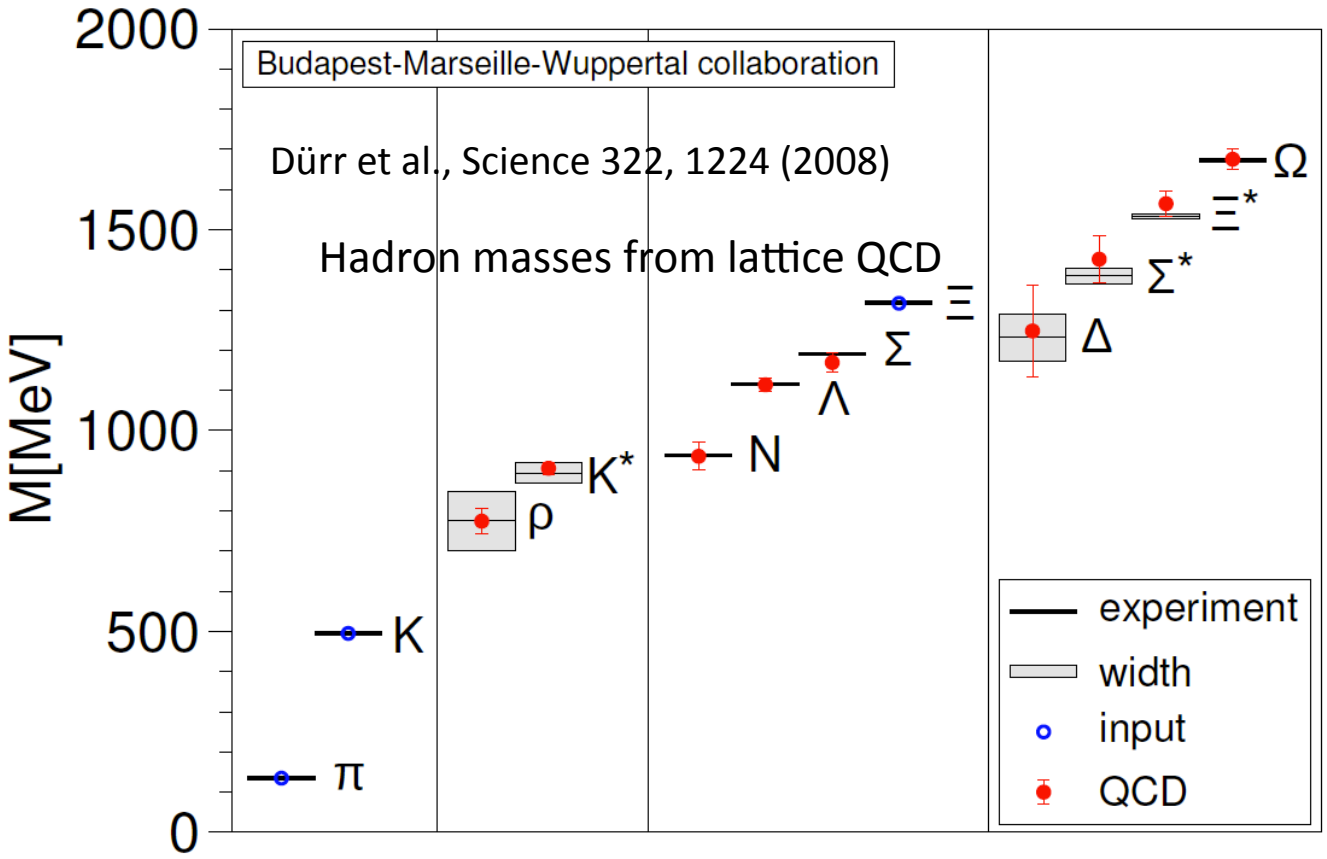
Chiral effective field theory and nuclear forces

- Machleidt & Entem, *Chiral effective field theory and nuclear forces,* Phys. Rept. 503, (2011); Machleidt, arXiv:0704.0807
- Epelbaum Hammer & Meißner, *Modern theory of nuclear forces,* Rev. Mod. Phys. **81**, 1773 (2009); arXiv:0811.1338

Low-momentum interactions and similarity transforms

- Bogner, Furnstahl & Schwenk, *From low-momentum interactions to nuclear structure,* Prog. Part. Nucl. Phys. **65**, 94 (2010); arXiv:0912.3688

Quantum chromo dynamics – theory of the strong interaction



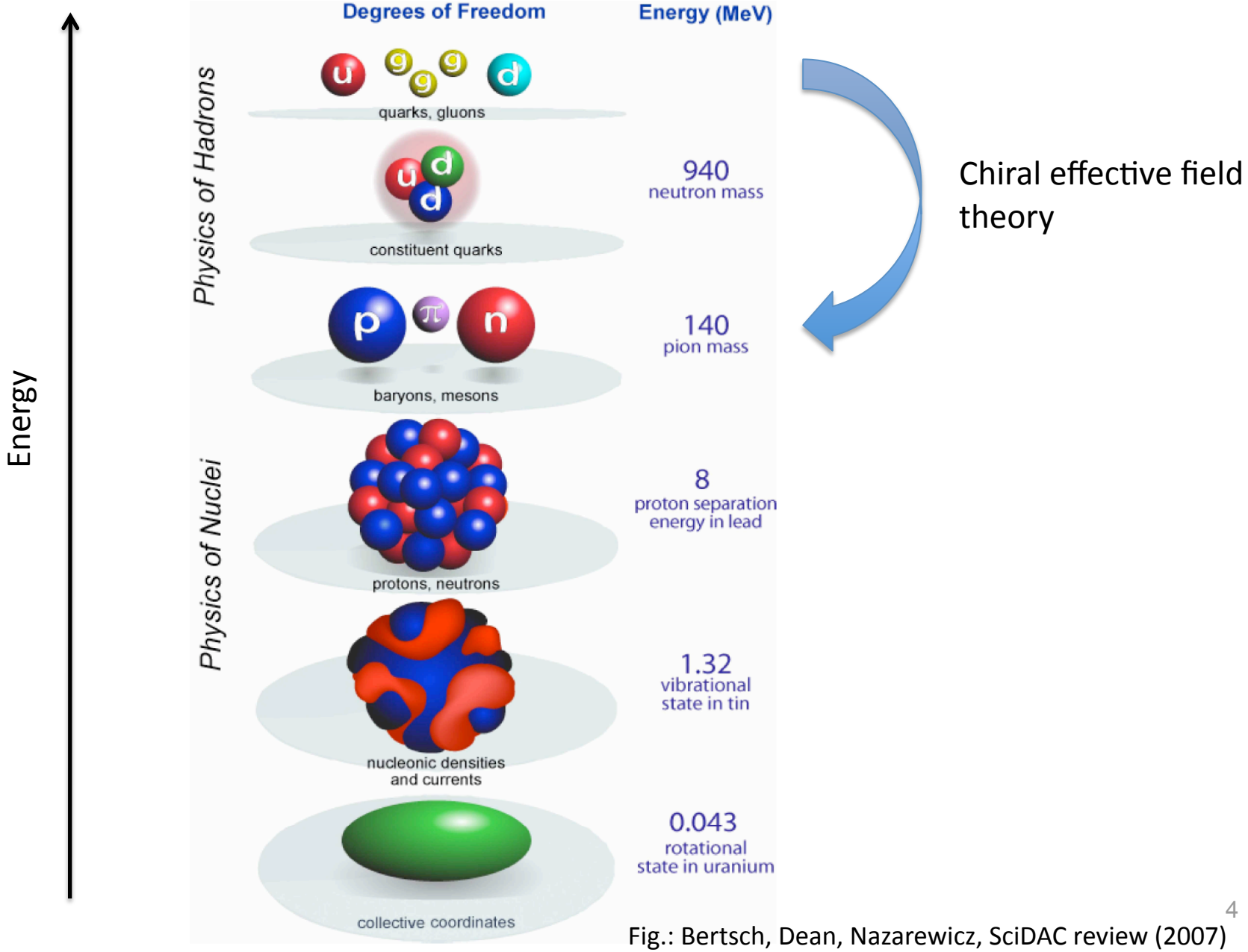
Most impressive progress

But: first-principle computation of nuclei from QCD are still far away …

Worse: Looking at the QCD Lagrangian, it is not obvious what the low-energy QCD physics is. Neither the spontaneous breaking of chiral symmetry nor the emergence of selfbound nuclei is obvious or predicted from QCD.

(The QED Lagrangian also does not tell us about emerging phenomena such as superconductivity or crystals.) We need another approach!

Energy scales and relevant degrees of freedom



Chiral effective field theory

Fig.: Bertsch, Dean, Nazarewicz, SciDAC review (2007)

Construction of nuclear potentials via chiral EFT

Weinberg, van Kolck, Epelbaum, Machleidt, …

1. Identify the **relevant degrees of freedom** for the resolution scale of atomic nuclei: **nucleons and pions**.
2. Identify the **relevant symmetries** of low-energy QCD and investigate if and how they are broken: **spontaneously broken chiral symmetry**
3. Construct the most general Lagrangian consistent with those symmetries and the symmetry breaking.
4. Design an **organizational scheme** that can distinguish between more and less important contributions: a low-momentum expansion: **power counting**
5. Guided by the expansion, calculate Feynman diagrams to the desired accuracy for the problem under consideration.

Reviews:

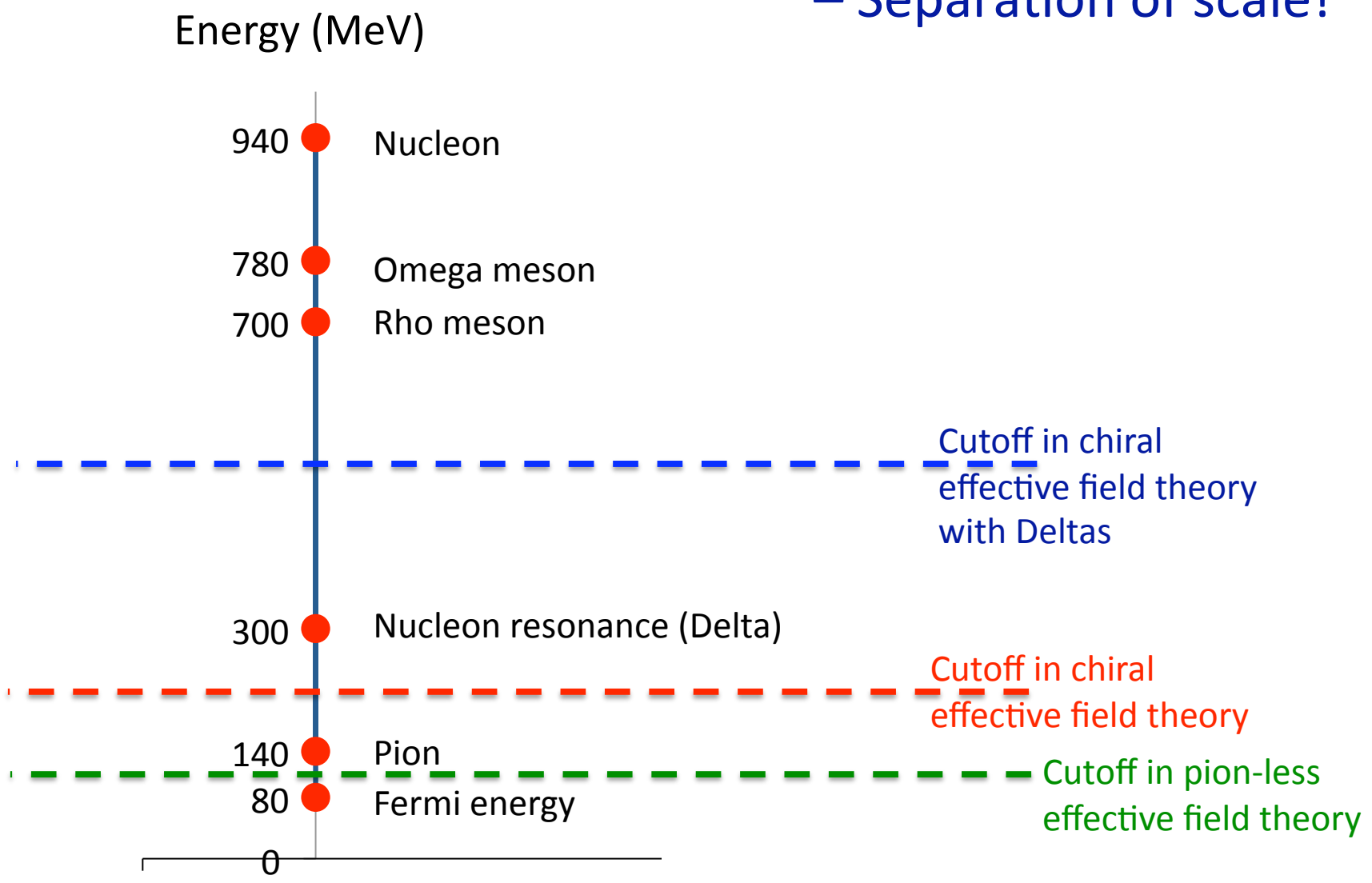
Bedaque and van Kolck, Ann. Rev. Nucl. Part. Sci. 52 (2002) 339, nucl-th/0205058.

Machleidt, & Entem, Phys. Rept. 503, 1 (2011); Machleidt, arxiv:0704.0807.

Epelbaum, Hammer, Meißner, Rev. Mod. Phys. 81, 1773 (2009); arXiv:0811.1338.

1. Identify relevant degrees of freedom

– Separation of scale!



2. Identification of relevant symmetries

1. **SU(3) color symmetry** from QCD
   (Nucleons and pions are color singlets)

2. **Chiral symmetry**: Left and right-handed massless u and d quarks do not mix: $SU(2)_L$ x $SU(2)_R$ symmetry. Expect left-right parity doublets in nature.

   Explicit breaking of chiral symmetry: u and d quarks have a small mass. Small corrections to above picture arise.

   But: There are no (left-right) parity doublets observed in nature!

   Reason**: Spontaneous breaking of chiral symmetry** (More is different!)

   - $SU(2)_L$ x $SU(2)_R$ symmetry spontaneously broken to $SU(2)_V$
   - Pions are the Nambu-Goldstone bosons of spontaneously broken chiral symmetry
   - Low-energy pion Lagrangian completely determined

$$\mathcal{L}_{\rm eff} = \mathcal{L}_{\pi\pi} + \mathcal{L}_{N\pi} + \mathcal{L}_{NN}$$

3. Construct most general Lagrangian consistent with symmetries; organizational scheme → power counting

$$\mathcal{L}_{\rm eff} = \mathcal{L}_{\pi\pi} + \mathcal{L}_{N\pi} + \mathcal{L}_{NN}$$

Derivative (low-momentum) expansion indicated by superscripts

Pion-pion Lagrangian: U is SU(2) matrix parameterized by three pion fields

$$\mathcal{L}^{(2)}_{\pi\pi} = \frac{f_\pi^2}{4}\,{\rm tr}\left[\partial^\mu U \partial_\mu U^\dagger + m_\pi^2 (U + U^\dagger)\right]$$

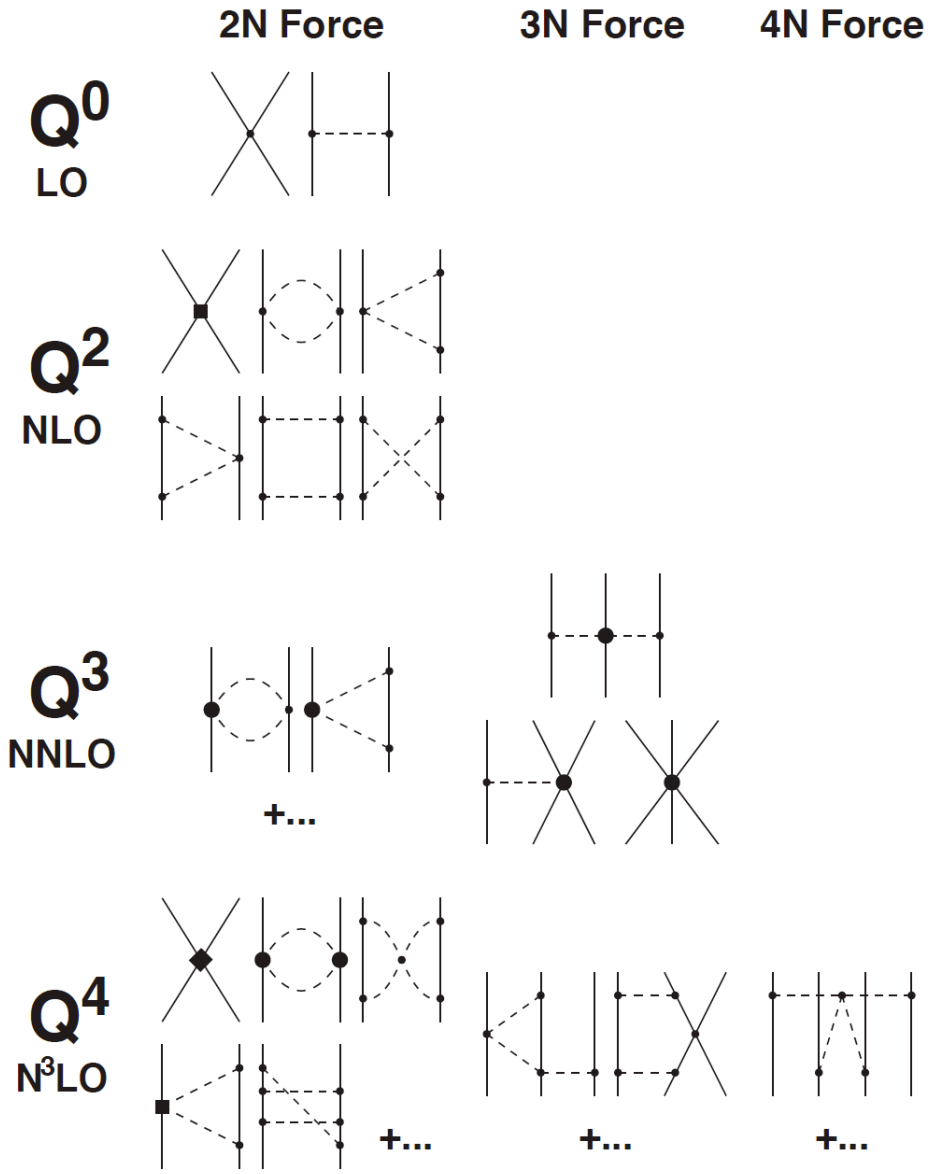
Leading order pion-nucleon Lagrangian

$$\mathcal{L}^{(1)}_{\pi N} = \bar\Psi \left(i\gamma^\mu D_\mu - M_N + \frac{g_A}{2}\gamma^\mu\gamma_5 u_\mu \right) \Psi$$

Leading order nucleon-nucleon Lagrangian (encodes unknown short-ranged physics)

$$\mathcal{L}^{(0)}_{NN} = -\frac{1}{2} C_S \bar N N \bar N N - \frac{1}{2} C_T \bar N \vec\sigma N \bar N \vec\sigma N$$

Effective field theory: chiral potential at order N^3LO



Nucleons: full lines
Pions: dashed lines

Features:

1. Systematic expansion of nucleon potential; small parameter (Q/Λ)
2. Low-energy constants from fit to data
3. Hierarchy of forces
   NN >> NNN >> NNNN

[from Machleidt arXiv:0704.0807]

Chiral nucleon-nucleon potential at leading order

One-pion exchange potential (p, p' are initial and final relative momenta)

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

$$\vec{q} \;\equiv\; \vec{p}\,' - \vec{p}$$

Leading order contact term (encode unknown short-range physics)

$$V^{(0)}(\vec{p'},\vec{p}) = C_S + C_T\,\vec{\sigma}_1\cdot\vec{\sigma}_2$$

Higher-order contact terms also serve as counter terms that renormalize loop integrals.

Why contact terms?

1. Only contact terms can model really short range physics.
2. Any short-range terms (e.g. delta functions, Gaussians …) with range smaller $1/\Lambda$ would do the job, but contacts are very convenient with analytical results.

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How does the momentum cutoff Λ enter the EFT?

1. The construction of the chiral potential involves solving the Lippmann-Schwinger equation. Λ is the cutoff in this equation.

$$\widehat{T}(\vec{p}\,',\vec{p}) = \widehat{V}(\vec{p}\,',\vec{p}) + \int d^3p''\, \widehat{V}(\vec{p}\,',\vec{p}\,'')\, \frac{M}{p^2 - p''^2 + i\epsilon}\, \widehat{T}(\vec{p}\,'',\vec{p})$$

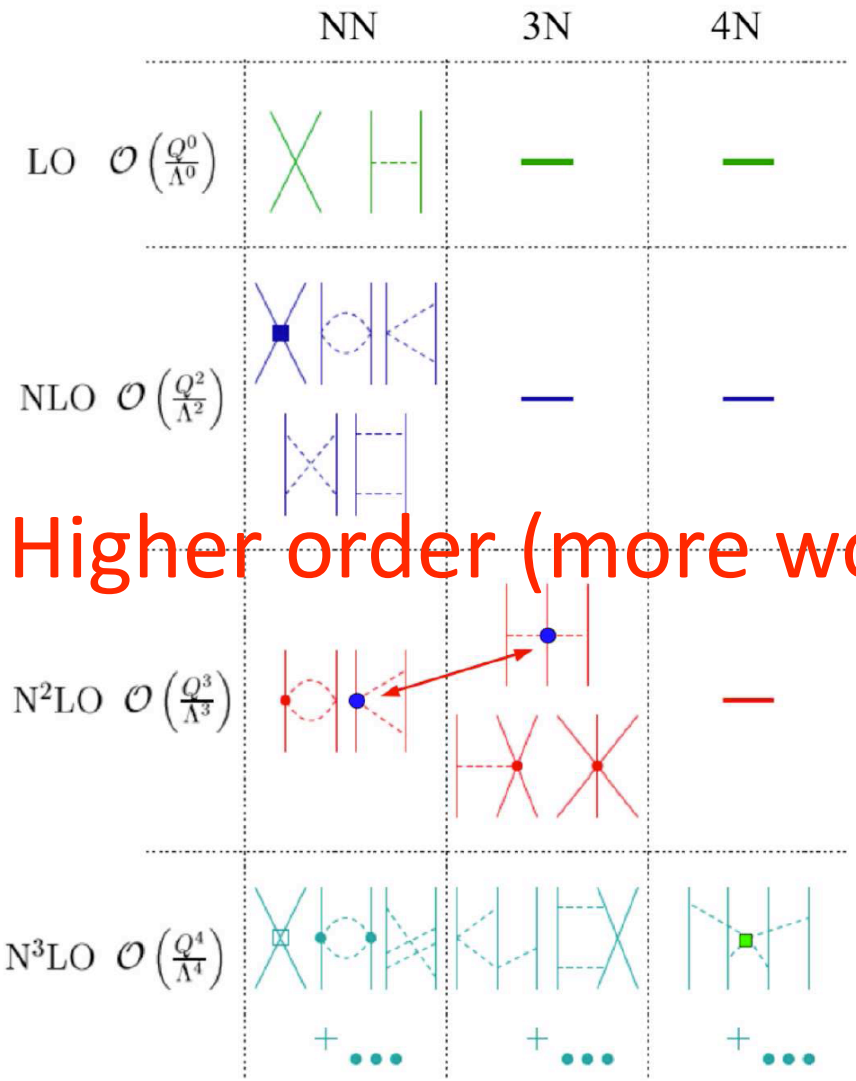
$$\widehat{V}(\vec{p}\,',\vec{p}) \quad \longmapsto \quad \widehat{V}(\vec{p}\,',\vec{p})\, e^{-(p'/\Lambda)^{2n}}\, e^{-(p/\Lambda)^{2n}}$$

2. The loop integrals that appear beyond leading order need to be regularized. One way of regularization is by imposing a cutoff of the order of Λ.

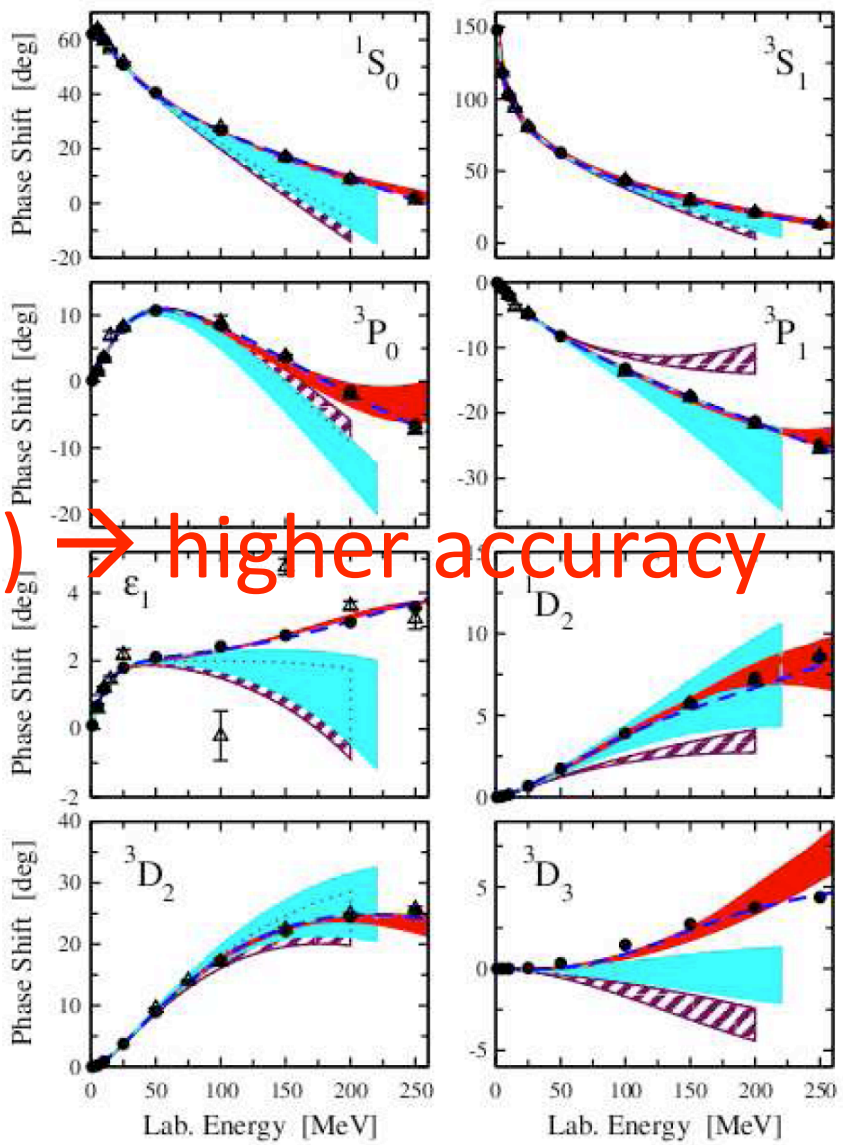
3. As a result, the low-energy constants depend implicitly on the regularization scheme and the cutoff.

4. There are (infinitely) many different chiral potentials! Differences of potentials that employ different values for the cutoff must be of higher order.

5. Regularization schemes, and form of potentials that encode short-ranged physics (contact potential or potentials with a very short range) are at the potential builder's discretion. **This makes the approach model independent**.



(a)



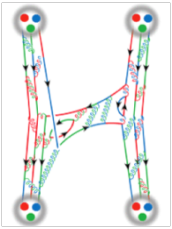
(b)

Higher order (more work) → higher accuracy

From Bogner et al, arXiv:0912.3688

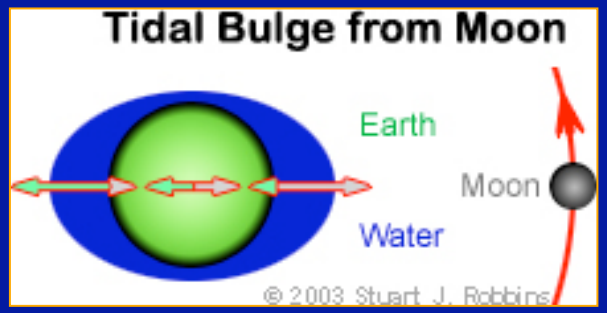
Figure 4: (a) Chiral EFT for nuclear forces. (b) Improvement in neutron-proton phase shifts sho by shaded bands from cutoff variation at NLO (dashed), N^{2}LO (light), and N^{3}LO (dark) compared extractions from experiment (points) [31]. The dashed line is from the N^{3}LO potential of Ref. [20].

Three-nucleon forces – Why?



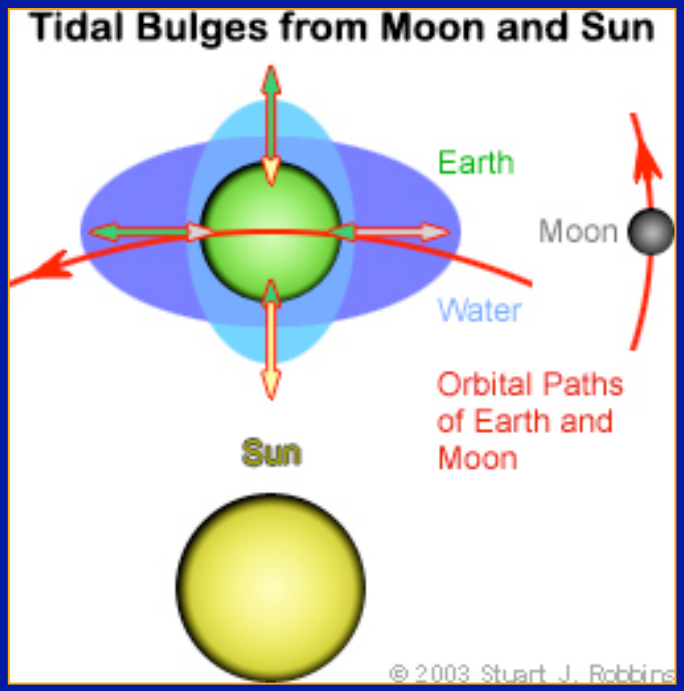
- Nucleons are not point particles (i.e. not elementary).
- We neglected some internal degrees of freedom (e.g. Δ-resonance, "polarization effects", …), and unconstrained high-momentum modes.

Example from celestial mechanics:
Earth-Moon system: point masses and modified two-body interaction



Renormalization group transformation:
Removal of "stiff" degrees of freedom at expense of additional forces.

Other tidal effects cannot be included in the two-body interaction! Three-body force unavoidable for point masses.



Three-body forces cont'd

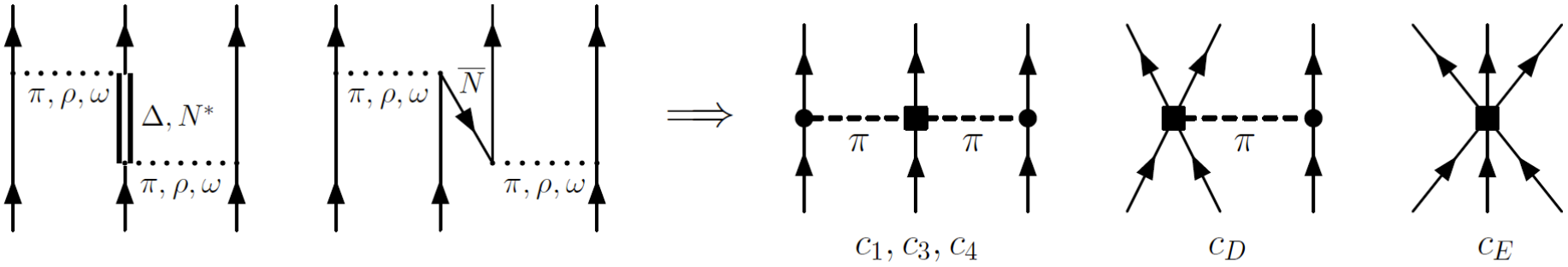


Figure 23: Eliminating degrees of freedom leads to three-body forces.

(taken from Bogner, Furnstahl, Schwenk, arXiv:0912.3688)

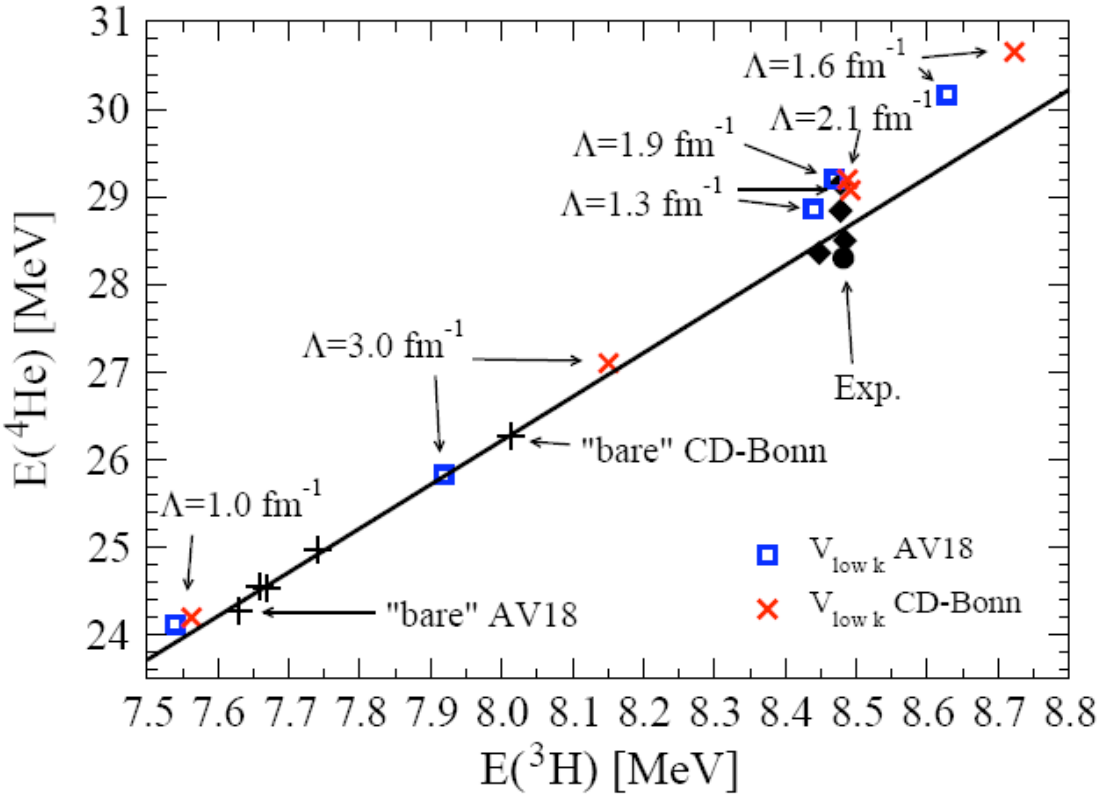
Leading three-nucleon force

1. Long-ranged two-pion term (Fujita & Miyazawa …)
2. Intermediate-ranged one-poin term
3. Short-ranged three-nucleon contact

The question is not: Do three-body forces enter the description?

The (only) question is: How large are three-body forces?

Non-uniqueness of three-nucleon forces



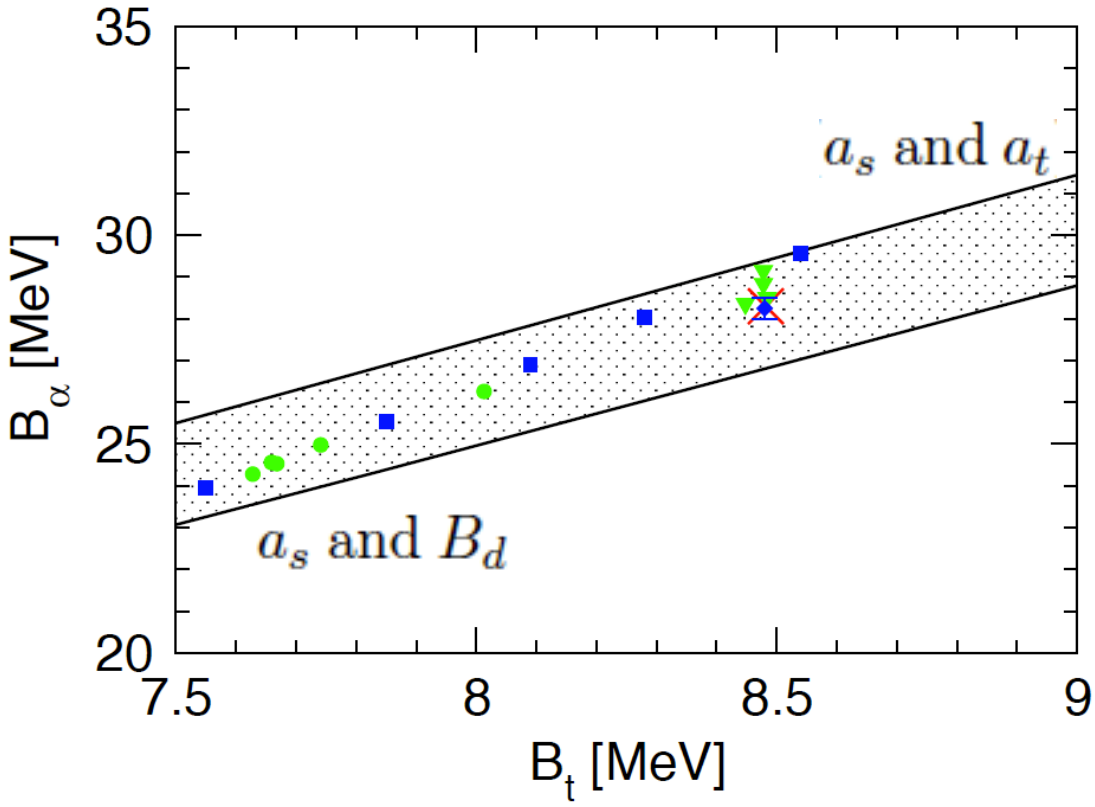
A. Nogga, S. K. Bogner, and A. Schwenk, Phys.Rev. C70 (2004) 061002

As cutoff Λ is varied, motion along "Tjon line".

Addition of Λ-dependent three-nucleon force yields (almost) agreement with experiment. **Q: What's missing?**

A: The complete description of ^{4}He would require four-nucleon forces!

Understanding the Tjon line



Blue square: EFT at NLO
Blue diamond: EFT at N^2LO
Other dots: phenomenological NN potentials

Large scattering length and absence of leading-order 4-body force explain Tjon line
Platter, Hammer, Meissner: Phys. Lett. B 607, 254 (2005)

Question: Your favorite physics friend comes to you and suggests to determine the effects of the three-body force on the structure of your favorite nucleus. You reply

1. Let's do this. This will put us on the fast track to Stockholm.
2. This is difficult to disentangle. But it can be done in a three-body system such as ^{3}H.
3. Which interaction are you looking at?
4. Answers 2 & 3 are correct.

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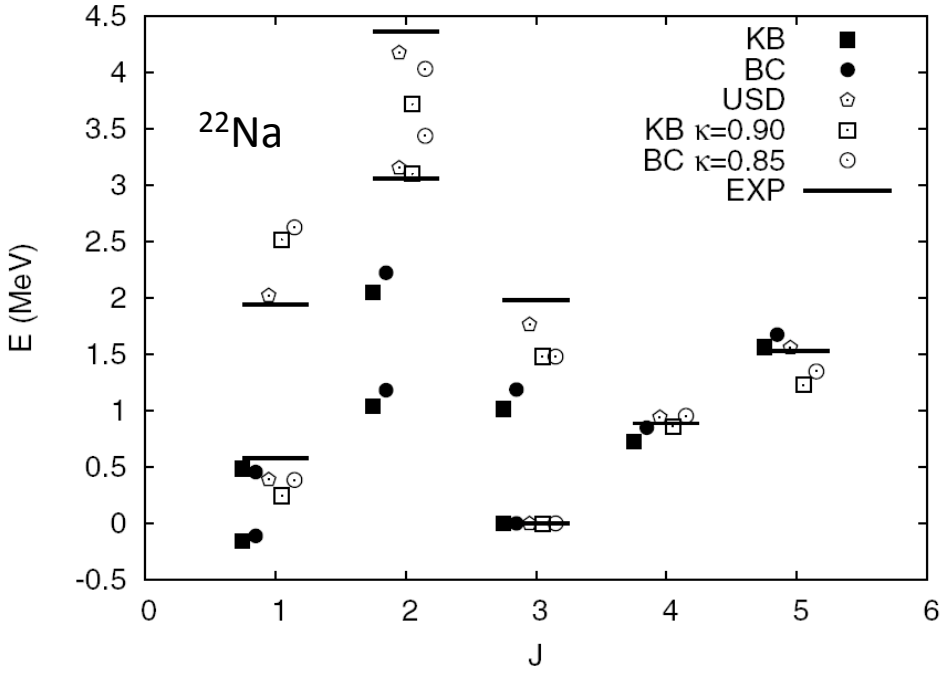
The size and form of three-body forces depends on the cutoff, and the chosen renormalization scheme. Different schemes ("implementations of the EFT at order n") yield predictions that expected to agree within the error estimate $(Q/\Lambda)^{n+1}$. **Only the sum of interactions can be probed**.

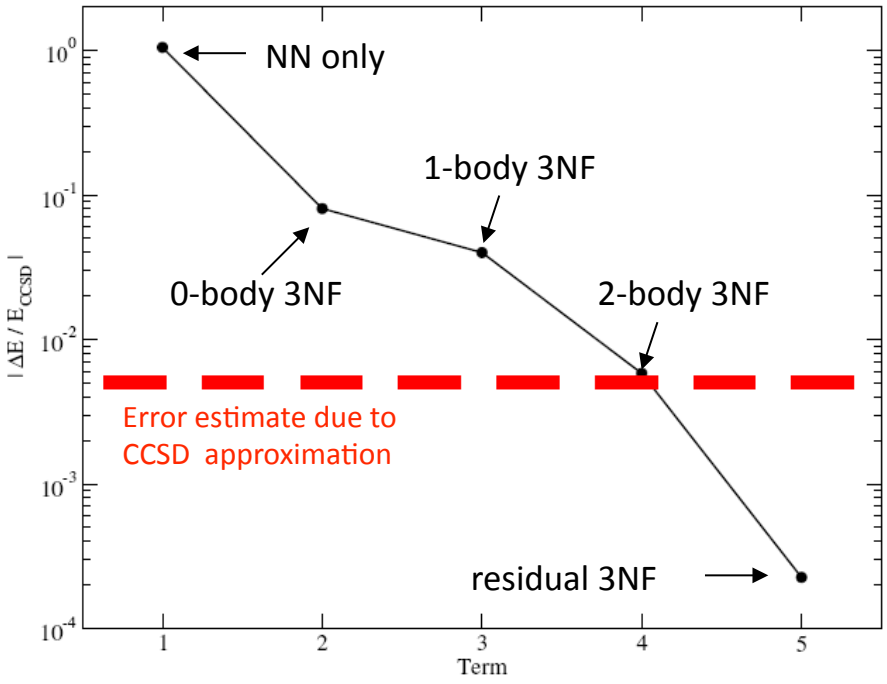
What's the role of three-nucleon forces?



Monopole shifts from 3NF as density-dependent NN force. [A.Zuker, PRL 90, 42502 (2003)]

Contributions to binding of ^{4}He. [Hagen, TP, Dean, Schwenk, Nogga, Wloch, Piecuch, PRC 76, 034302 (2007); Roth et al, arXiv:1112.0287]

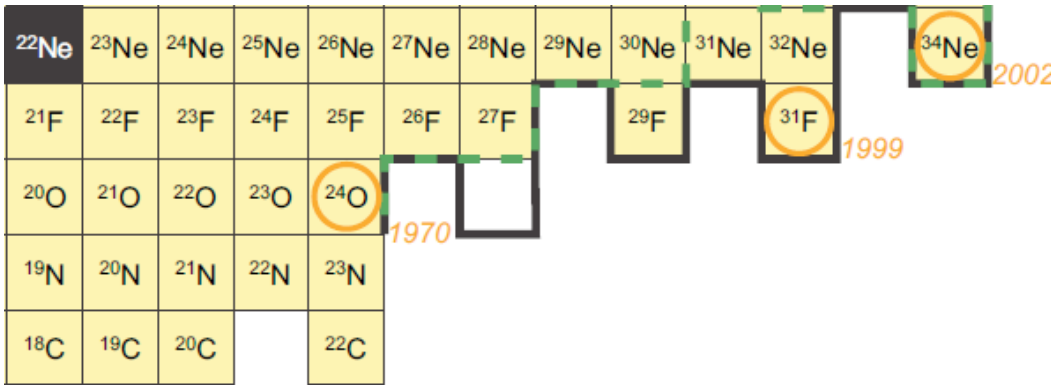
$$\hat{H}_3 = \frac{1}{6}\sum_{ijk}\langle ijk||ijk\rangle + \frac{1}{2}\sum_{ijpq}\langle ijp||ijq\rangle\{\hat{a}_p^\dagger \hat{a}_q\} + \frac{1}{4}\sum_{ipqrs}\langle ipq||irs\rangle\{\hat{a}_p^\dagger \hat{a}_q^\dagger \hat{a}_s \hat{a}_r\} + \hat{h}_3\,,$$



Is ^{28}O a bound nucleus?

Experimental situation

- "Last" stable oxygen isotope ^{24}O
- ^{25}O unstable (Hoffman et al 2008)
- ^{26}O unstable (Lunderberg et al 2012)
- ^{31}F exists (adding on proton shifts drip line by 6 neutrons)



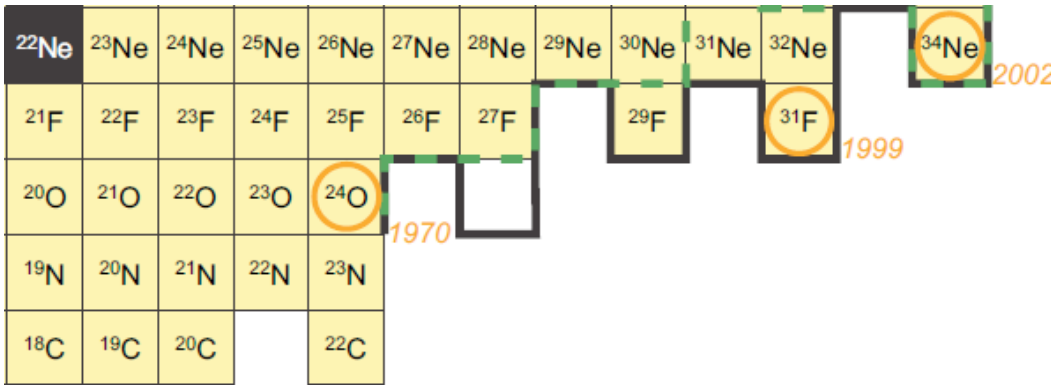
Theoretical description challenging (proximity of continuum, 3NFs)

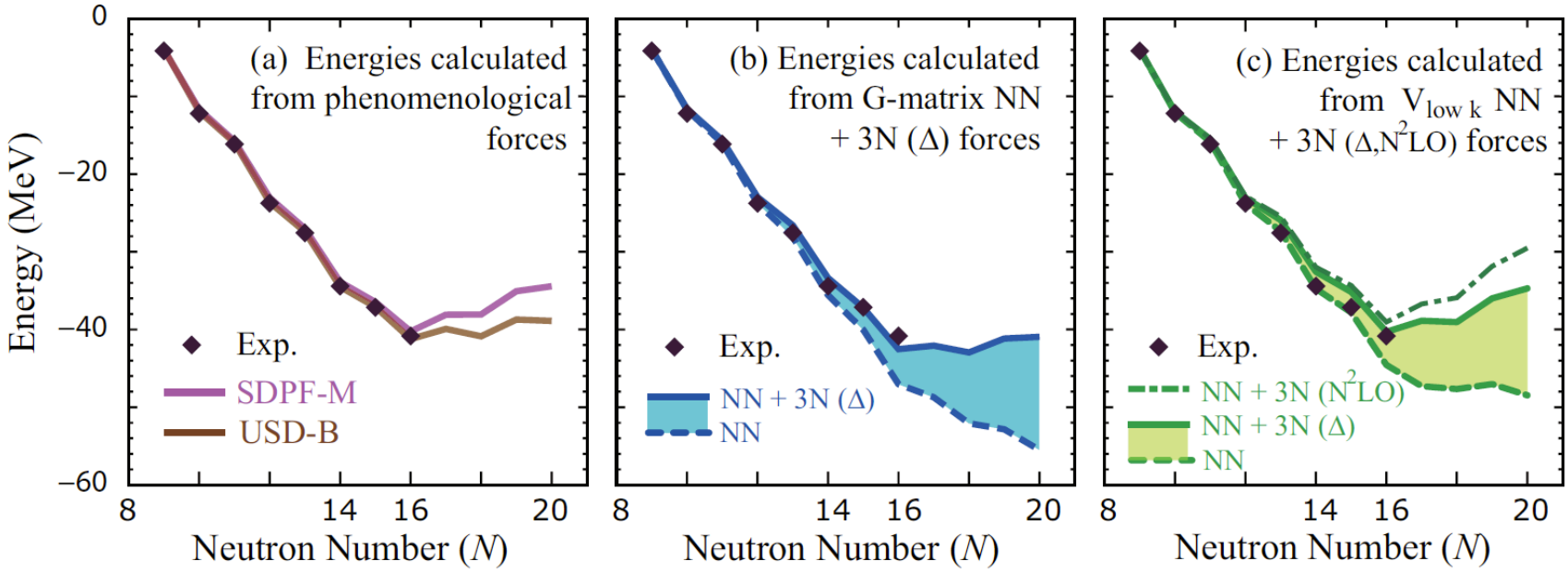
- Continuum shell model [Volya & Zelevinsky, PRL 94, 052501 (2005)]
- Chiral NN interactions [Hagen et al., PRC 80, 021306 (2009)].
- Effects of 3NFs [Otsuka, Suzuki, Holt, Schwenk, Akaishi, PRL 105, 032501 (2010)]
- More complete calculation desirable (3NFs, continuum, large model space, minimum adjustments to interaction)

Is ^{28}O a bound nucleus?

Experimental situation

- "Last" stable oxygen isotope ^{24}O
- ^{25}O unstable (Hoffman et al 2008)
- ^{26}O unstable (Lunderberg et al 2012)
- ^{31}F exists (adding on proton shifts drip line by 6 neutrons)





Shell model (sd shell) with monopole corrections based on three-nucleon force predicts 2nd O as last stable isotope of oxygen. [Otsuka, Suzuki, Holt, Schwenk, Akaishi, PRL (2010), arXiv: 0908.2607]

Intermission

- Systematic construction of nuclear forces within (chiral) effective field theory
- There is a recipe to follow
- Highlights: power counting, hierarchy of NN >> NNN >> NNNN forces
- Approach is model independent
- Resulting potential depends on regularization scheme and cutoff
- There are (infinitely) many good ways to implement this

Estimate for model spaces and Hamiltonian matrix dimensions

Assume we want to compute the binding energy of a nucleus with mass number A in a wave function based approach. Assume that the interaction has a momentum cutoff Λ.

Q: What are the minimum requirements for the model space / What basis would you choose?

A:

1. The basis must be sufficiently extended in position space to capture a nucleus with radius $R \approx 1.2\, A^{1/3}$ fm
2. The basis must be sufficiently extended in momentum space to capture the cutoff Λ.
3. THUS: we need approximately $K=(R\Lambda/(2\pi))^3$ single-particle states (phase space volume!) In practice $K \approx (R\Lambda/2)^3 \sim \Lambda^3 A$.

Estimate: computation of oxygen: $\Lambda = 4$/fm and $R \approx 2.5$fm

Thus, our model space has about $K=5^3 = 125$ single-particle states.

Matrix dimension: $D=K!/(K-A)!/A! \approx (K/A)^A \approx 8^{16} \approx 2^{48} \approx 10^{14}$.

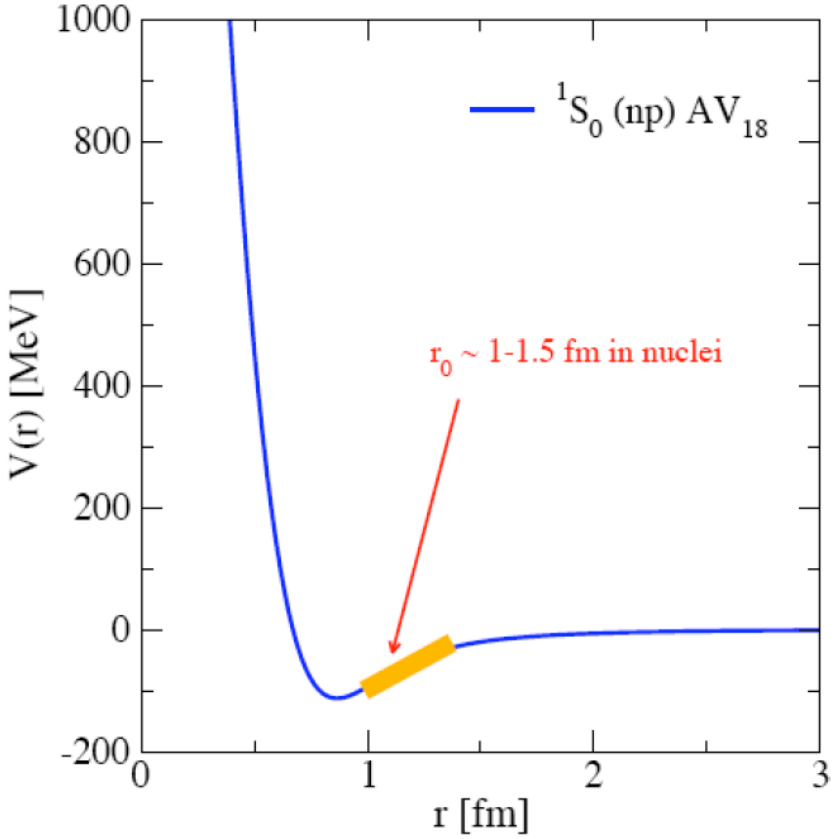
Some conclusions

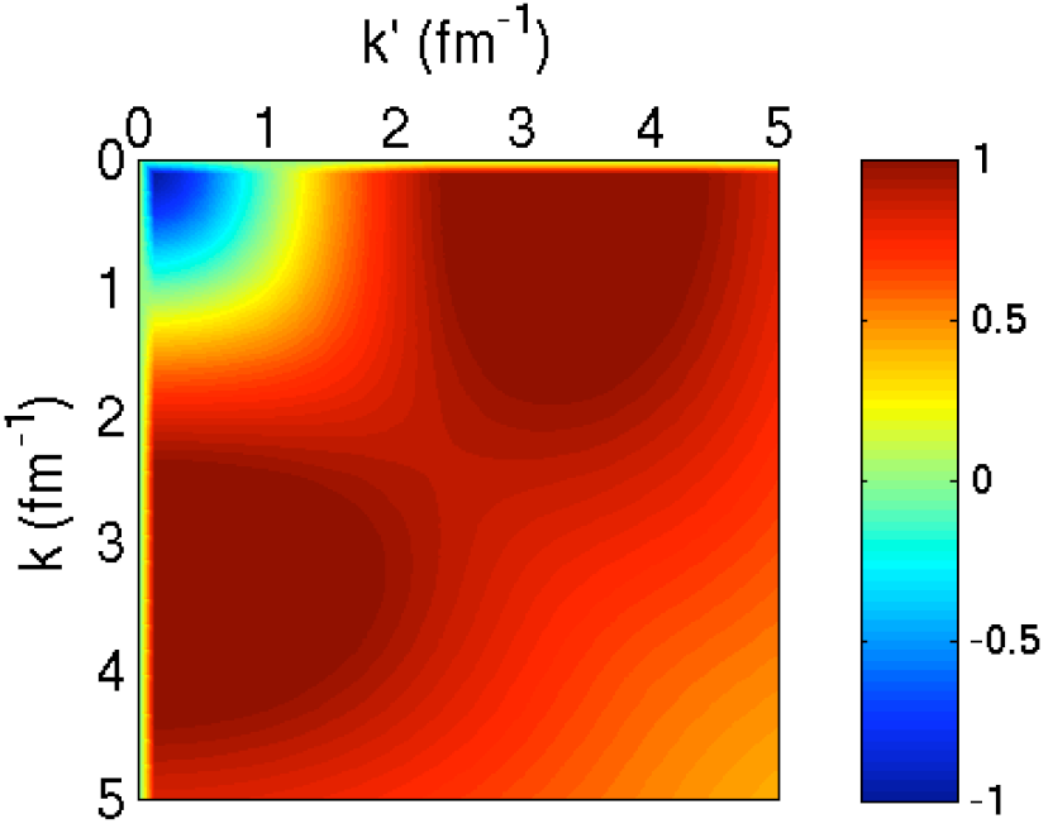
1. For “bare” chiral interactions (e.g. Entem and Machleidt), matrix diagonalization is possible only for light nuclei. One either needs a much more efficient method or a lower cutoff.
2. The factorial scaling with *A* is not matched by Moore’s law (doubling of FLOPS about every 18 month → factor 1000 in 15 years).
3. For wave-function based methods, the most effective way to heavier nuclei is to decrease the phase-space volume $K \sim (\Lambda R)^3 \sim \Lambda^3 A$ by decreasing the cutoff.

→ Low-momentum interactions & similarity renormalization group transformations that lower the cutoff Λ.

Homework: Consider an oscillator basis. How has one choose the oscillator frequency ω and the number of oscillator shells N for a given momentum cutoff Λ and mass number A?

Momentum-dependence of phenomenological potentials





Configuration space ←→ momentum space

Hard core ←→ high-momentum modes

Bogner/Furnstahl (2007)

Similarity renormalization group (SRG) transformation

Glazek, & Wilson, PRD **48** (1993) 5863; **49** (1994) 4214; Wegner, Ann. Phys. **3** (1994) 77; Perry, Bogner, & Furnstahl (2007)

Main idea: decouple low from high momenta via a (unitary) similarity transformation

Unitary transformation

$$\hat{H}(s) = U(s)\hat{H}U^{\dagger}(s) = U(s)\left(\hat{T} + \hat{V}\right)U^{\dagger}(s)$$

Evolution equation

$$\frac{d\hat{H}(s)}{ds} = \left[\eta(s), \hat{H}(s)\right] \qquad \text{with} \qquad \eta(s) \equiv \frac{dU(s)}{ds}U^{\dagger}(s) = -\eta^{\dagger}(s)$$

Choice of unitary transformation through (one does not need to construct U explicitly).

$$\eta(s) = \left[\hat{T}, \hat{H}(s)\right]$$

yields scale-dependent potential that becomes more and more diagonal

$$\hat{H}(s) = \hat{T} + \hat{V}(s)$$

Note: Baker-Campbell-Hausdorff expansion implies that SRG of 2-body force generates many-body forces

$$e^{-\eta}\hat{H}e^{\eta} = \hat{H} + \left[\hat{H}, \eta\right] + \frac{1}{2!}\left[\left[\hat{H}, \eta\right], \eta\right] + \ldots$$

SRG evolution of a chiral potential

(use cutoff $\lambda \equiv s^{-1/4}$ as evolution variable)

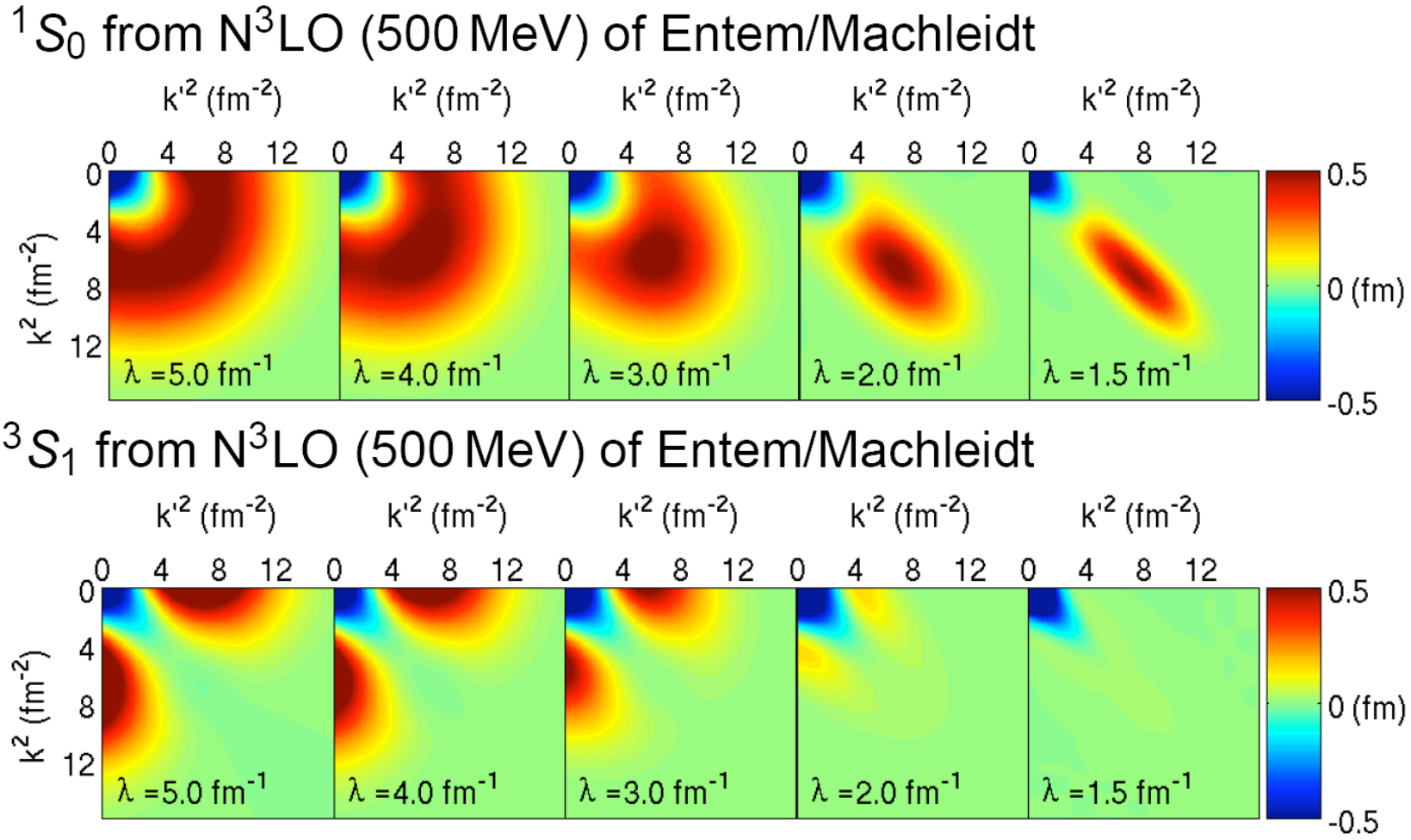


Fig.: Bogner & Furnstahl. See http://www.physics.ohio-state.edu/~ntg/srg

Understanding SRGs

Question: Which statement is correct?

1. The SRG is a unitary transformation, and no information is lost.
2. The SRG is only accurate up to the cutoff.

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When performing the SRG, up to A-body forces are created in an A-body system ("no free lunch theorem") . In practice, one hopes (with view to the chiral power counting) that the computation of 2-body and 3-body forces might be sufficient.

Q: How can we check in practice, that keeping 2-body and 3-body forces is sufficient?

1. Perform a computation with and without SRG an compare.
2. Check how results in the A-body system depend on the cutoff/evolution parameter

Understanding SRGs

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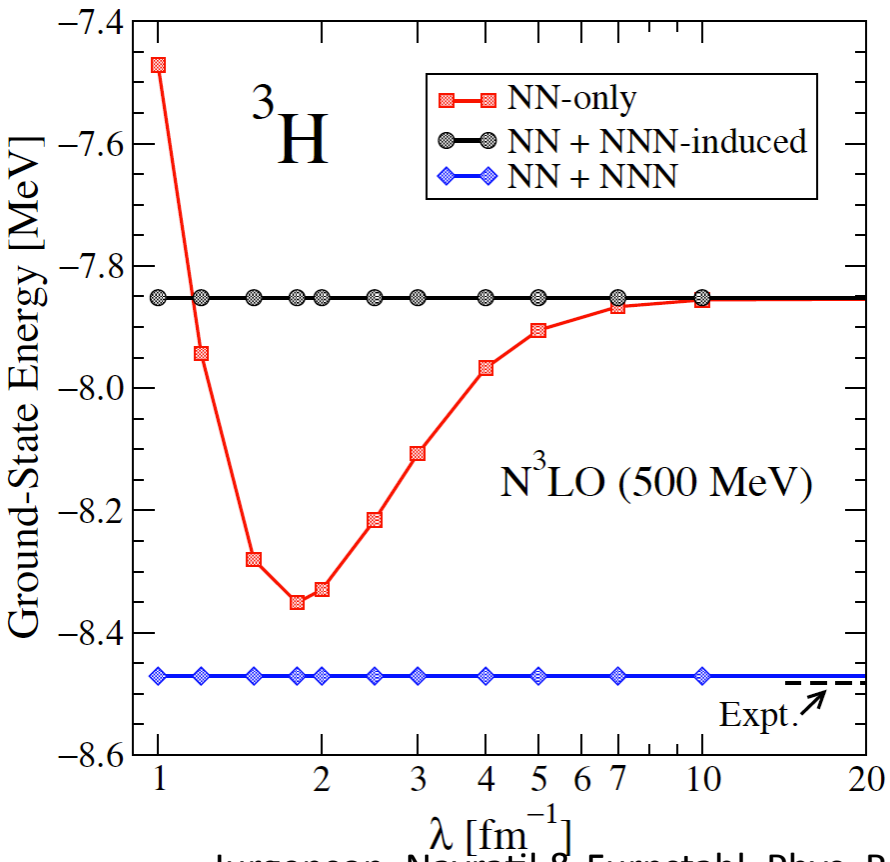
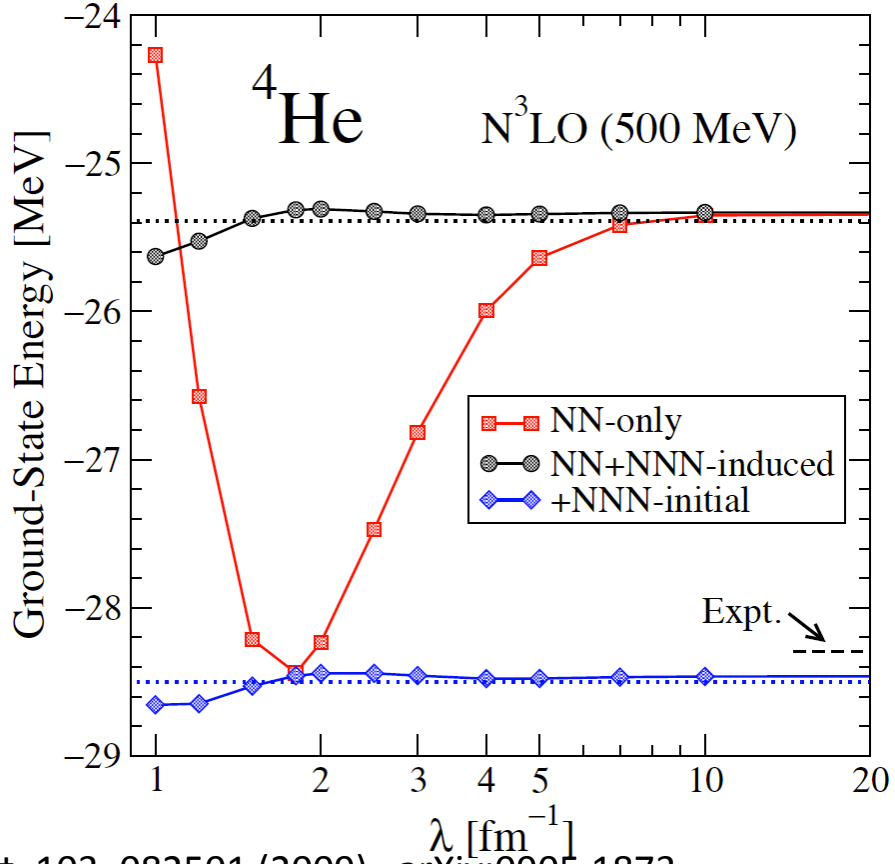
1. Perform a computation with and without SRG an compare.
2. Check how results in the A-body system depend on the cutoff/evolution parameter ✔

Of course: Any observable other than the Hamiltonian also needs to be transformed.

Solution of ^{3}H and ^{4}He with induced and initial 3NF





Jurgenson, Navratil & Furnstahl, Phys. Rev. Lett. 103, 082501 (2009), arXiv:0905.1873

Q: What is the effect of (omitted) 4NF and forces of even higher rank?

A: In ^{4}He, (short ranged) 4NF yield about 200 keV (see energies at small momentum)

Note: This is consistent with deviation from experiment!

Summary

- Introduction to main ideas behind nuclear forces from chiral EFT
- Model-independent approach
- Potentials are not observables, and one can shuffle things around (e.g. via different regularization and renormalization schemes, or via unitary transformations)
- A high cutoff carries a high computational price tag
- Similarity renormalization group transformations very useful tools for study and practical computations

Solving the nuclear many-body problem: coupled-cluster theory

Thomas Papenbrock

and OAK RIDGE NATIONAL LABORATORY

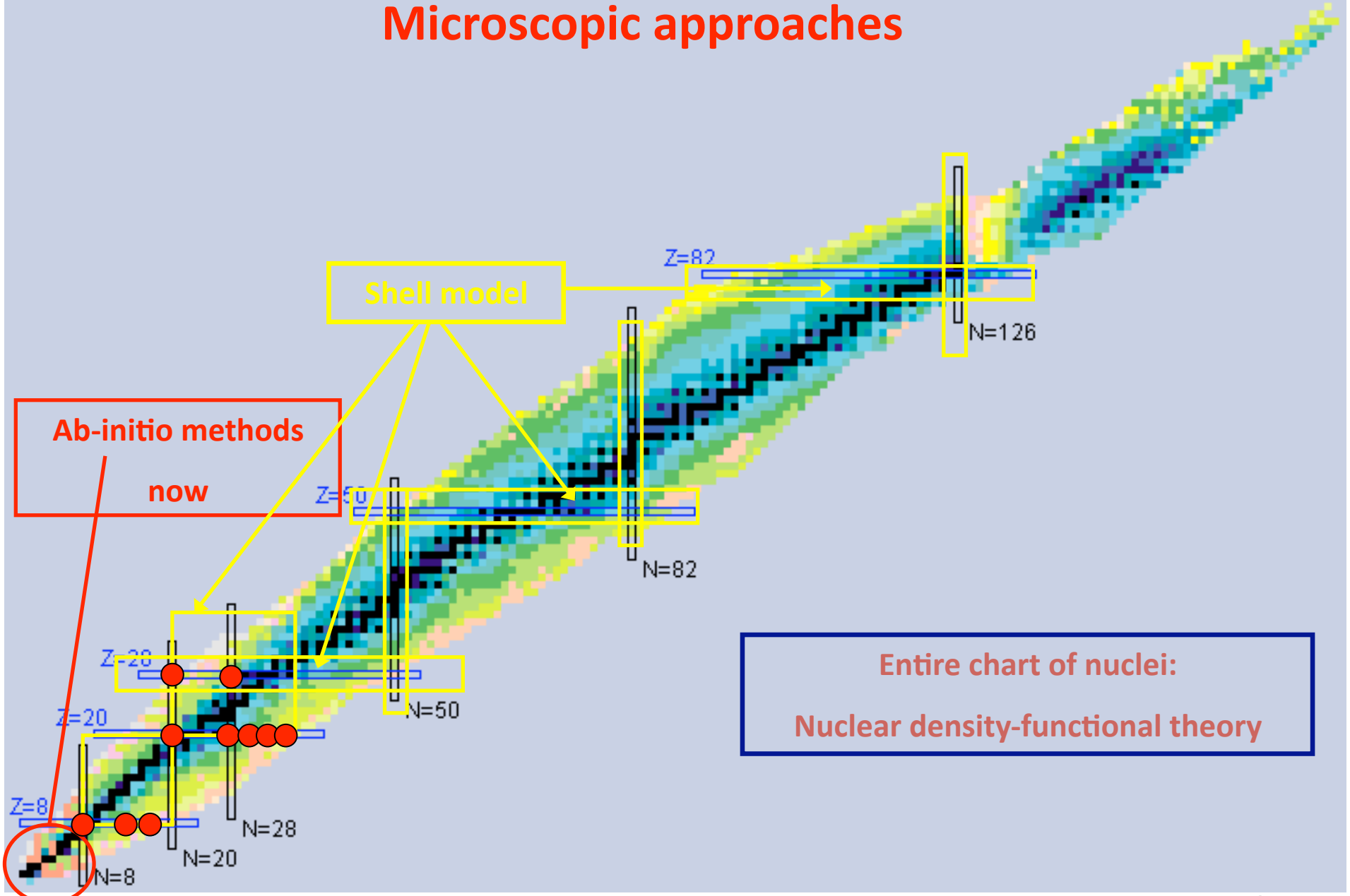
Aim of this lecture:

Present some results from *ab initio* computations with emphasis of the coupled-cluster method

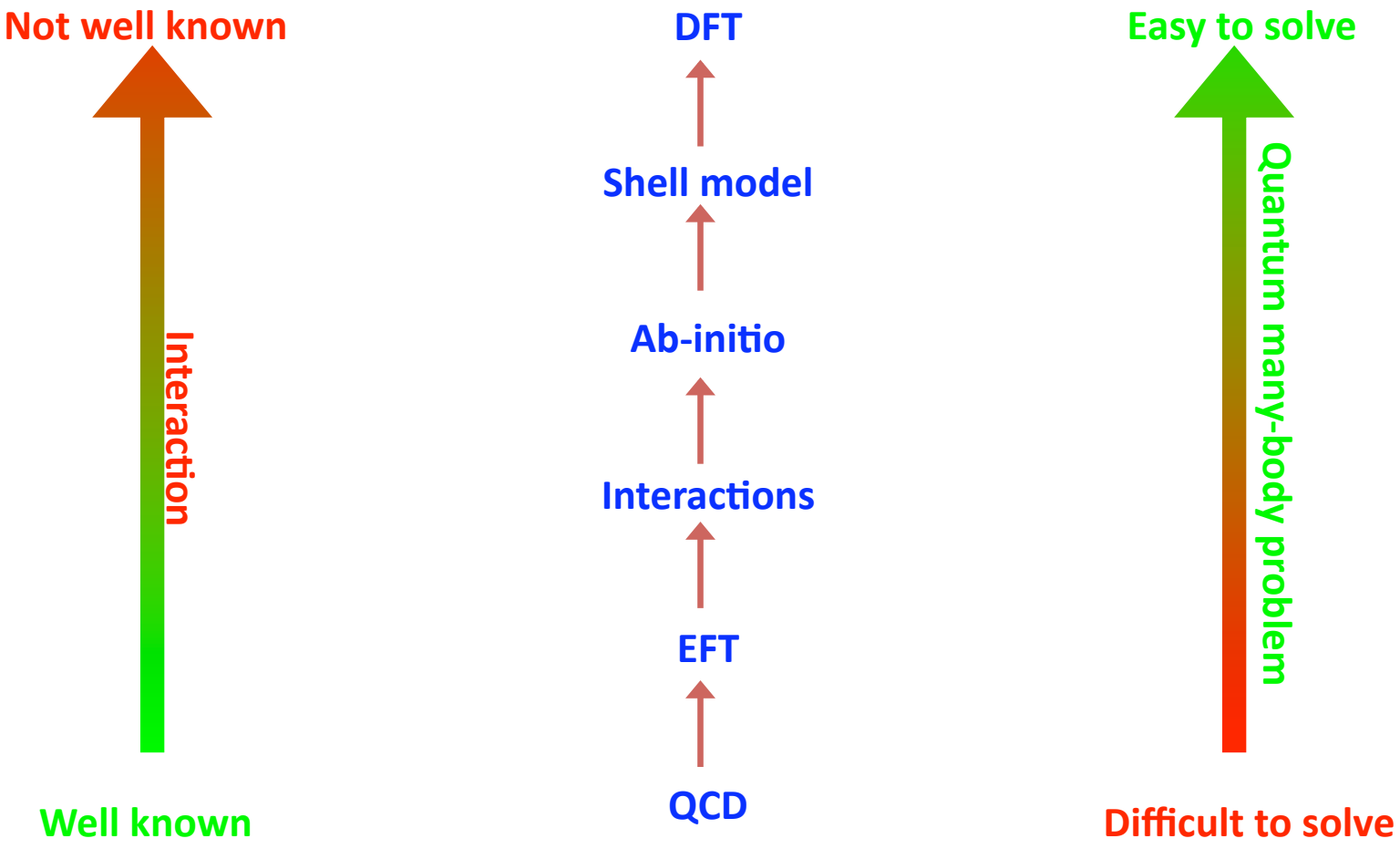
13th CNS Summer School

August 21–27, 2014 at Tokyo University, Wako Campus

Microscopic approaches



No free lunch



This lecture week presents several aspects of this duality.

Light nuclei from a chiral interaction (N^{3}LO by Entem & Machleidt) with no-core shell model

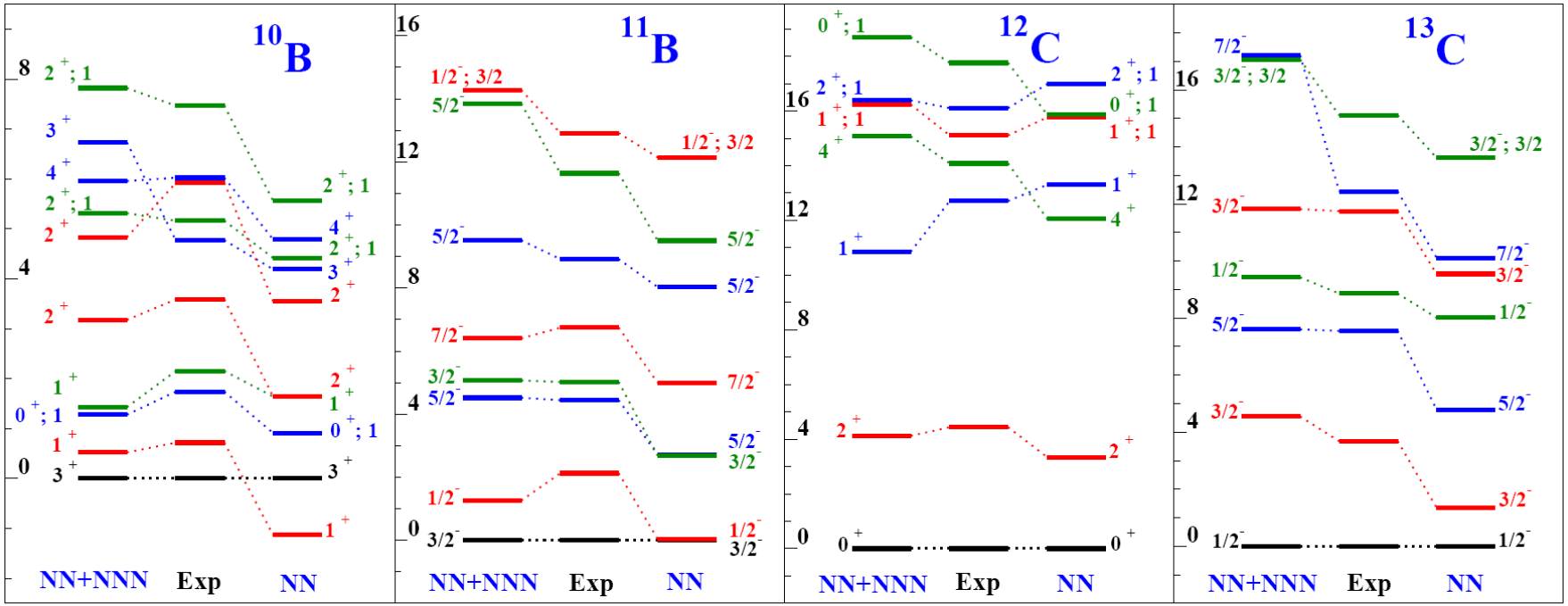


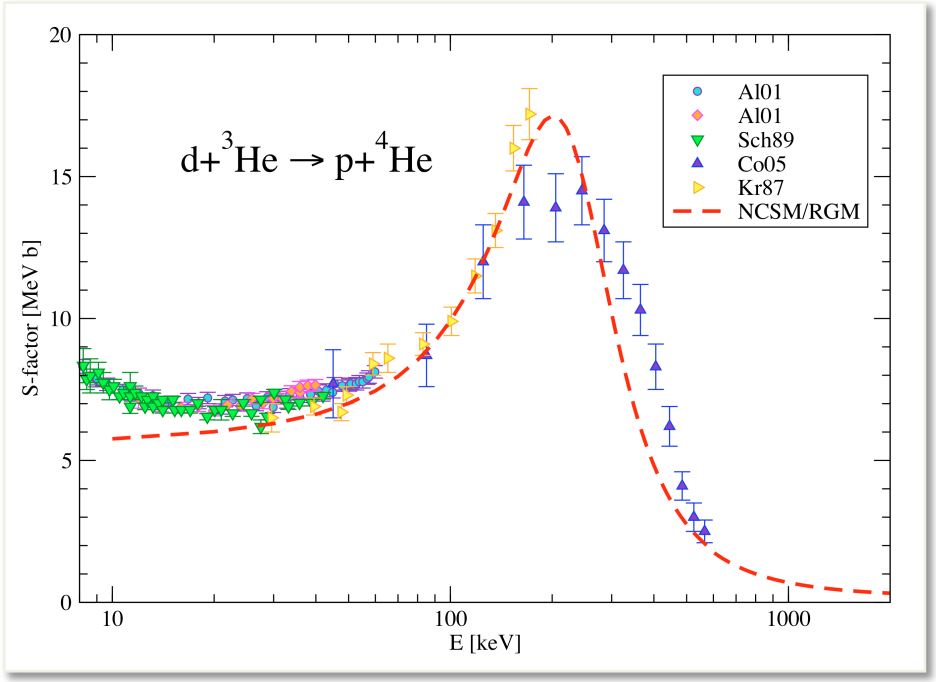
Figure 5. States dominated by p-shell configurations for ^{10}B, ^{11}B, ^{12}C, and ^{13}C calculated at $N_{\max} = 6$ using $\hbar\Omega = 15$ MeV (14 MeV for ^{10}B). Most of the eigenstates are isospin T=0 or 1/2, the isospin label is explicitly shown only for states with T=1 or 3/2. The excitation energy scales are in MeV.

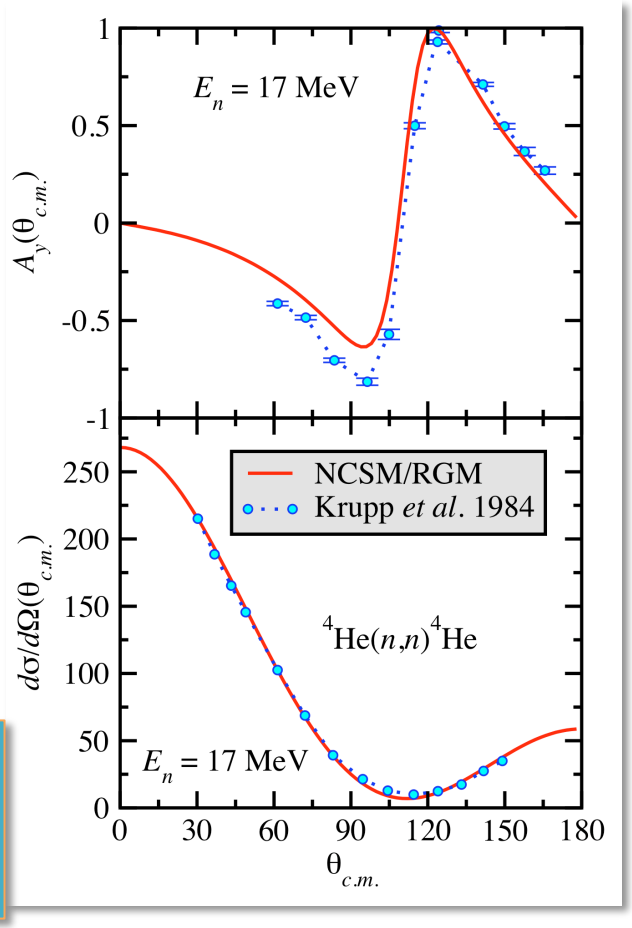
P. Navratil et al., Phys. Rev. Lett. 99, 042501 (2007), nucl-th/0701038.
Review: Navratil, Quaglioni, Stetcu, Barrett, J. Phys. G 36, 083101 (2009); arXiv:0904.0463.

Ab initio description of nuclear reactions

[S. Quaglioni and P. Navrátil, PRL101, 092501 (2008); PRC79, 044606 (2009)]

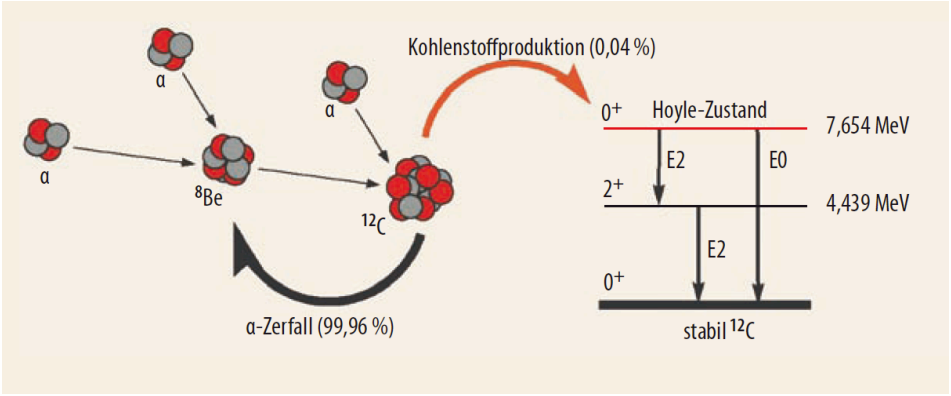
$$\int dr\, r^2 \begin{pmatrix} \left\langle n\, r' \alpha \left| \hat{A}_1 (H-E) \hat{A}_1 \right| \alpha\, r\, n \right\rangle & \left\langle n\, r' \alpha \left| \hat{A}_1 (H-E) \hat{A}_2 \right| {}^3\mathrm{H}\, r\, d \right\rangle \\ \left\langle d\, r' {}^3\mathrm{H} \left| \hat{A}_2 (H-E) \hat{A}_1 \right| \alpha\, r\, n \right\rangle & \left\langle d\, r' {}^3\mathrm{H} \left| \hat{A}_2 (H-E) \hat{A}_2 \right| {}^3\mathrm{H}\, r\, d \right\rangle \end{pmatrix} \begin{pmatrix} \frac{g_1(r)}{r} \\ \frac{g_2(r)}{r} \end{pmatrix} = 0$$



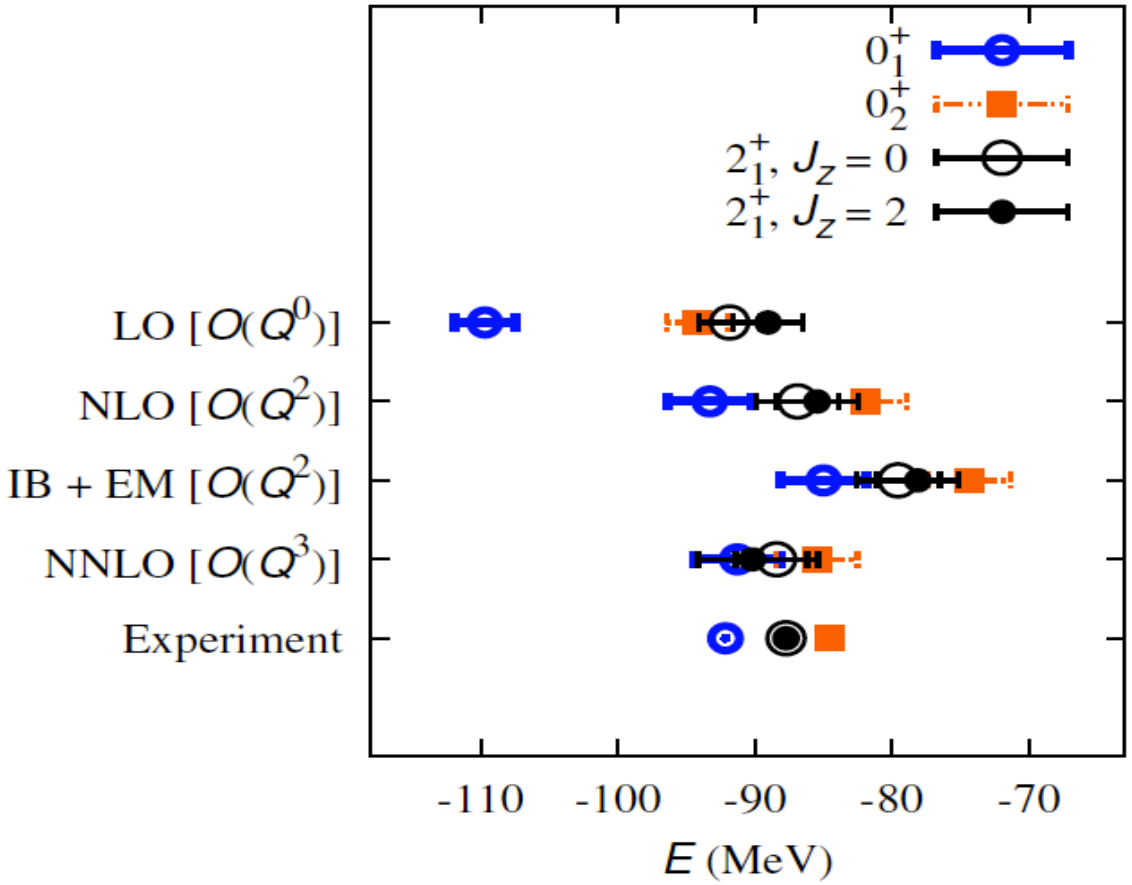


Combination of no-core shell model and the resonating group method
Accurate nuclear Hamiltonian, consistent cluster wave functions
Correct asymptotic expansion, Pauli principle and translational invariance
[Slide courtesy of P. Navratil]

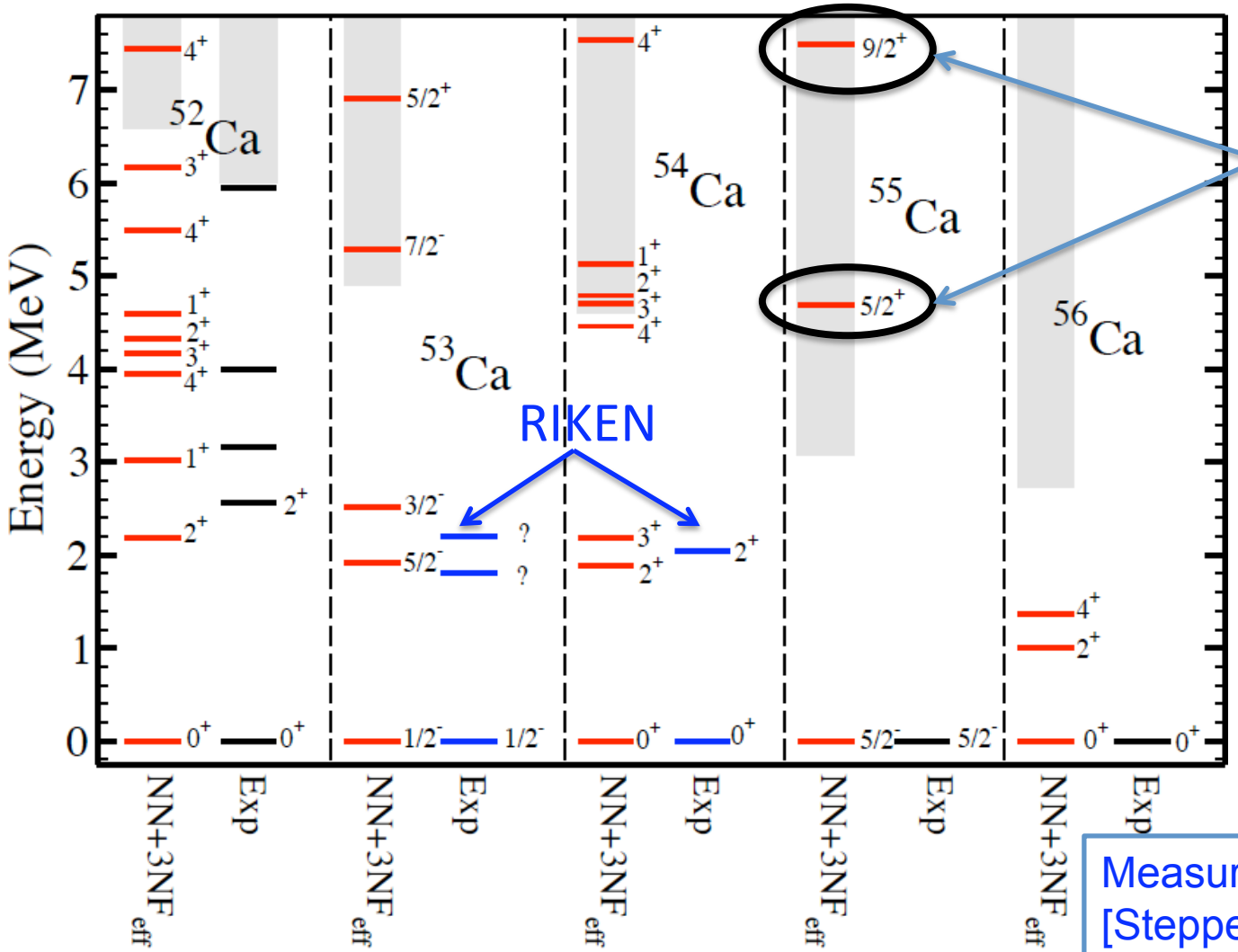
^{12}C Hoyle state from lattice EFT



Epelbaum et al, Phys. Rev. Lett. 106, 192501 (2011); arXiv:1101.2547



Spectra and shell evolution in Calcium isotopes



1. Our prediction for excited $5/2^-$ and $½^-$ states in ^{53}Ca seen at RIKEN
2. Inversion of $9/2^+$ and $5/2^+$ states in neutron rich calcium isotopes
3. Harmonic oscillator gives the naïve shell model order

Measurement at RIKEN [Steppenbeck et al., J. Phys. G 2013; Nature 502, 207 (2013);] confirms our prediction.

Continuum coupling crucial for level ordering

Solving the nuclear many-body problem

- Coupled-cluster method
- No-core shell model
- Greens function Monte Carlo
- Lattice Monte Carlo

Reading suggestions:

Coupled cluster method:
T. Crawford and H. Schaefer, Rev. Comp. Chem. 14, 33 (2000); I. Shavitt and R. Bartlett, *Many-Body Methods in Chemistry and Physics: MBPT and Coupled-Cluster Theory* (Cambridge, 2009); Hagen, Papenbrock, Hjorth-Jensen & Dean, arXiv: 1312.7872.
No-core shell model:
Navratil, Quaglioni, Stetcu, Barrett, J. Phys. G 36, 083101 (2009); arXiv:0904.0463.
GFMC:
Pieper & Wiringa: Ann. Rev. Nucl. Part.Sci. 51, 53 (2001); nucl-th/0103005
Lattice Monte Carlo:
Dean Lee, Prog. Part. Nucl. Phys. 63 117-154 (2009); arXiv:0804.3501

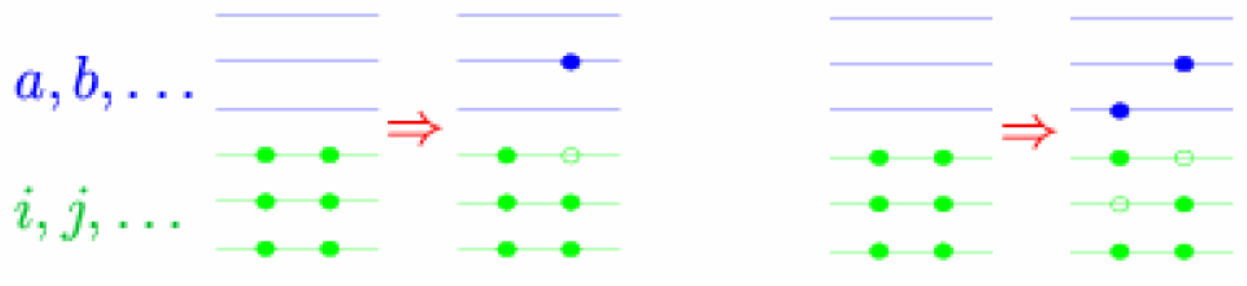
Coupled-cluster theory (CCSD)

Ansatz:

$$
\begin{aligned}
|\Psi\rangle &= e^{T}|\Phi\rangle \\
T &= T_1 + T_2 + \dots \\
T_1 &= \sum_{ia} t_i^a a_a^\dagger a_i \\
T_2 &= \sum_{ijab} t_{ij}^{ab} a_a^\dagger a_b^\dagger a_j a_i
\end{aligned}
$$

- ☺ Scales gently (polynomial) with increasing problem size o^2u^4 .
- ☺ Truncation is the only approximation.
- ☺ Size extensive (error scales with A)

Correlations are *exponentiated* 1p-1h and 2p-2h excitations. Part of np-nh excitations included!



How do we deal with this ansatz / how do we choose the parameters of the cluster operator?

Coupled-cluster method

Schrödinger equation

$$\hat{H}|\Psi\rangle = E|\Psi\rangle$$

Exponential ansatz for correlation operator

$$\hat{H}e^{\hat{T}}|\Phi_0\rangle = Ee^{\hat{T}}|\Phi_0\rangle$$

yields Schrödinger equation for similarity transformed Hamiltonian

$$e^{-\hat{T}}\hat{H}e^{\hat{T}}|\Phi_0\rangle = E|\Phi_0\rangle$$

Similarity-transformed Hamiltonian is not Hermitian.

$$\overline{H} \equiv e^{-\hat{T}}\hat{H}e^{\hat{T}}$$

Coupled-cluster equations (in CCSD approximation)

Multiply with 0p0h, 1p1h, and 2p2h bras and obtain coupled-cluster equations.

$$\begin{aligned}
\langle \Phi_0 | \overline{H} | \Phi_0 \rangle &= E \\
\langle \Phi_i^a | \overline{H} | \Phi_0 \rangle &= 0 \\
\langle \Phi_{ij}^{ab} | \overline{H} | \Phi_0 \rangle &= 0
\end{aligned}$$

The 1p1h and 2p2h excitations are defined as

$$\begin{aligned}
|\Phi_i^a\rangle &= \hat{a}_a^\dagger \hat{a}_i |\Phi_0\rangle \\
|\Phi_{ij}^{ab}\rangle &= \hat{a}_a^\dagger \hat{a}_b^\dagger \hat{a}_j \hat{a}_i |\Phi_0\rangle
\end{aligned}$$

CCSD approximation: The similarity-transformed Hamiltonian has no 1p1h and no 2p2h excitations from the reference state.

First, one needs to solve the CCSD equations. This yields the cluster amplitudes t_i^a and t_{ij}^{ab} that define the similarity-transformed Hamiltonian.

Second, the ground-state energy can be computed.

It's all about the similarity-transformed Hamiltonian

Structure of similarity-transformed Hamiltonian after the CCSD equations are solved

$$\bar{H}_{\mathrm{CCSD}} = \begin{array}{c} \begin{array}{ccc} \text{0p0h} & \text{1p1h} & \text{2p2h} \end{array} \\ \begin{pmatrix} E_{\mathrm{CCSD}} & \bar{H}_{0S} & \bar{H}_{0D} \\ 0 & \bar{H}_{SS} & \bar{H}_{SD} \\ 0 & \bar{H}_{DS} & \bar{H}_{DD} \end{pmatrix} \end{array} \begin{array}{l} \text{0p0h} \\ \text{1p1h} \\ \text{2p2h} \end{array}$$

For excited states and expectation values: Solve the right and left eigenvalue problems

$$\begin{aligned} \overline{H}|R_n\rangle &= E_n|R_n\rangle \\ \langle L_n|\overline{H} &= E_n\langle L_n| \end{aligned}$$

Benefits:

- small model space (2p-2h) excitations are not to numerous)
- similarity transformed Hamiltonian has up to three-body operators in this space

Computation of the similarity-transformed Hamiltonian

Baker Campbell Hausdorff relation to compute similarity-transformed Hamiltonian

$$e^{-\hat{T}}\hat{H}e^{\hat{T}} = \hat{H} + \left[\hat{H},\hat{T}\right] + \frac{1}{2!}\left[\left[\hat{H},\hat{T}\right],\hat{T}\right] + \frac{1}{3!}\left[\left[\left[\hat{H},\hat{T}\right],\hat{T}\right],\hat{T}\right] + \frac{1}{4!}\left[\left[\left[\left[\hat{H},\hat{T}\right],\hat{T}\right],\hat{T}\right],\hat{T}\right] + \ldots.$$

Q: When does this expansion terminate for a two-body Hamiltonian H?

Answers:

1. This is an infinite series that does not terminate.
2. It terminates at 4-fold nested commutators (as shown above) because we deal with a two-body Hamiltonian

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Q: What is the rank (two-body, three-body, four-body …) of the similarity-transformed Hamiltonian for $T=T_1+T_2$ and a two-body Hamiltonian H?

Answers:

1. Two body
2. Three body
3. Four body
4. Six body

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Key observation:

1. When expressed in a diagrammatic way, no unlinked diagrams will be produced by the exponential similarity transform → size extensive approach
2. All terms of the cluster operator *T* commute with each other as annihilation and creation operators refer to different sets of single-particle orbitals (occupied and unoccupied single-particle states)

Consequences (of second point)

1. **The BCH expansion is finite** (at 2k nested commutators for k-body forces) This makes the method very efficient. No ODE needs to be integrated.
3. Solution by iteration (keeping fingers crossed that Banach's fixed point theorem applies): rewrite as t=f(t) and iterate. (usually 15-50 iteration needed)

Who likes to commute? Can we get there fast, please?

$$e^{-\hat{T}}\hat{H}e^{\hat{T}} = \hat{H} + \left[\hat{H},\hat{T}\right] + \frac{1}{2!}\left[\left[\hat{H},\hat{T}\right],\hat{T}\right] + \frac{1}{3!}\left[\left[\left[\hat{H},\hat{T}\right],\hat{T}\right],\hat{T}\right] + \frac{1}{4!}\left[\left[\left[\left[\hat{H},\hat{T}\right],\hat{T}\right],\hat{T}\right],\hat{T}\right] + \ldots.$$

First attempted: Apply Wick's theorem and work it out.

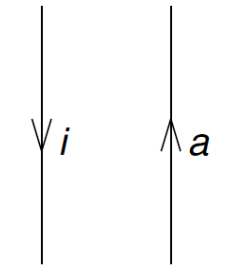
$$\begin{aligned}
\langle\Phi_0|\overline{H}|\Phi_0\rangle &= E \\
\langle\Phi_i^a|\overline{H}|\Phi_0\rangle &= 0 \\
\langle\Phi_{ij}^{ab}|\overline{H}|\Phi_0\rangle &= 0
\end{aligned}$$

More efficient approach: use diagrams!

Diagrammatics

hole line

particle line

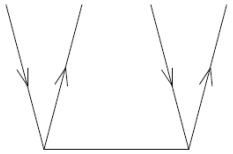


$\hat{a}_i \quad \hat{a}_a^\dagger$

Cluster operators ("T amplitudes")

$$\hat{T}_1 = \sum_{ia} t_i^a \{a_a^\dagger a_i\} =$$

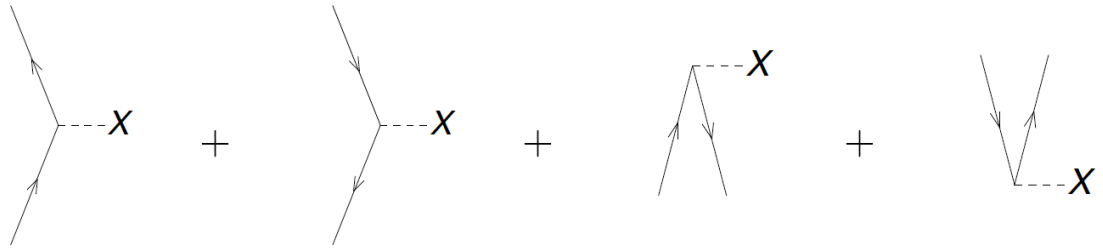
$$\hat{T}_2 = \frac{1}{4} \sum_{ijab} t_{ij}^{ab} \{a_a^\dagger a_b^\dagger a_j a_i\} =$$



Normal-ordered one-body Hamiltonian

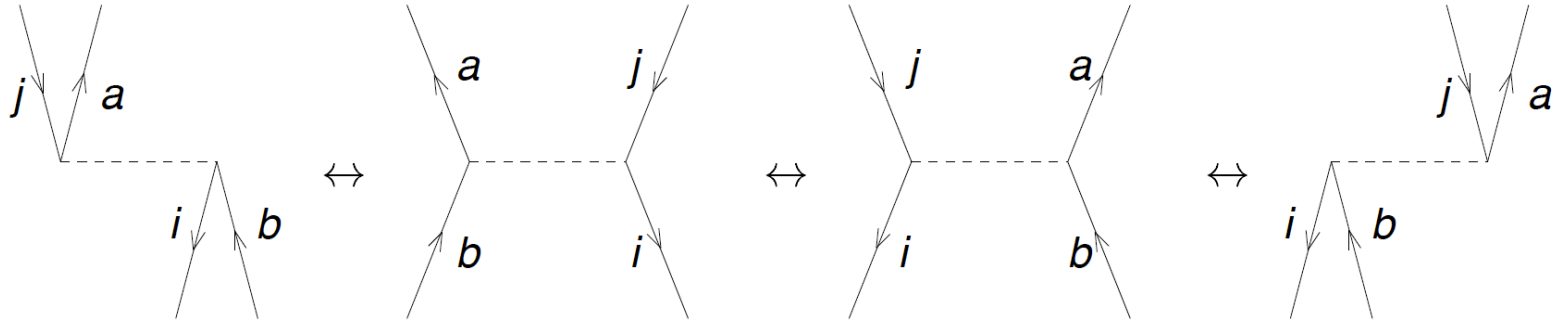
$$\hat{F}_N = \sum_{ab} f_{ab} \{a_a^\dagger a_b\} + \sum_{ij} f_{ij} \{a_i^\dagger a_j\} + \sum_{ia} f_{ia} \{a_i^\dagger a_a\} + \sum_{ia} f_{ai} \{a_a^\dagger a_i\}$$

$=$



Diagrammatics cont'd

Antisymmetric two-body operator <ai|V|jb> = < left out, right out|| left in, right in>



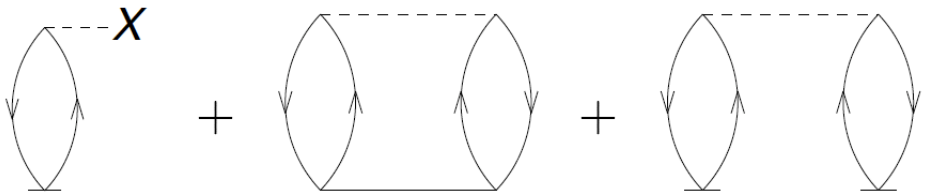
<ai|V|jb> <ai|V|bj> <ia|V|jb> <ia|V|bj>

CCSD energy equation

$$\langle \Phi_0 | \overline{H} | \Phi_0 \rangle = E$$

All diagrams that are fully contracted (no open lines)

$$E_{\mathrm{CCSD}} - E_0 =$$



$$= \sum_{ia} f_{ia} t_i^a + \frac{1}{4} \sum_{ijab} \langle ij||ab\rangle t_{ij}^{ab} + \frac{1}{2} \sum_{ijab} \langle ij||ab\rangle t_i^a t_j^b$$

Question: What is the computational cost (in number of occupied and unoccupied states of the model space) for the computation of the energy?

Answers:

1. o*u
2. $(o*u)^2$
3. $o^2 * u^4$

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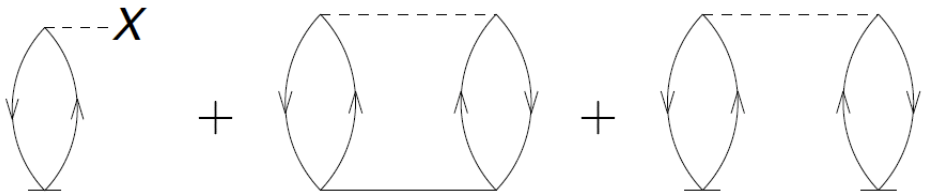


$$= \sum_{ia} f_{ia} t_i^a + \frac{1}{4} \sum_{ijab} \langle ij||ab\rangle t_{ij}^{ab} + \frac{1}{2} \sum_{ijab} \langle ij||ab\rangle t_i^a t_j^b$$

Question: What is the computational cost (in number of occupied and unoccupied states of the model space) for the computation of the energy?

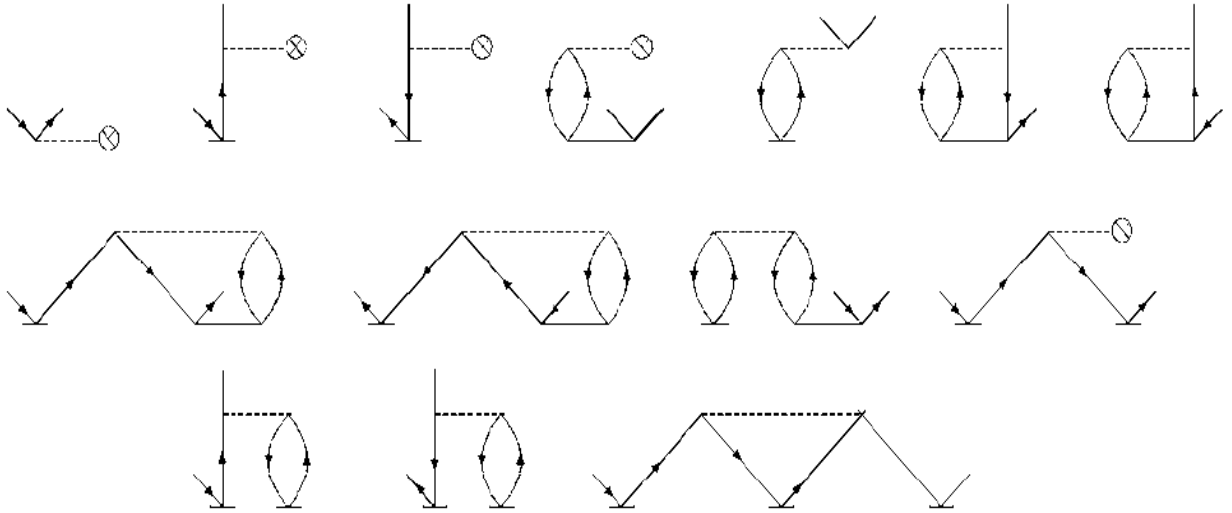
Answers:

1. o*u
2. $(o*u)^2$ ✔ (last two diagrams)
3. $o^2 * u^4$

T_1 equation (within CCSD)

$$\langle \Phi_i^a | \overline{H} | \Phi_0 \rangle \quad = \quad 0$$

All linked diagrams with one incoming hole line and one outgoing particle line.



$$\begin{aligned}
0 \quad = \quad & f_{ai} + \sum_c f_{ac} t_i^c - \sum_k f_{ki} t_k^a + \sum_{kc} \langle ka||ci\rangle t_k^c + \sum_{kc} f_{kc} t_{ik}^{ac} + \frac{1}{2} \sum_{kcd} \langle ka||cd\rangle t_{ki}^{cd} - \\
& \frac{1}{2} \sum_{klc} \langle kl||ci\rangle t_{kl}^{ca} - \sum_{kc} f_{kc} t_i^c t_k^a - \sum_{klc} \langle kl||ci\rangle t_k^c t_l^a + \sum_{kcd} \langle ka||cd\rangle t_k^c t_i^d - \\
& \sum_{klcd} \langle kl||cd\rangle t_k^c t_i^d t_l^a + \sum_{klcd} \langle kl||cd\rangle t_k^c t_{li}^{da} - \frac{1}{2} \sum_{klcd} \langle kl||cd\rangle t_{ki}^{cd} t_l^a - \frac{1}{2} \sum_{klcd} \langle kl||cd\rangle t_{kl}^{ca} t_i^d ,
\end{aligned}$$

T_2 equation (within CCSD)

$$\langle \Phi_{ij}^{ab} | \overline{H} | \Phi_0 \rangle \quad = \quad 0$$

All linked diagrams with two incoming hole lines and two outgoing particle lines.

At this point, one has to consider re-use of intermediate diagrams and order of contractions for numerical efficiency.

→ "factorization" of diagrams (Kucharski & Bartlett 1991)

Homework: Write down all diagrams for the equation above!

Summary: Ab-initio method

- Size extensive
- Computational cost $n_o^2\, n_u^4 \sim \Lambda^{12} A^6$(in CCSD)
- Within CCSD, one only computes the matrix elements of a similarity-transformed two-body Hamiltonian (shell model needs matrix elements between many-body states)

No core shell model

Main idea: build and diagonalize the Hamiltonian matrix of the many-body system in an oscillator basis

Oscillator basis: The only localized basis, in which a wave function

$\Phi_{com}(r1+r2)\,\Phi_{rel}(r1-r2)$

can be written as a ***finite*** sum of products

$\Phi_n(r1)\Phi_m(r2)$

of oscillator wave functions Φ.

Consequence: An intrinsic wave function can be computed that makes no reference to the center of mass

- Rotational and translational invariance exactly preserved
- Matrix dimensions scales factorial in the number of single-particle states

Navratil, Quaglioni, Stetcu & Barrett, *Recent developments in no-core shell-model calculations*, J. Phys. G 36, 083101 (2009); arXiv:0904.0463

Green's Function Monte Carlo

Idea:

1. Determine accurate approximate wave function via variation of the energy (The high-dimensional integrals are done via Monte Carlo integration).

$$E_T = \frac{\langle \Psi_{\text{trial}} | \hat{H} | \Psi_{\text{trial}} \rangle}{\langle \Psi_{\text{trial}} | \Psi_{\text{trial}} \rangle}$$

2. Refine wave function and energy via projection with Green's function

$$|\Psi\rangle = \lim_{\tau \to \infty} e^{-\tau(\hat{H} - E_T)} |\Psi_{\text{trial}}\rangle$$

Nice review: "Lectures on Quantum Monte Carlo" by David M. Ceperley:
http://people.physics.uiuc.edu/Ceperley/papers/175.pdf

Great lecture:

Werner Krauth, *Introduction To Monte Carlo Algorithms*, cond-mat/9612186

Green's function Monte Carlo details

- Idea: Function of the Hamiltonian projects out the ground state from a trial wave function.
- Method: A wave function at imaginary "time" (n+1)t is obtained from a trial wave function at time nt via Green's function $G(R,R') \equiv \langle R|e^{-\tau(\mathcal{H}-E_T)}|R'\rangle$

$$\psi_{n+1}(R) = e^{-\tau(\mathcal{H}-E_T)}\psi_n(R) = \int dR' G(R,R')\psi_n(R')$$

- Note: ψ_n results from a 3n-dimensional integral over ψ_0.

$$\psi_n(R_n) = \int dR_{n-1}\ldots dR_1 dR_0 G(R_n,R_{n-1})\ldots G(R_2,R_1)G(R_1,R_0)\psi_0(R_0)$$

- Understanding of the method: Expansion in terms of exact eigenstates ϕ_a

$$\psi_n(R) = \sum_\alpha \phi_\alpha(R) < \phi_\alpha|\Psi > e^{-n\tau(E_\alpha - E_T)}$$

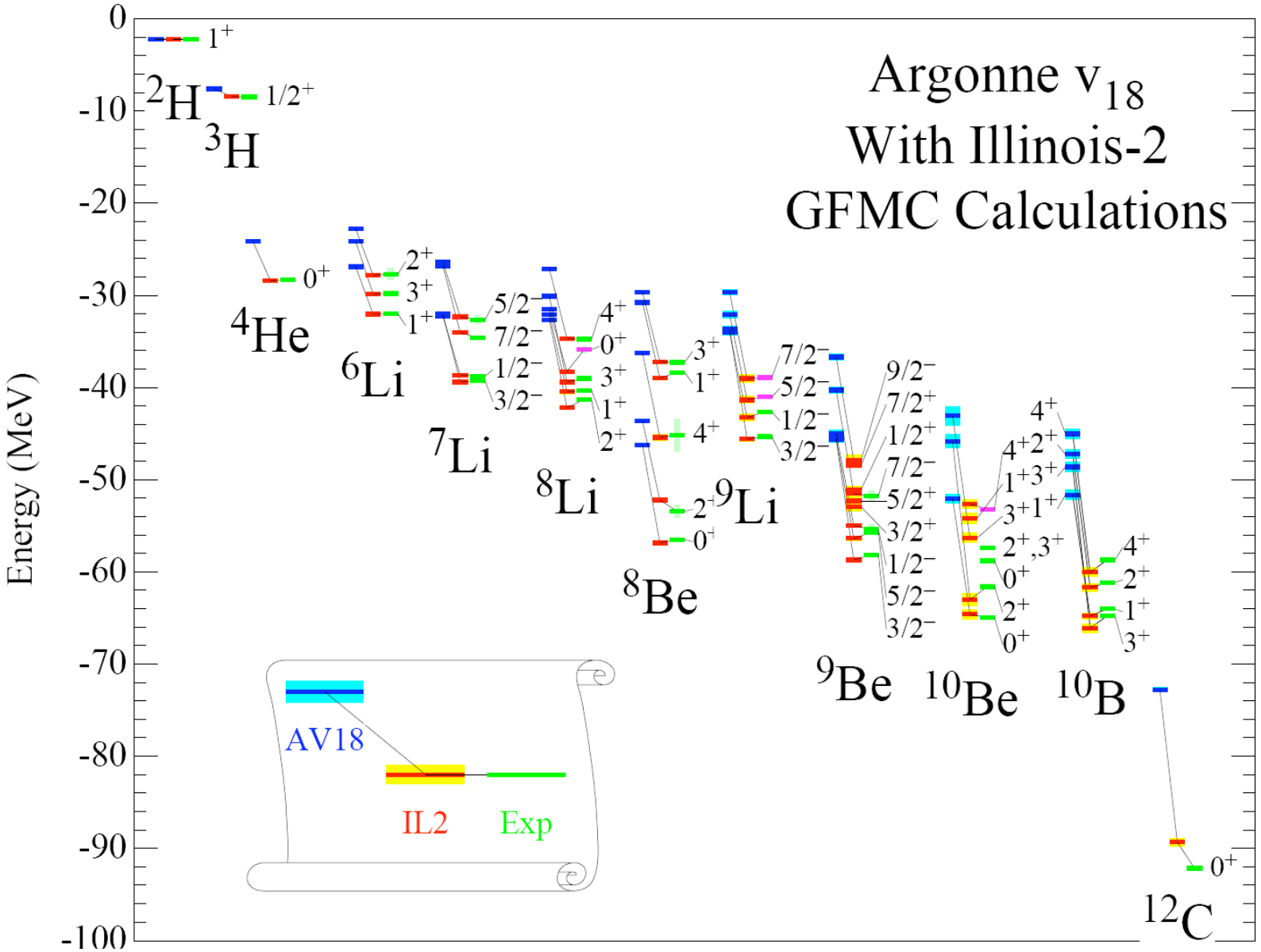
$$\lim_{n\to\infty} \psi_n(R) = \phi_0(R) < \phi_0|\Psi > e^{-n\tau(E_0 - E_T)}$$

- <u>Key insight</u>: Green's function in the limit of zero time step is exactly known for Hamiltonians H=T+V(R) with <u>local</u> potential V(R)

$$< R|e^{-\tau(\mathcal{H}-E_T)}|R' >= (4\pi\lambda\tau)^{-3N/2} e^{-\frac{(R-R')^2}{4\lambda\tau}} e^{-\tau(V(R)-E_T)} + O(\tau^2)$$

- "Only" need to perform a high-dimensional integration → Monte Carlo

Green's function Monte Carlo results



Pieper and Wiringa, Ann.Rev.Nucl.Part.Sci. 51 (2001) 53

Accomplishments of ab-initio nuclear structure calculations

- Demonstration that nuclei can be built from scratch
- Demonstration that three-nucleon forces must be included in the description
- Determination of low-energy constants of potentials from chiral EFT
- Probing of effective interactions in medium-mass nuclei
- Bridging the gap to (ab-initio) reactions in light systems
- Providing a solid basis that other methods can build on and link to (→ UNEDF www.unedf.org, NUCLEI www.computingnuclei.org projects)

Several methods with complementary properties available

Computing the nuclear mass table: density functional theory

Thomas Papenbrock

and OAK RIDGE NATIONAL LABORATORY

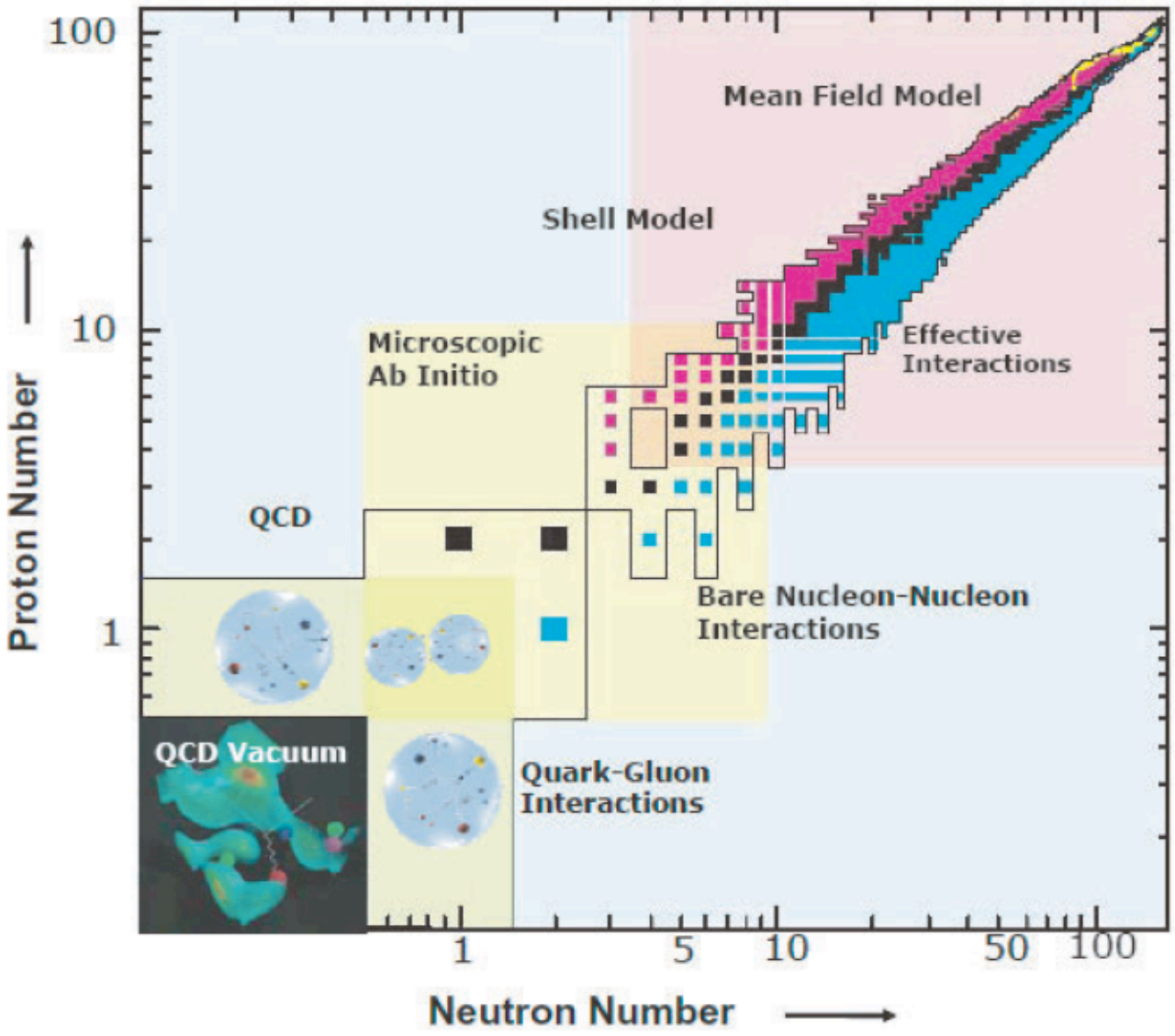
Aim of this lecture:

Introduction to nuclear mean-field methods

13th CNS Summer School

August 21–27, 2014 at Tokyo University, Wako Campus

Bottom-up approach to nuclear structure



DFT

↑

Shell model

↑

Ab-initio

↑

Interactions

↑

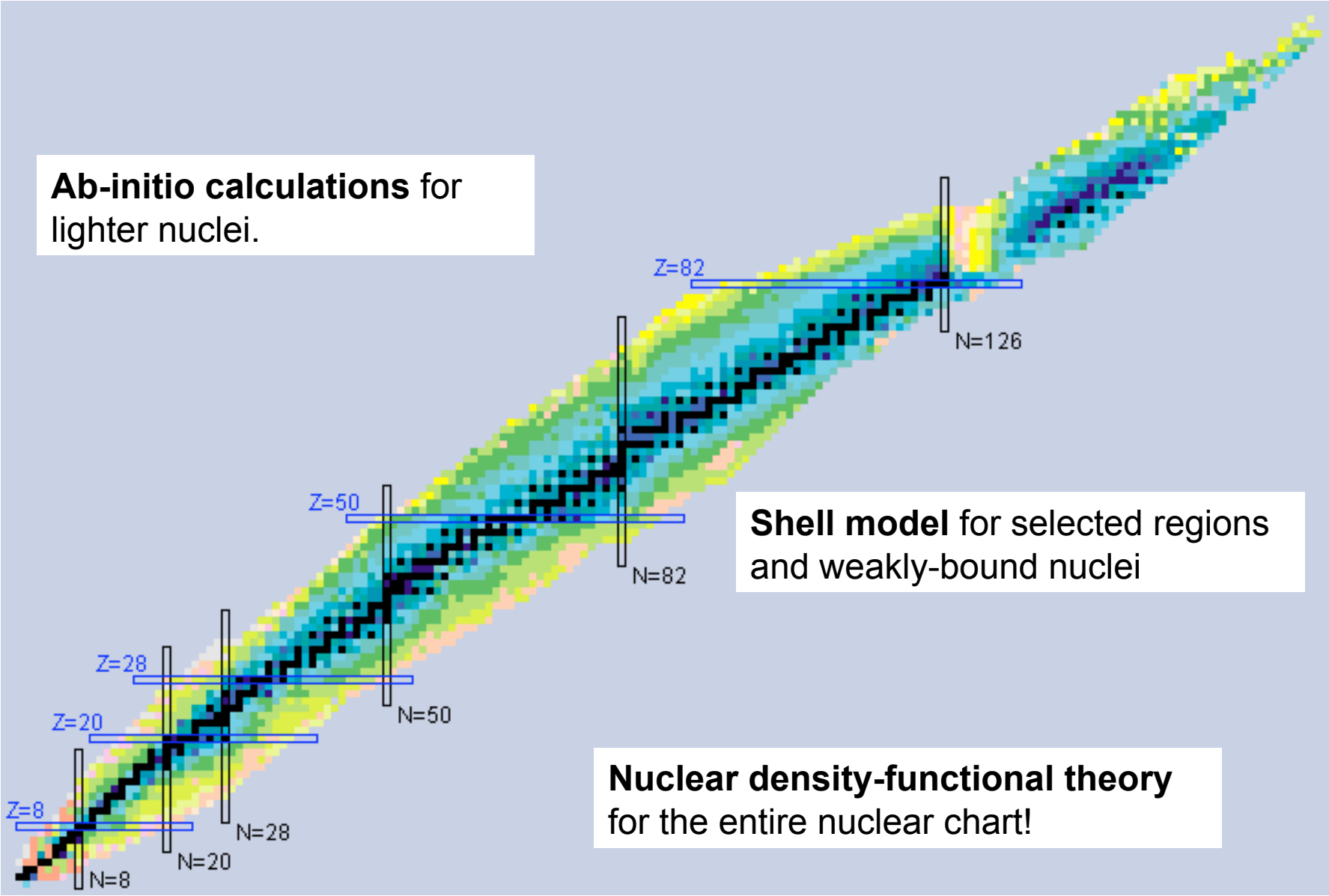
EFT

↑

QCD

Figure from A. Richter (2004)

Methods (th)at work



Nobel Prize in chemistry 1998

Walter Kohn

"for his development of the density-functional theory"

Two quotes from Kohn's Nobel lecture:

I begin with a provocative statement. *In general the many-electron wavefunction* $\Psi(r_1,...,r_N)$ *for a system of N electrons is not a legitimate scientific concept, when* $N \geq N_0$, *where* $N_0 \approx 10^3$.

I will use two criteria for defining "legitimacy": a) That Ψ can be calculated with sufficient accuracy and b) can be recorded with sufficient accuracy.

In concluding this section I remark that DFT, while *derived* from the N-particle Schroedinger equation, is finally expressed entirely in terms of the density $n(r)$, in the Hohenberg-Kohn formulation,[1] and in terms of $n(r)$ and *single*-particle wavefunctions $\psi_j(r)$, in the Kohn-Sham formulation[2]. This is why it has been most useful for systems of very many electrons where wavefunction methods encounter and are stopped by the "exponential wall".

Density-functional theory (DFT)

Theoretical basis: Hohenberg-Kohn theorem (1964)

Map from ground-state wave function to density

$$\psi(r) \rightarrow \rho(r)$$

Map from density to set of all corresponding wave functions

$$\rho(r) \rightarrow \{\psi(r)\}|_\rho$$

Energy functional: energy is minimum in this set

$$F[\rho(r)] = \min_{\{\psi\}|_\rho} \langle\psi|\hat{H}|\psi\rangle$$

Ground-state energy from minimization of the functional

$$E_{\mathrm{gs}} = \min_\rho \{F[\rho] + \int \mathrm{d}r v(r)\rho(r)\}$$

Density-functional theory

Alternative view: Energy functional is a Legendre transform (Lieb, 1983)

Find ground-state energy for all external potentials (this is a functional)

$$v(r) \rightarrow E[v(r)]$$

Perform functional Legendre transform

1. Compute density as functional derivative

$$\rho(r) = \frac{\delta E[v(r)]}{\delta v(r)}$$

2. Inversion: Find potential in terms of density

3. Construct Legendre transform

$$F[\rho(r)] \;=\; E[v(r)] - \int \mathrm{d}r v(r)\rho(r)$$

This path of construction can actually be followed for dilute Fermi gases [Puglia et al (2003)], the pairing Hamiltonian [TP, Bhattacharyya (2007)], or the Lipkin model [Bertolli, TP (2008)].

Example: Energy of a non-interacting fermions

(Thomas-Fermi approximation)

$$E[\rho] = \int d^3r \left(\frac{3}{10}(3\pi^2)^{2/3}\frac{\hbar^2}{2m}\rho^{5/3}(r) + V_{\text{ext}}(r)\rho(r) \right)$$

energy functional

kinetic energy density
(Thomas-Fermi approximation)

external potential

Note: Hohenberg-Kohn DFT not a practical (i.e. accurate) tool

- Local approximations of the density functional are too inaccurate
- Problem is particular with the kinetic energy density

Systematic construction of density functional for dilute Fermi gas

Dilute Fermi gas:

All parameters of the potential (scattering length, effective range, …) much smaller than the Fermi wave length (or average two-particle distance) → small expansion parameter exist, namely $\mathbf{k_F a}$.

Use EFT to systematically construct energy density functional in terms of these small parameters.

$$\mathcal{E} = \rho \frac{\hbar^2 k_F^2}{2m} \left\{ \frac{3}{5} + \left[\frac{2}{3\pi} k_F a + \frac{4}{35\pi^2} (11 - 2\log 2)(k_F a)^2 \right] \right\}$$

$$\rho = \frac{k_F^3}{3\pi^2}$$

Contributions from interaction

This systematic approach gives valuable insights into the construction of density functionals. However, it is at present limited to “solvable” Hamiltonians.

See, e.g., R. J. Furnstahl and H.-W. Hammer, Annals Phys. 302 (2002) 206.
S. J. Puglia et al, Nucl.Phys. A723 (2003) 145.

Kohn-Sham DFT [W. Kohn & L. Sham, Phys. Rev. 140 (1965) A1133]

- Kohn-Sham: The form of the density functional is

$$E[\rho] = \int d^3r\,(\tau(r) + V_{\text{ext}}(r)\rho(r)) + E_{\text{int}}[\rho]$$

$$\rho(r) = \sum_{k=1}^{A} |\psi_k(r)|^2 \quad \text{density}$$

$$\tau(r) = \frac{\hbar^2}{2m} \sum_{k=1}^{A} |\nabla\psi_k(r)|^2 \quad \text{kin. energy density of free fermions (nonlocal!)}$$

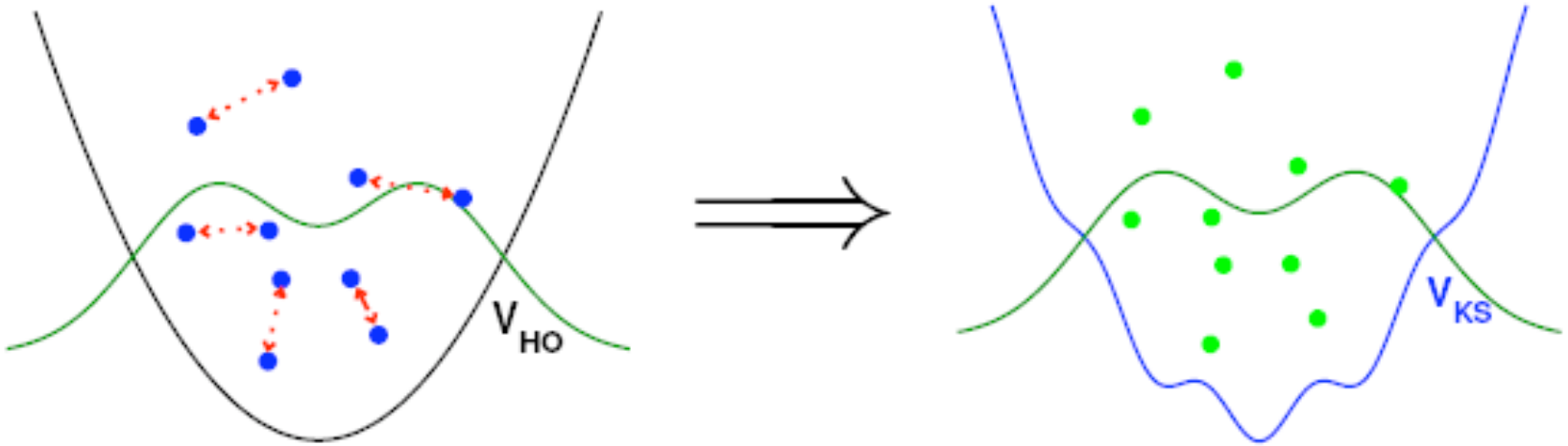
- Kohn-Sham equations: dE[ρ] = 0

$$\left(-\frac{\hbar^2}{2m}\Delta + \frac{\delta E_{\text{int}}[\rho]}{\delta\rho(r)} + V_{\text{ext}}(r)\right)\psi_k(r) = \mu\psi_k(r)$$

- Remarks: Single-particle Schrödinger equation has to be solved.
- For nuclei, one uses the *local density approximation* (LDA), and gradient corrections.

$$E_{\text{int}} = E_{\text{int}}[\rho, \nabla\rho] = \int d^3r\mathcal{E}(\rho, \nabla\rho)$$

Idea behind Kohn-Sham DFT



Ground state density of interacting fermions in external harmonic trap.

Turn off the interaction, but change external potential such that the density remains that of the interacting system. The additional potential is the Kohn-Sham potential.

Picture from R. Furnstahl: http://trshare.triumf.ca/~schwenk/ECT/furnstahl1.pdf

Nuclear DFT

Problem: Local density approximation not accurate (e.g. pairing would require highly nonlocal functional)

Approach: Include anomalous pairing densities and work with quasi-particle states

1. Add sources to the Hamiltonian

$$\begin{aligned} \hat{H} &\rightarrow \hat{H} + \int d^3r \hat{\psi}^\dagger(r)\hat{\psi}(r)v(r) + \int d^3r \left(\hat{\psi}(r)\hat{\psi}(r) + \hat{\psi}^\dagger(r)\hat{\psi}^\dagger(r)\right) w(x) \\ E_{g.s.} &= E[v(r), w(r)] \end{aligned}$$

2. Perform Legendre transform with respect to all sources

$$F[\rho(r), \kappa(r)] = E[v(r), w(r)] - \int d^3r v(r)\rho(r) - \int d^3r w(r)\kappa(r)$$

Practical approach: Skyrme Hartree Fock theory

Refs.: T.H.R. Skyrme, Phil. Mag. 1 (1956) 1043; D. Vautherin and D. M. Brink, PRC 5 (1972) 626; J. W. Negele and D. Vautherin, PRC 5 (1972) 1472; Bogner and Furnstahl (2006)

Main idea: Use mean-field Hamiltonian that depends on densities and currents, and solve self-consistently.

$$
\begin{aligned}
E &= \int d^3r\, n\left\{\mathcal{E}_{\rm kin} + \mathcal{E}_{\rm Skyrme} + \mathcal{E}_{\rm Skyrme,odd}\right\} + E_{\rm Coulomb} + E_{\rm pair} + E_{\rm cm} \quad , \\
n\mathcal{E}_{\rm kin} &= \frac{\hbar^2}{2m}\int d^3\,\tau \quad , \\
n\mathcal{E}_{\rm Skyrme} &= \frac{B_0 + B_3 n^\alpha}{2} n^2 - \frac{B'_0 + B'_3 n^\alpha}{2}\tilde{n}^2 \\
&\quad + B_1\left(n\tau - \mathbf{j}^2\right) - B'_1\left(\tilde{n}\tilde{\tau} - \tilde{\mathbf{j}}^2\right) - \frac{B_2}{2} n\Delta n + \frac{B'_2}{2}\tilde{n}\Delta\tilde{n} \\
&\quad - B_4 n\nabla\cdot\mathbf{J} - (B_4 + B'_4)\tilde{n}\nabla\cdot\tilde{\mathbf{J}} + \frac{C_1}{2}\mathbf{J}^2 - \frac{C'_1}{2}\tilde{\mathbf{J}}^2 \quad , \\
n\mathcal{E}_{\rm Skyrme,odd} &= -\frac{C_0 + C_3 n^\alpha}{2}\boldsymbol{\sigma}^2 + \frac{C'_0 + C'_3 n^\alpha}{2}\tilde{\boldsymbol{\sigma}}^2 + \frac{C_2}{2}\boldsymbol{\sigma}\cdot\Delta\boldsymbol{\sigma} - \frac{C'_2}{2}\tilde{\boldsymbol{\sigma}}\cdot\Delta\tilde{\boldsymbol{\sigma}} \\
&\quad - C_1\boldsymbol{\sigma}\cdot\boldsymbol{\tau} + C'_1\tilde{\boldsymbol{\sigma}}\cdot\tilde{\boldsymbol{\tau}} - B_4\boldsymbol{\sigma}\cdot(\nabla\times\mathbf{j}) - (B_4 + B'_4)\tilde{\boldsymbol{\sigma}}\cdot(\nabla\times\tilde{\mathbf{j}}) \quad , \\
E_{\rm Coulomb} &= e^2\frac{1}{2}\int d^3r\, d^3r' \frac{n_{\rm p}(\mathbf{r}) n_{\rm p}(\mathbf{r}')}{|\mathbf{r} - \mathbf{r}'|} - \frac{3}{4}e^2\left(\frac{3}{\pi}\right)^{1/3}\int d^3r \left[n_{\rm p}\right]^{4/3} \quad .
\end{aligned}
$$

Functional or Hamiltonian?

In modern parlance, one speaks of nuclear energy density functionals and not of density-dependent Hamiltonians.

1. This is just modern vocabulary
2. This is of a correct expression because there are no density-dependent Hamiltonians (Hamiltonians depend on field operators in general, but not on densities)

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Which symmetries does the mean-field break?

1. …
2. …
3. …
4. …

Which symmetries does the mean-field break?

1. Translation invariance
2. Rotation invariance (deformation)
3. Particle number conservation (pairing)
4. Isospin invariance (deformation in isospin space; worth considering close to N=Z line)

The “best” mean-field theory allows for all symmetries to be broken.

Reminder: Symmetry-breaking in mean-field theories

- HF states usually break symmetries, e.g., translational invariance and rotational invariance.
- HFB quasi-particle states do not exhibit a definite number of particles (breaking of U(1) gauge symmetry).

Question: Is the symmetry breaking in HF(B) a feature or a nuisance?

Answer:

1. It's a feature because it displays the most relevant properties of the ground state (e.g. deformation, pairing)
2. It's a nuisance because nuclei have definite spin and particle numbers, and the symmetry-breaking solutions miss these points.

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2. It's a nuisance because nuclei have definite spin and particle numbers, and the symmetry-breaking solutions miss these points.

However: Symmetry restoration becomes an important (and not yet fully solved) problem

Summary: Symmetry-breaking in mean-field theories

- HF states usually break symmetries, e.g., translational invariance and rotational invariance.
- HFB quasi-particle states do not exhibit a definite number of particles (breaking of U(1) gauge symmetry).
- The breaking of symmetry is desired, as it allows the single-particle state to capture relevant correlations.
- Restoration of symmetries becomes an important issue.

Publicly available program

HFODD

J. Dobaczewski et al, Computer Physics Communications 167 (2005) 214

http://www.fuw.edu.pl/~dobaczew/hfodd/hfodd.html

Skyrme functionals, example: UNEDF0

Kortelainen, Lesinski, Moré, Nazarewicz, Sarich, Schunck, Stoitsov, Wild, Phys. Rev. C 82, 024313 (2010)

- Energy functional based on Skyrme SLy4 parametrization

$$E = \int \mathcal{H}(\boldsymbol{r}) d^3\boldsymbol{r}$$

- usual kinetic part (with 1/A mass shift); interaction: $\chi = \chi_0 + \chi_1$
- interaction energy functional (with isospin labels): 13 parameters

$$\begin{aligned}\chi_t(\boldsymbol{r}) \;=\; & C_t^{\rho\rho}\rho_t^2 + C_t^{\rho\tau}\rho_t\tau_t + C_t^{J^2}\boldsymbol{J}_t^2 \\ & + C_t^{\rho\Delta\rho}\rho_t\Delta\rho_t \;+ C_t^{\rho\nabla J}\rho_t\boldsymbol{\nabla}\cdot\boldsymbol{J}_t \\ & C_t^{\rho\rho} = C_{t0}^{\rho\rho} + C_{t\mathrm{D}}^{\rho\rho}\;\rho_0^{\gamma}\end{aligned}$$

- Pairing part depends on local pairing density: 2 parameters

$$\breve{\chi}(\boldsymbol{r}) = \sum_{q=n,p} \frac{V_0^q}{2}\left[1 - \frac{1}{2}\frac{\rho(\boldsymbol{r})}{\rho_0}\right]\breve{\rho}^2(\boldsymbol{r})$$

UNEDF0 functional

- Pairing parameters from odd-even staggering (OES); Lipkin-Nagomi for particle number projections
- Optimization employs POUNDerS [Practical Optimization Using No Derivatives (of Squares)]
- (pseudo) observables: nuclear matter properties, binding energies, radii, OES of 44 well-deformed even-even nuclei and 28 spherical nuclei

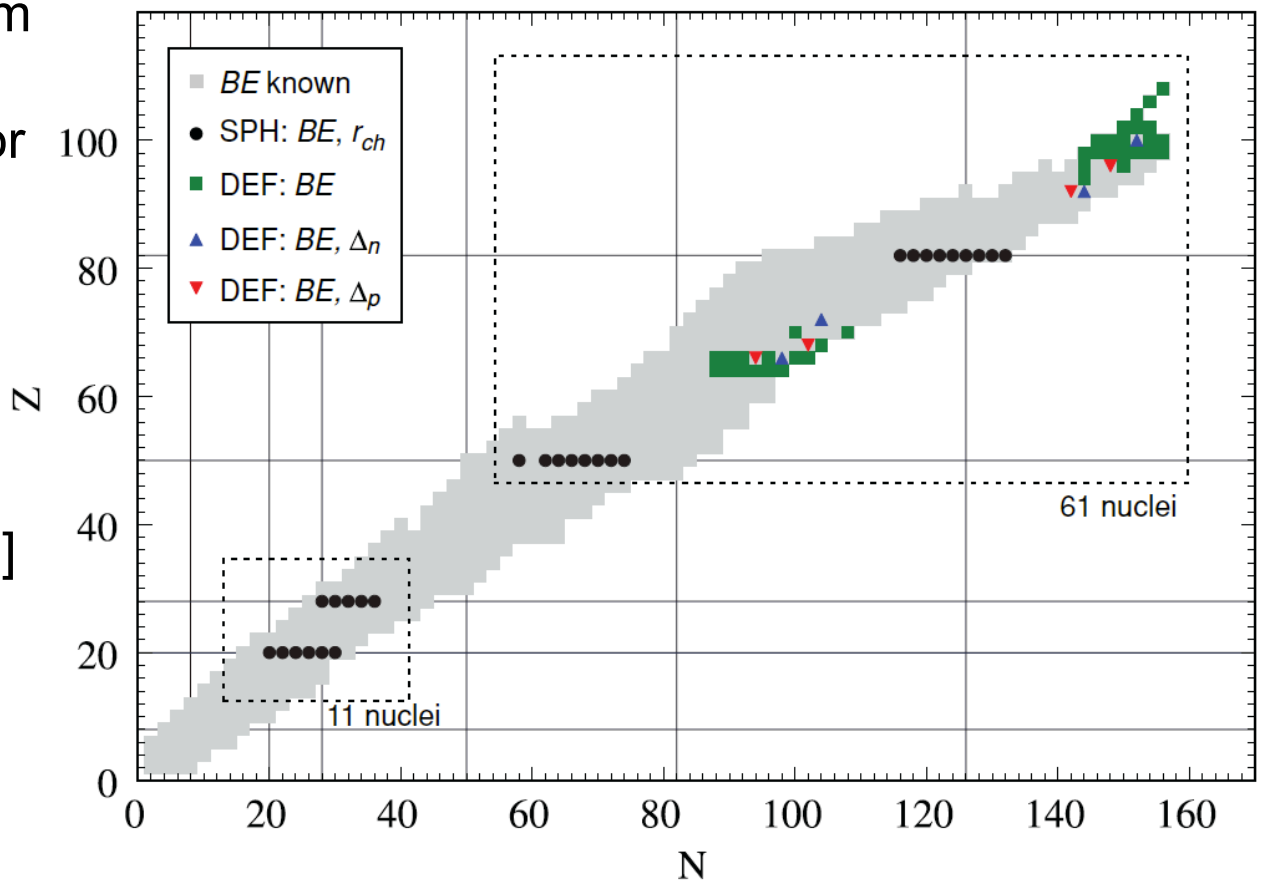


FIG. 1. (Color online) Experimental set of fit observables used in this work. The set contains data for 11 nuclei with $A < 66$ and 61 nuclei with $A > 106$.

Kortelainen, Lesinski, Moré, Nazarewicz, Sarich, Schunck, Stoitsov, Wild, Phys. Rev. C 82, 024313 (2010)

Sensitivity analysis exhibits correlations of the model

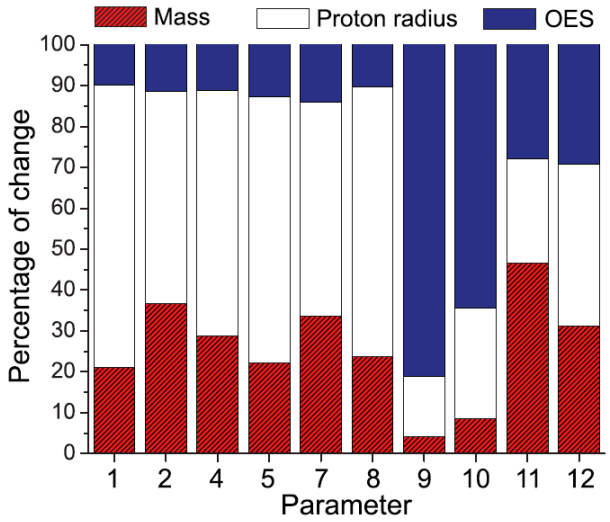
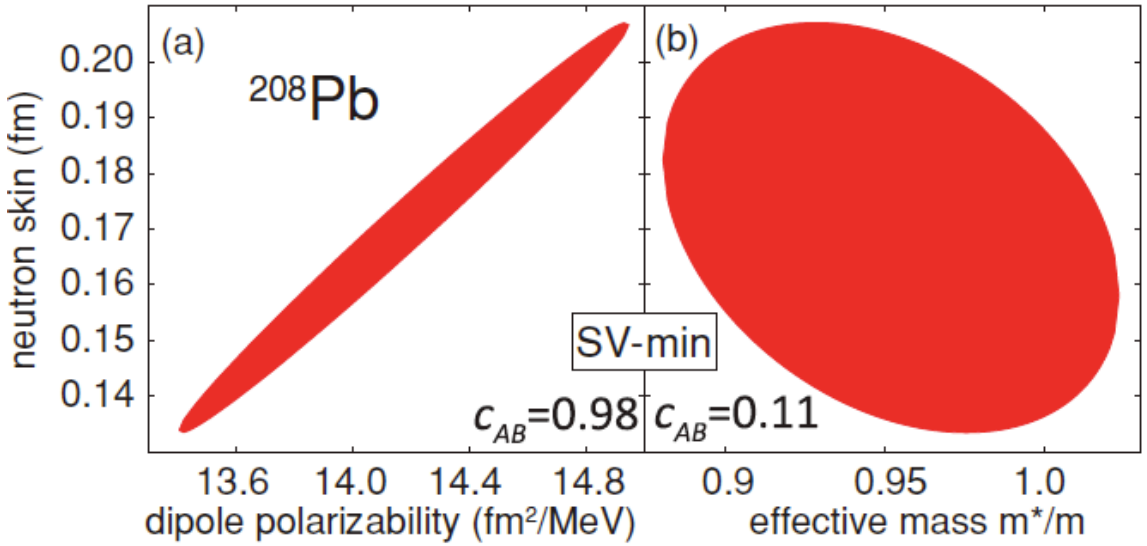


FIG. 10. (Color online) Sensitivity of the parameters of UNEDF0 to different data types entering χ^2. The EDF parameters are labeled as in Table VII.

← Sensitivity of parameters to changes in mass, proton radius, odd-even staggering [Kortelainen et al (2010)]

Correlation of observables within the model →
[Nazarewicz & Reinhard (2010)]

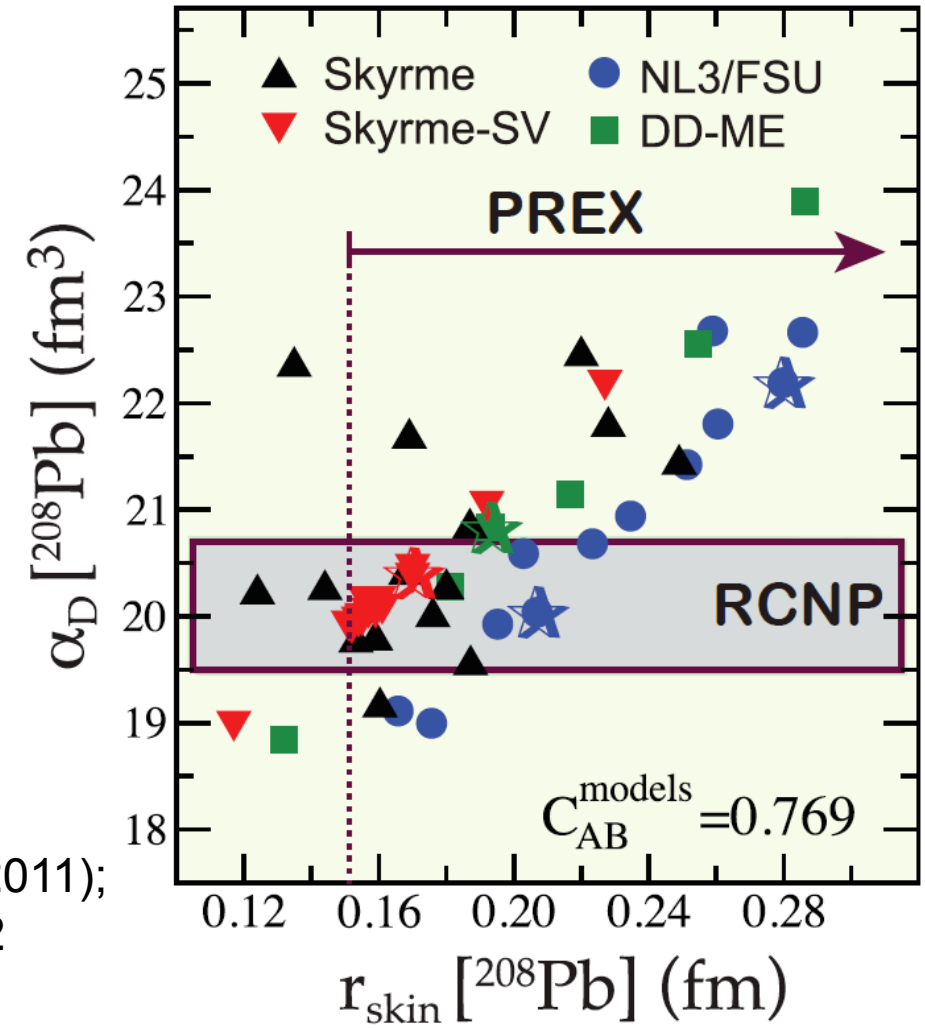


Dipole polarizability and neutron skin

$$\alpha_{\rm D} = \frac{8\pi}{9} e^2 \int_0^\infty \omega^{-1} R_{\rm E1}(\omega)\, d\omega$$

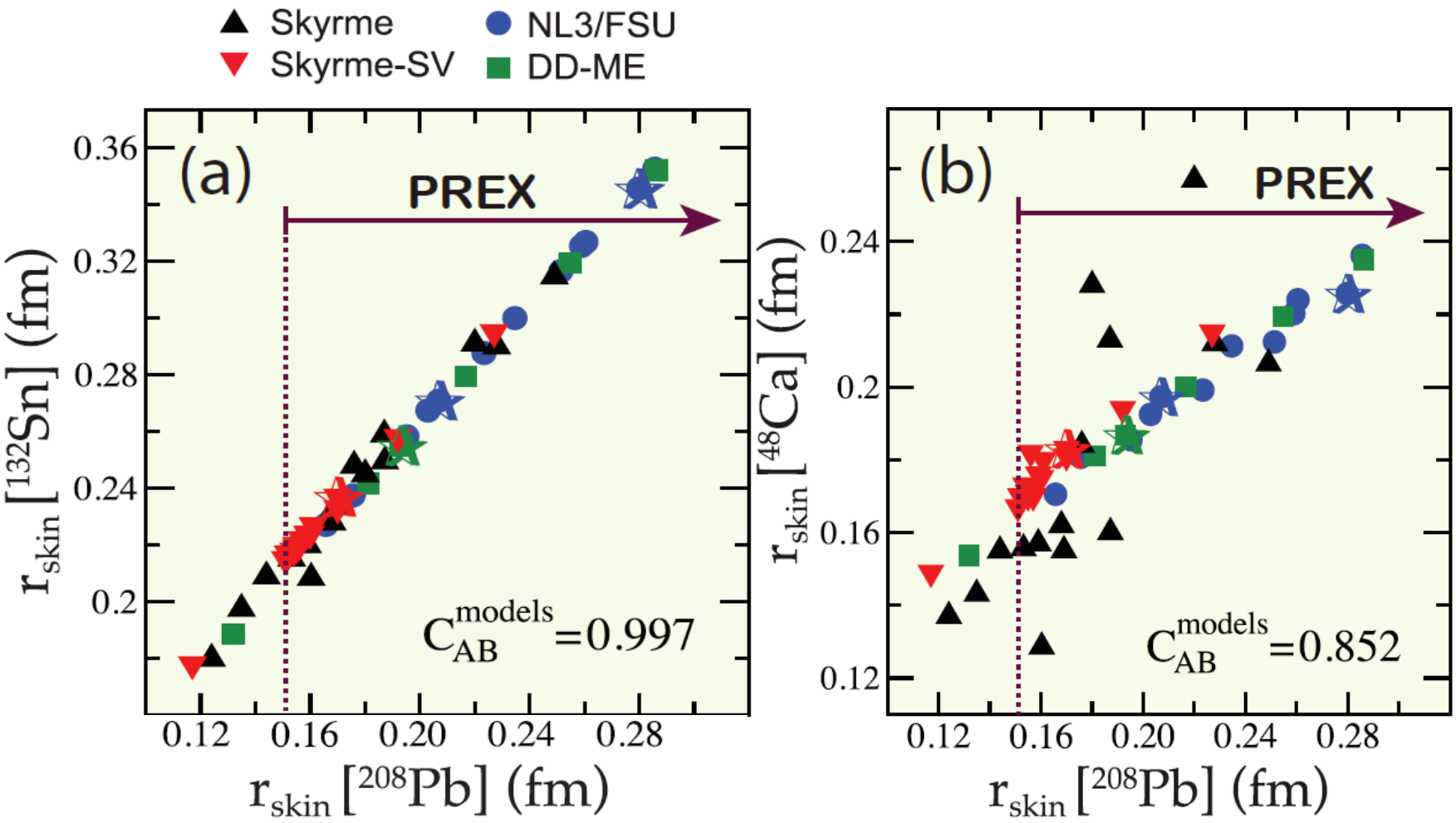
Correlations between observables based on an ensemble of ~18 functionals

$$C_{AB} = \frac{|\overline{\Delta A\, \Delta B}|}{\sqrt{\overline{\Delta A^2}\ \overline{\Delta B^2}}}$$



Tamii et al., Phys. Rev. Lett. 107, 062502 (2011); Piekarewicz et al., Phys. Rev. C 85, 041302 (2012)

Strong correlations between neutron skins in different nuclei

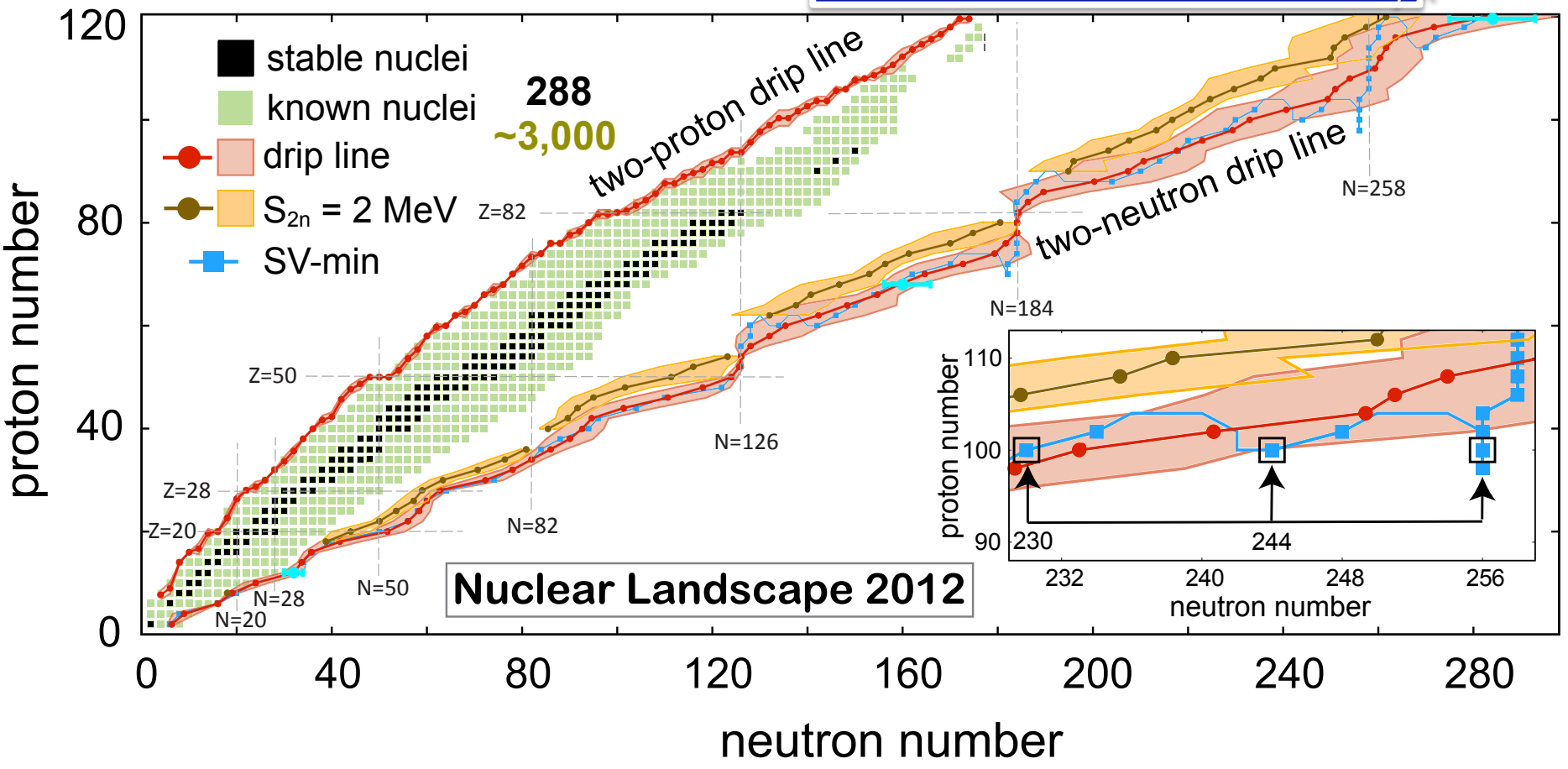


J. Piekarewicz et al., Phys. Rev. C 85, 041302(R) (2012)

How many atomic nuclei exist?

Literature: 5,000-12,000

Skyrme-DFT: 6,900±500$_{syst}$

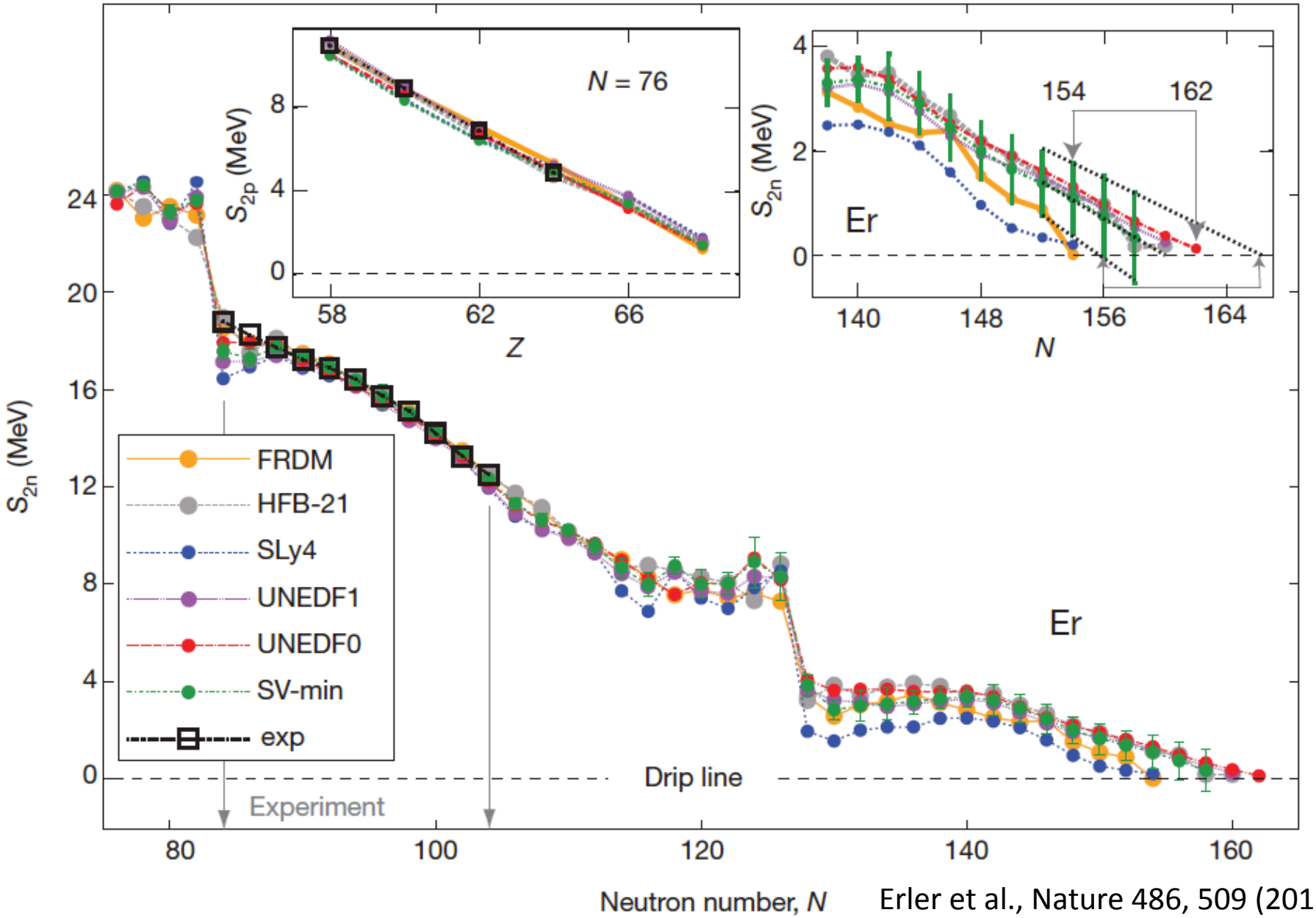


Models: SLy4, Svmin,UNEDF0, UNEDF1, FRDM and HFB-21

- Systematic errors (due to incorrect assumptions/poor modeling)
- Statistical errors (optimization and numerical errors)

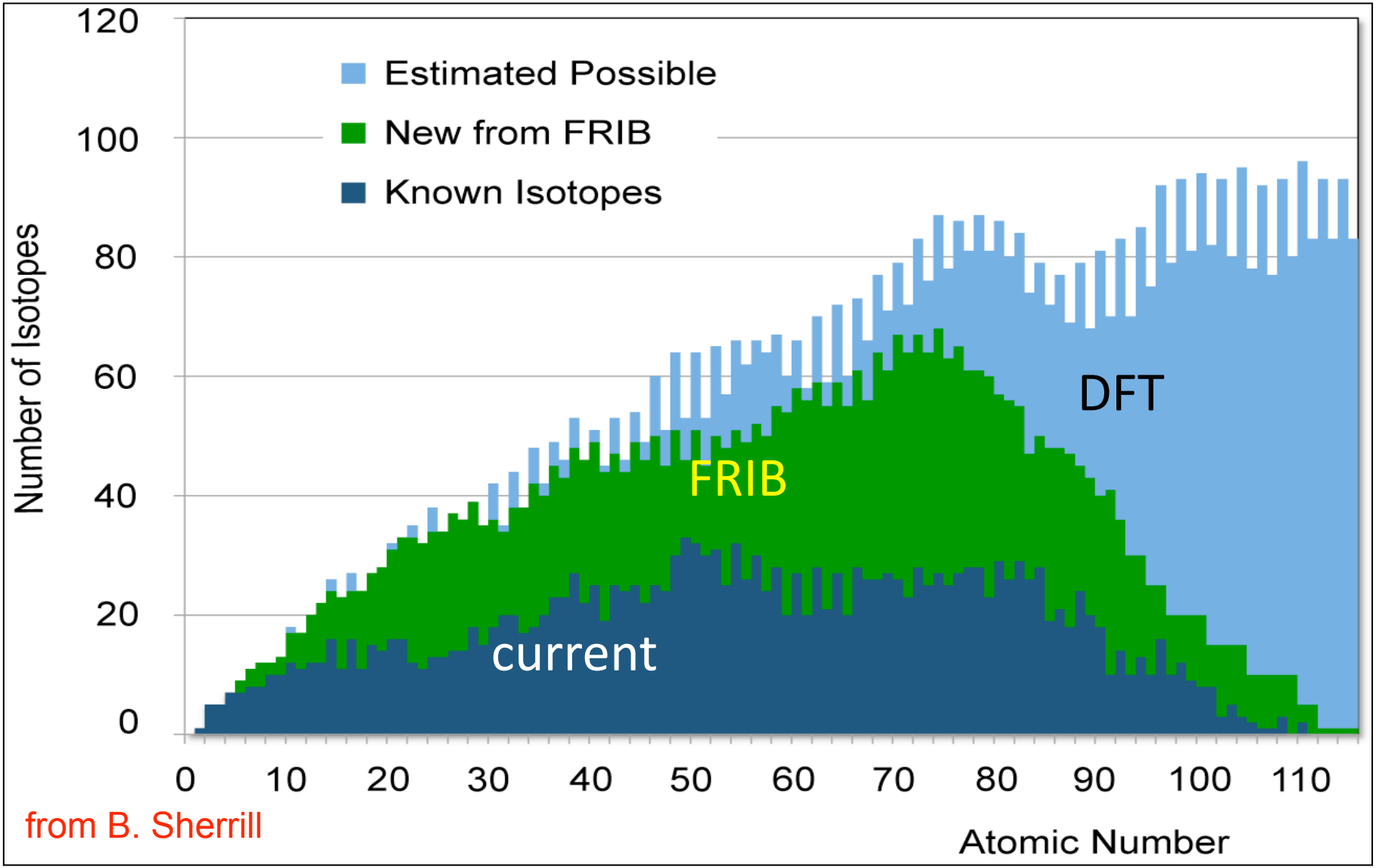
Erler et al., Nature 486, 509 (2012)

Separation energies illustrate challenges



Erler et al., Nature 486, 509 (2012)

How many nuclei can be produced?



NUCLEI

Nuclear Computational Low-Energy Initiative

- 15 institutions
- ~60 researchers
  - physics
  - computer science
  - applied mathematics
- foreign collaborators
- annual budget M$2+
- 5 years

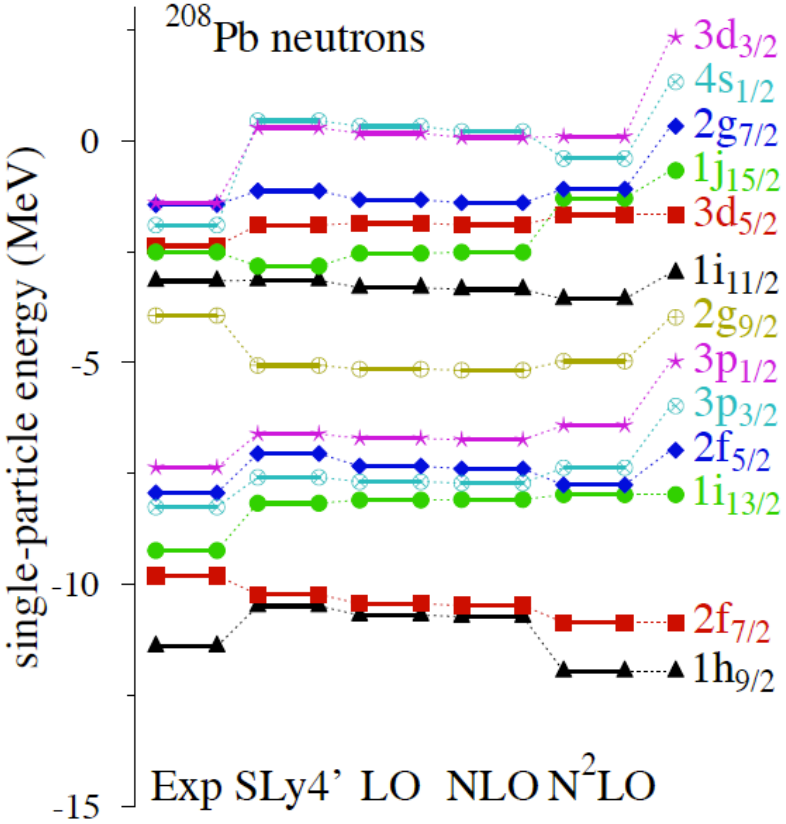
http://computingnuclei.org/

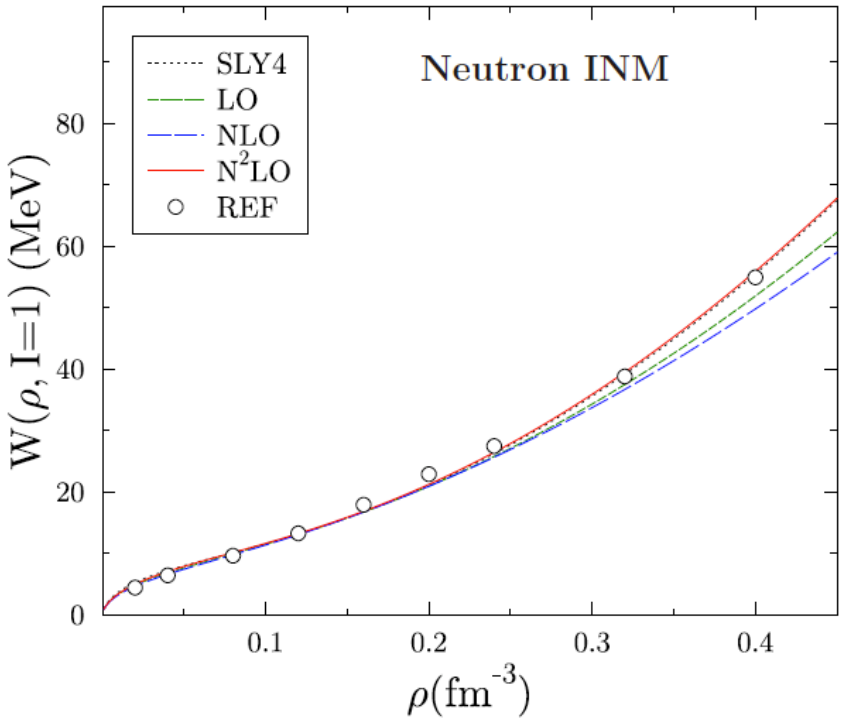
Theoretical improvements of the energy functional: density-matrix expansion using soft interactions

Basic idea:
Vautherin & Negele (1972)

$$\rho\left(\vec{R}+\frac{\vec{s}}{2},\vec{R}-\frac{\vec{s}}{2}\right)=\rho_{SL}(sk_F)\rho(\vec{R})+\frac{35}{2sk_F{}^3}\,j_3(sk_F)\left[\tfrac{1}{4}\nabla^2\rho(\vec{R})-\tau(\vec{R})+\tfrac{3}{5}\,k_F{}^2\rho(\vec{R})\right]$$

See also: Holt, Kaiser & Weise; Gebremariam, Duguet & Bogner; …





Stoitsov et al., Phys. Rev. C 82, 054307 (2010)

Summary

Self-consistent mean-field models

- Theoretical foundation within Kohn-Sham DFT.
- Applicable across nuclear chart.
- Phenomenological approach; fit to data.
- Yield impressive results (given their simplicity) in regions that entered the fit.
- Form of functional needs improvement to cover drip line physics
- Future theoretical and experimental advances for neutron-rich nuclei necessary.

Outlook

Enthusiastic and lively field

Moving towards a unified description of all atomic nuclei

Plenty of opportunities and challenges