Ab initio computations and effective theory for deformed nuclei

Thomas Papenbrock

The University of Tennessee and Oak Ridge National Laboratory

Gaute Hagen (Oak Ridge), Morten Hjorth-Jensen (Oslo), Øyvind Jensen (Bergen), Hai Ah Nam (Oak Ridge), David Pigg (Oak Ridge)

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- YITP program “Dynamics and Correlations in Exotic Nuclei” official JUSTIPEN activity, ~6 US participants partially supported
- JUSTIPEN now in its 6^{th} year, 70k$ annual budget
- Statistics for past three years:
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  - total of about 50 visits by ~30 individuals from 15 US institutions
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- Other programs (JUSEIPEN & FUSTIPEN [operating], CUSTIPEN [proposed]) modeled after JUSTIPEN

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Overview

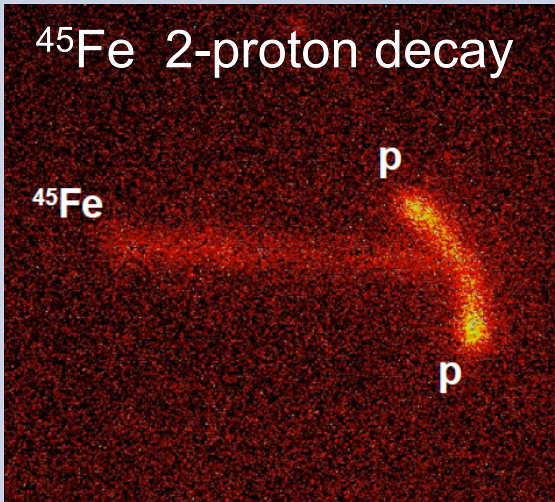
1. Introduction
2. Proton halo state in ^{17}F
3. Coupled-clusters as a similarity renormalization group transformation
4. Effective theory for deformed nuclei
5. Summary

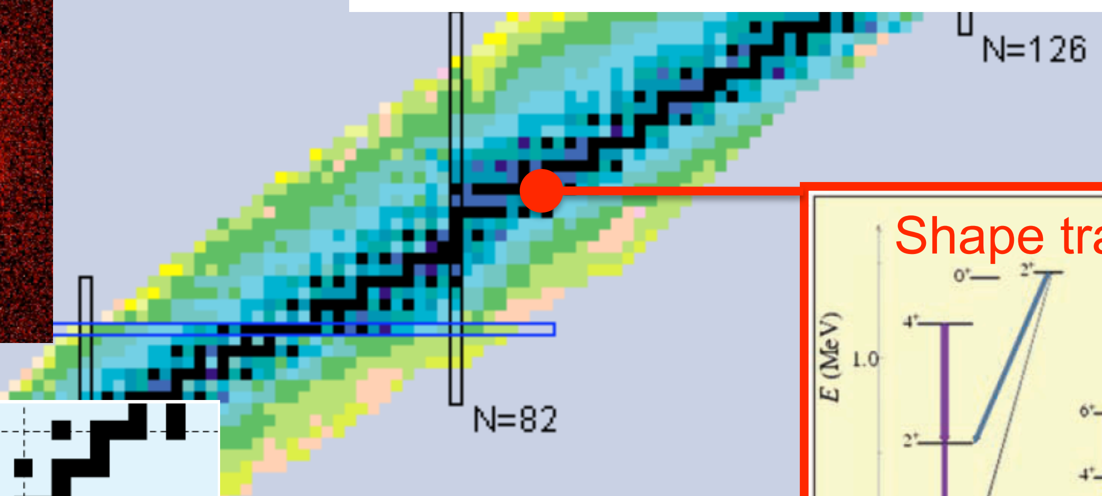
Nuclei across the chart

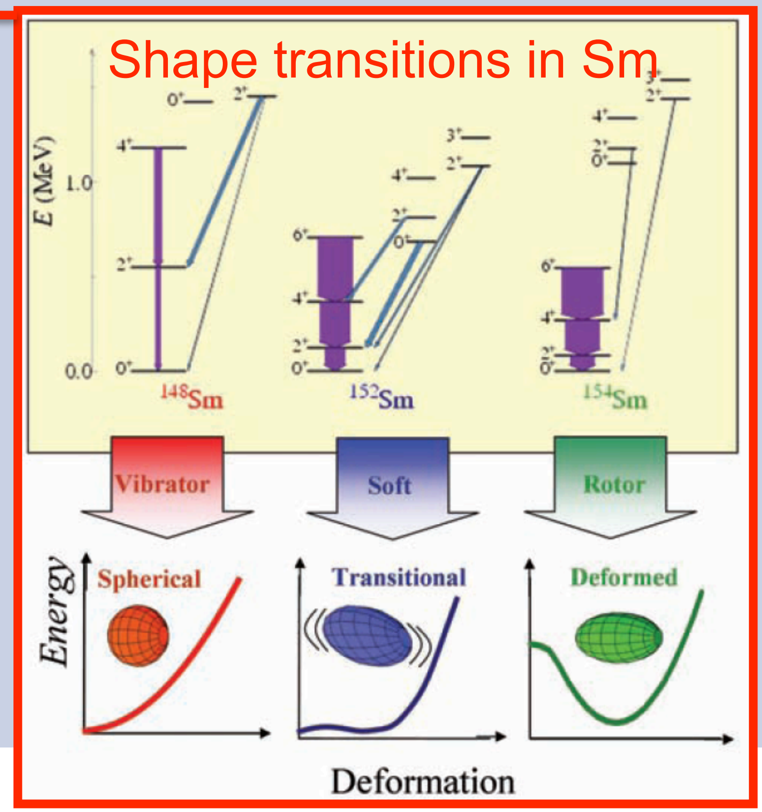
118 chemical elements (94 naturally found on Earth)
288 stable (primordial) isotopes

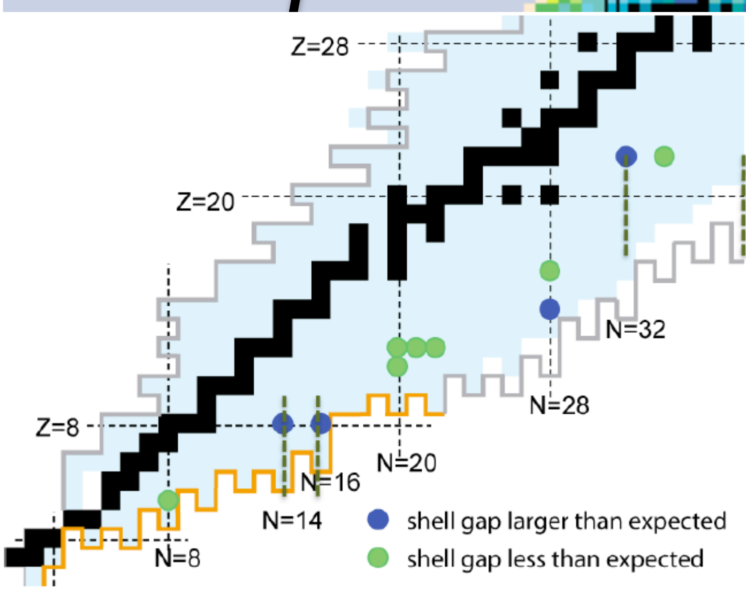
Thousands of short-lived isotopes – many with interesting properties

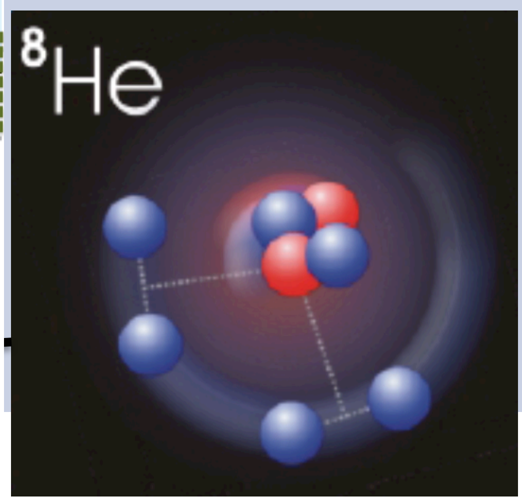
continuum effects relevant
novel clustering behavior
new aspects in evolution of structure



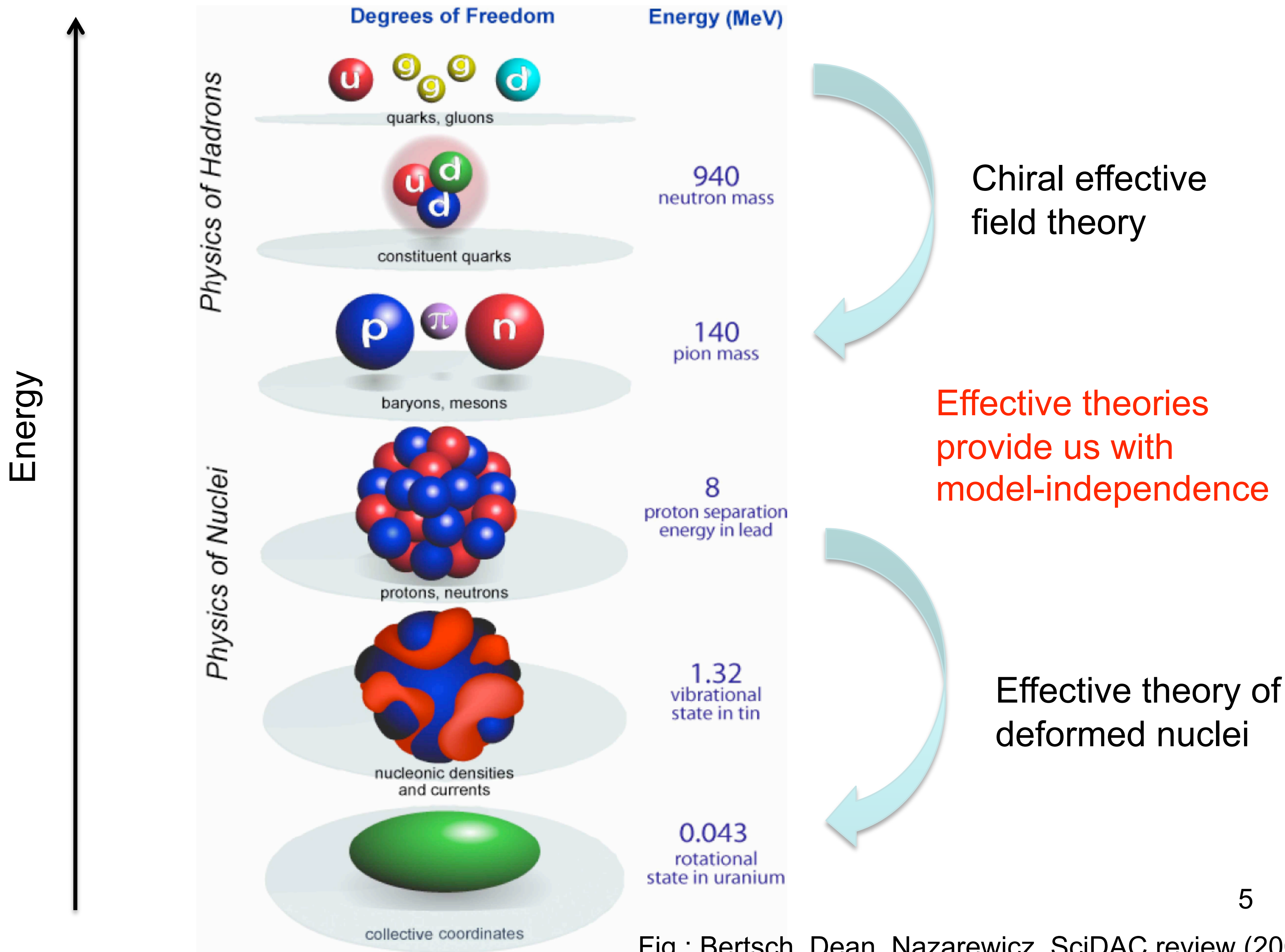








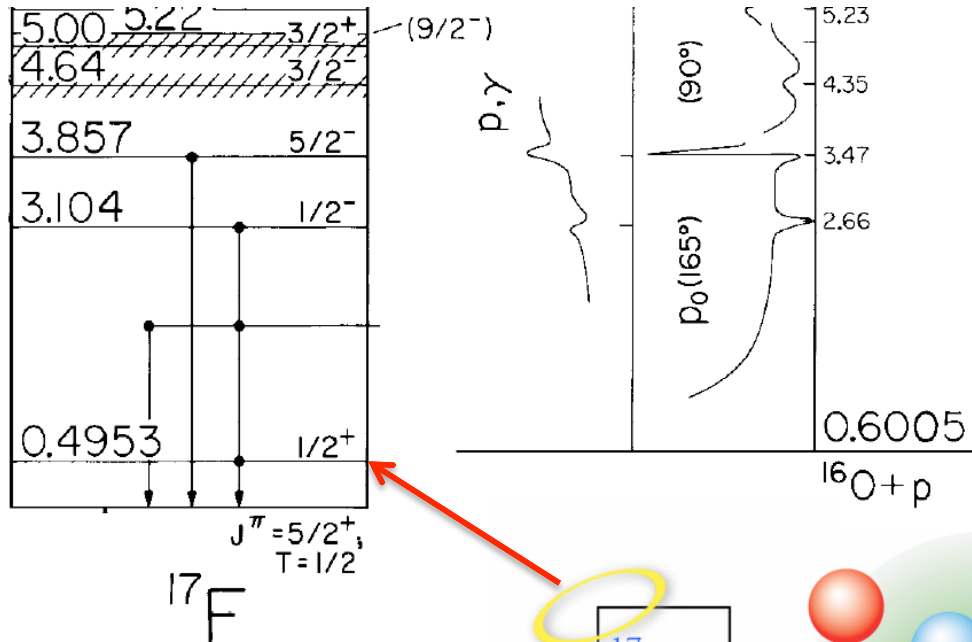
Energy scales and relevant degrees of freedom

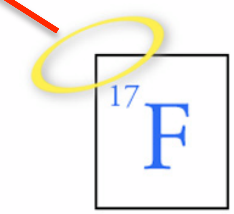


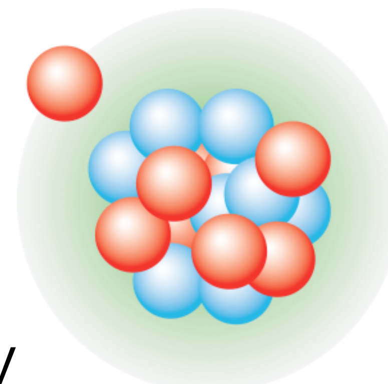
Effective theories provide us with model-independence

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

Ab initio description of proton-halo state in ^{17}F







- Separation energy of halo state is only 105 keV
- Continuum has to be treated properly
- Focus is on single-particle states
- Previous study: shell model in the continuum with ^{16}O core

[K. Bennaceur, N. Michel, F. Nowacki, J. Okolowicz, M. Ploszajczak, Phys. Lett. B 488, 75 (2000)]

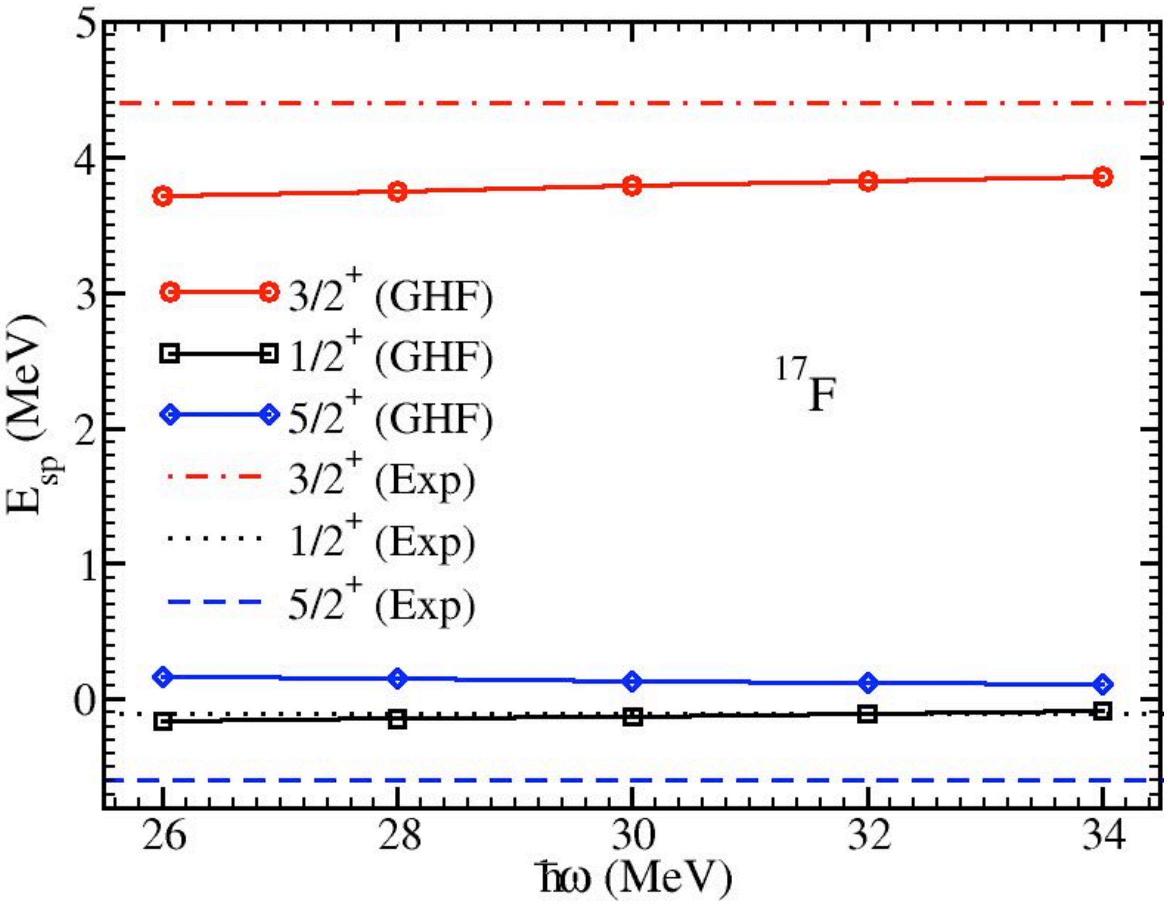
Bound states and resonances in ^{17}F

Single-particle basis consists of bound, resonance and scattering states

- Gamow basis for $s_{1/2}$ $d_{5/2}$ and $d_{3/2}$ single-particle states
- Harmonic oscillator states for other partial waves

Computation of single-particle states via “Equation-of-motion CCSD”

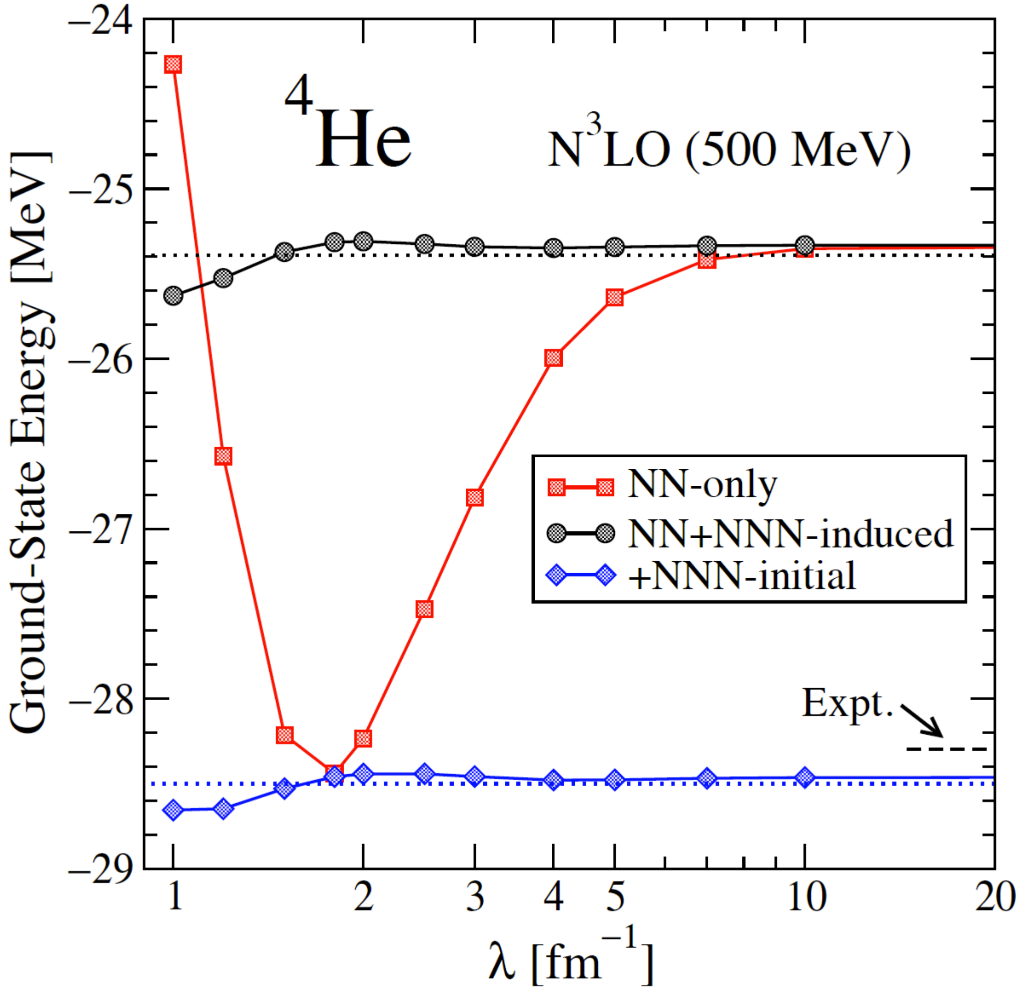
- Excitation operator acting on closed-shell reference
- Here: superposition of one-particle and 2p-1h excitations



- Gamow basis weakly dependent on oscillator frequency
- $d_{5/2}$ not bound; spin-orbit splitting too small
- $s_{1/2}$ proton halo state close to experiment

[G. Hagen, TP, M. Hjorth-Jensen, Phys. Rev. Lett. 104, 182501 (2010)]

Size of three-nucleon forces from variation of high-momentum (renormalization group)



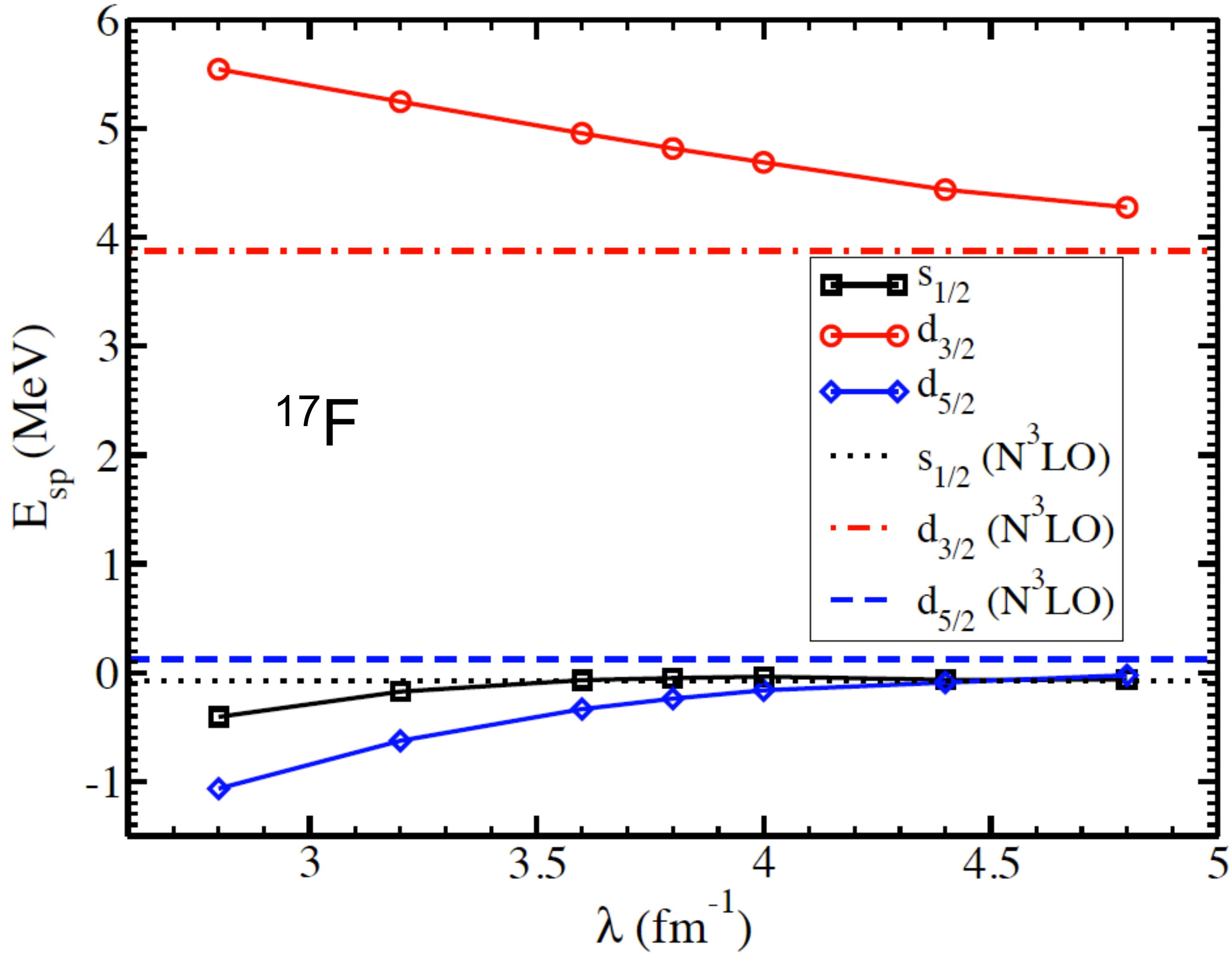
Similarity RG transformation [S.K. Bogner, R.J. Furnstahl, R.J. Perry, PRC 75, 061001(2007); Hergert & Roth 2007; Wegner 1994; Glazek & Wilson 1994]

- RG transformation of NN force induces NNN
- RG of NN and NNN almost independent of cutoff
- Small cutoff dependence → NNNN forces small

[Jurgenson, Navratil & Furnstahl, Phys. Rev. Lett. 103, 082501 (2009)]

Cutoff-dependence implies missing physics from short-ranged many-body forces.

Variation of cutoff probes omitted short-range forces



- Proton-halo state ($s_{1/2}$) only weakly sensitive to variation of cutoff
- Spin-orbit splitting increases with decreasing cutoff

[G. Hagen, TP, M. Hjorth-Jensen, Phys. Rev. Lett. 104, 182501 (2010)]

Time-dependent CC method

[Hoodbhoy & Negele 1978]

Imaginary-time propagation is a (non-unitary) SRG transformation

$$H(\tau) = e^{-S(\tau)} H e^{S(\tau)}$$

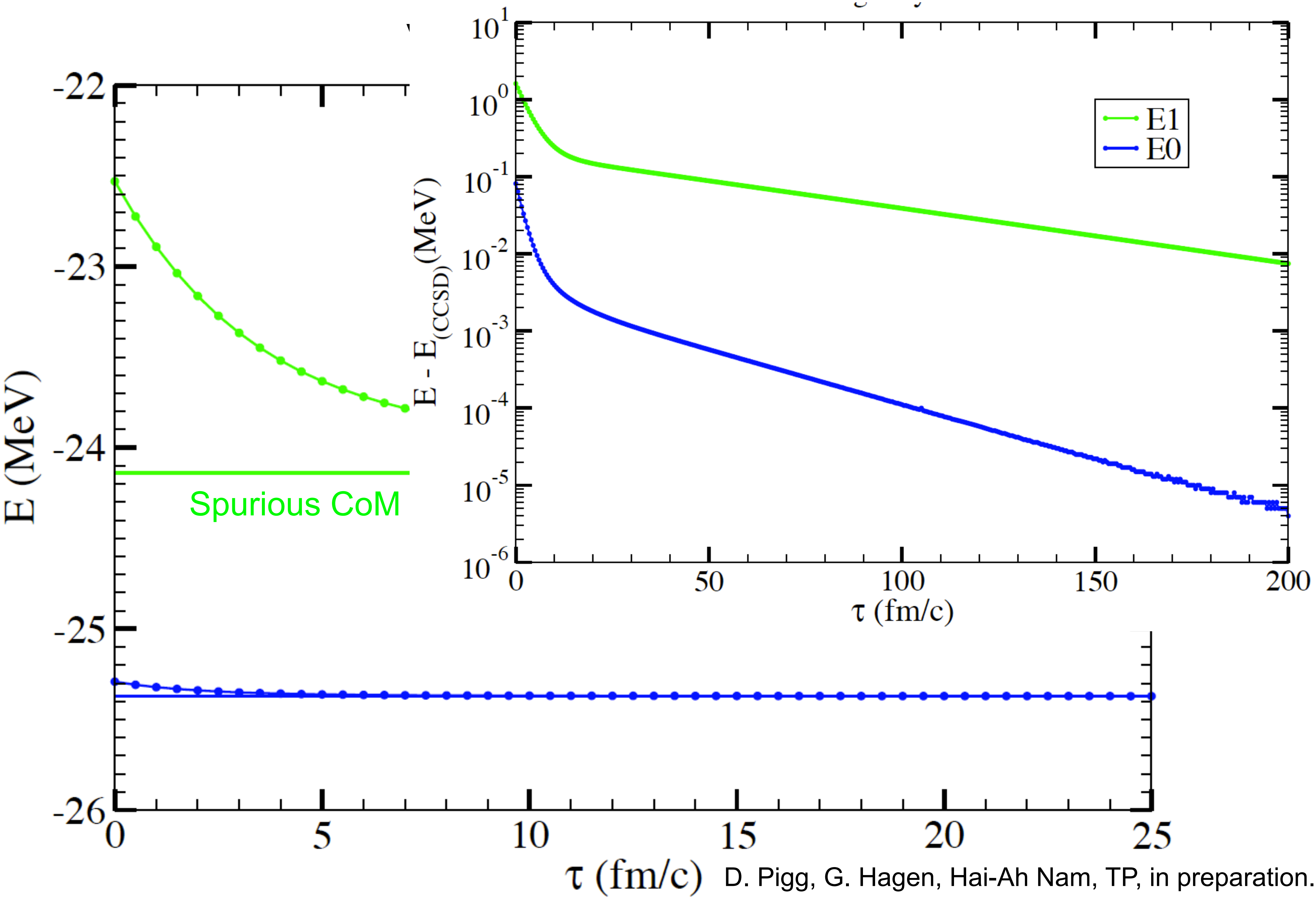
$$\partial_\tau H(\tau) = [H(\tau), \partial_\tau S]$$

Generator of this SRG:
1p-1h & 2p-2h excitations of the similarity-transformed Hamiltonian

$$\begin{aligned}
\partial_\tau s_0 &= -\langle\Phi| e^{-S} H e^S |\Phi\rangle \ , \\
\partial_\tau s_i^a &= -\langle\Phi_i^a| e^{-S} H e^S |\Phi\rangle \ , \\
\partial_\tau s_{ij}^{ab} &= -\langle\Phi_{ij}^{ab}| e^{-S} H e^S |\Phi\rangle
\end{aligned}$$

SRG: Glazek & Wilson 1993; Wegner 1994; Bogner, Furnstahl, Perry 2007; Tsukiyama, Bogner, Schwenk 2011.

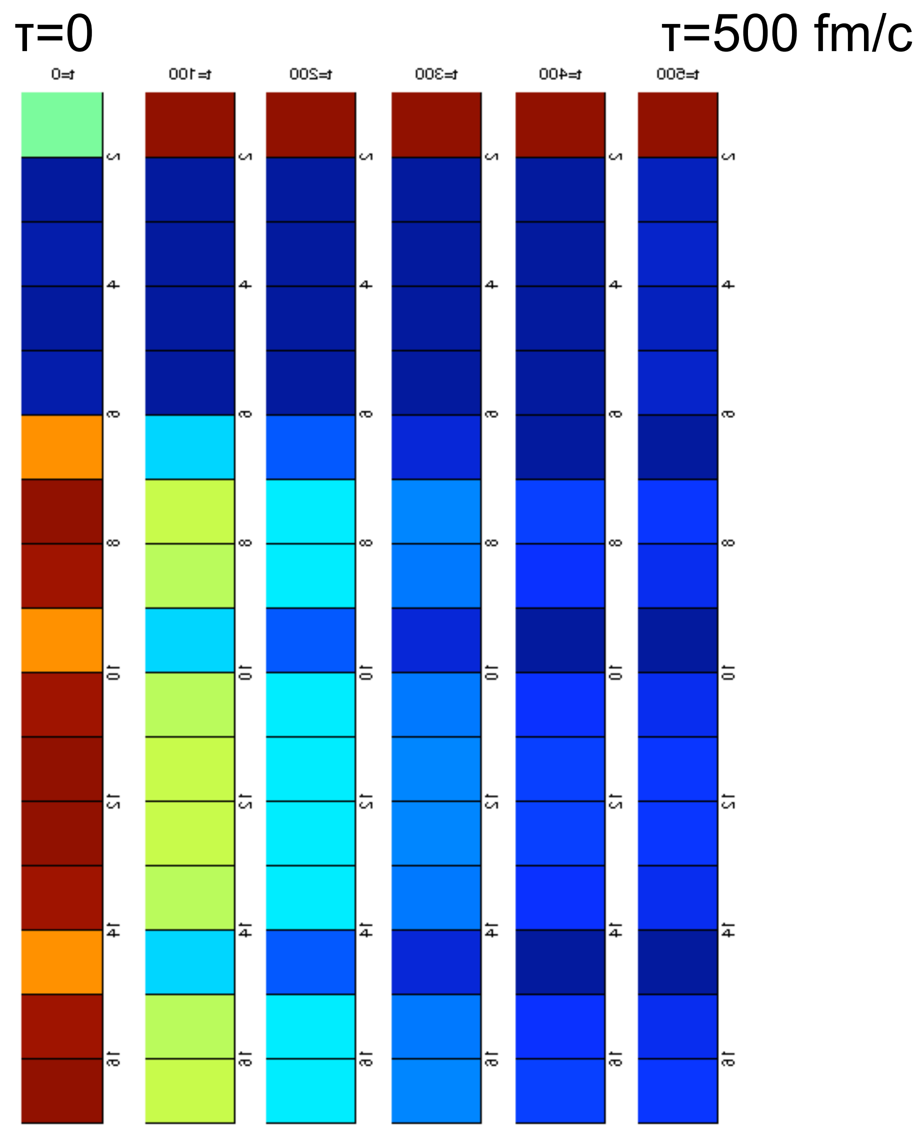
Imaginary time evolution



D. Pigg, G. Hagen, Hai-Ah Nam, TP, in preparation.

Imaginary time evolution as similarity renormalization group flow

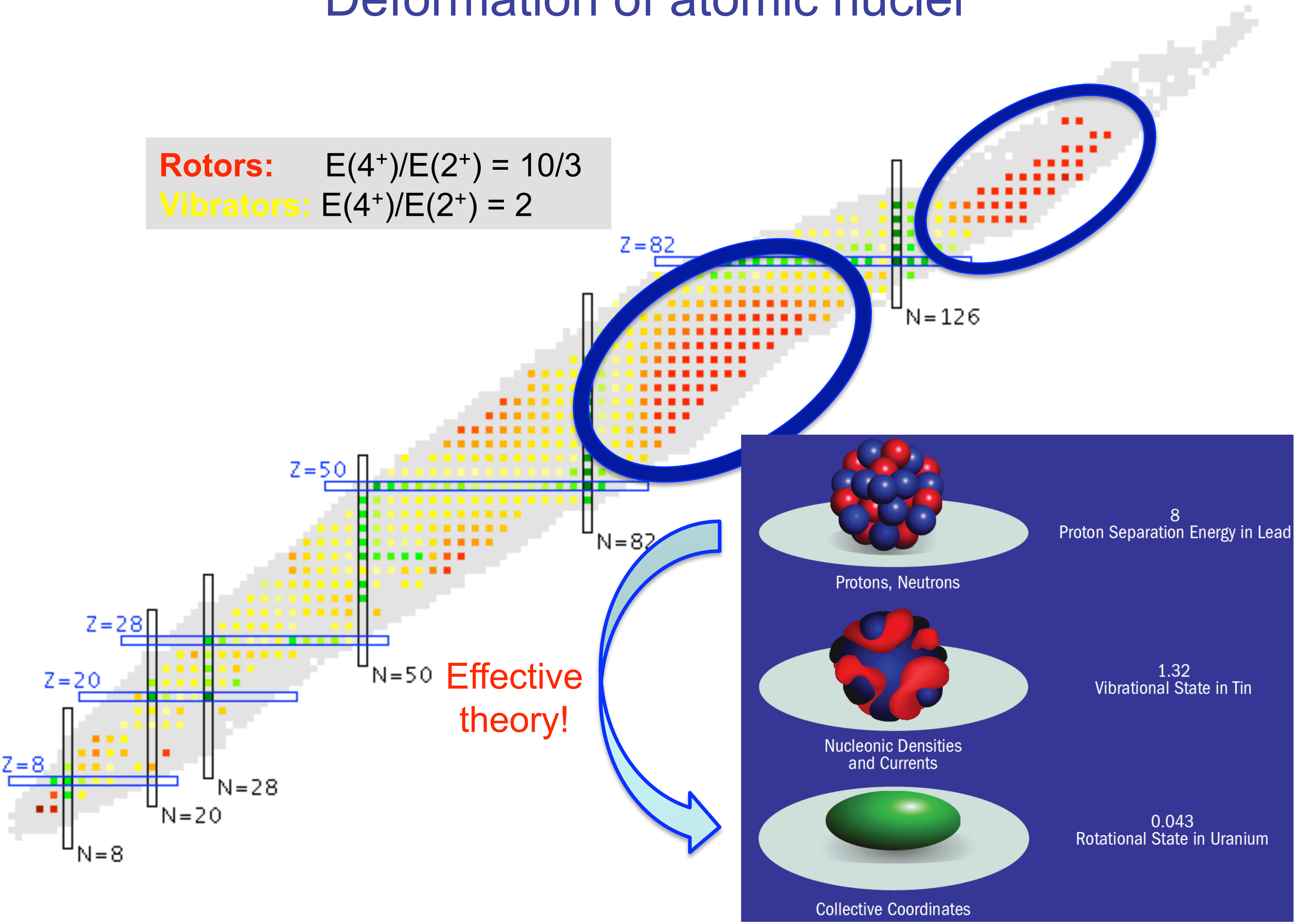
Evolution of first column of Hamiltonian matrix



Deformation of atomic nuclei

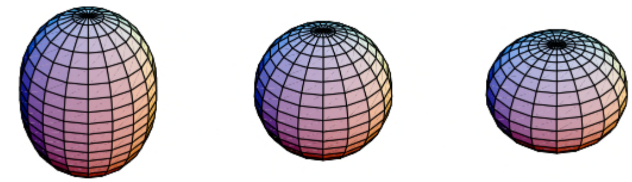
Rotors: E(4⁺)/E(2⁺) = 10/3

Vibrators: E(4⁺)/E(2⁺) = 2



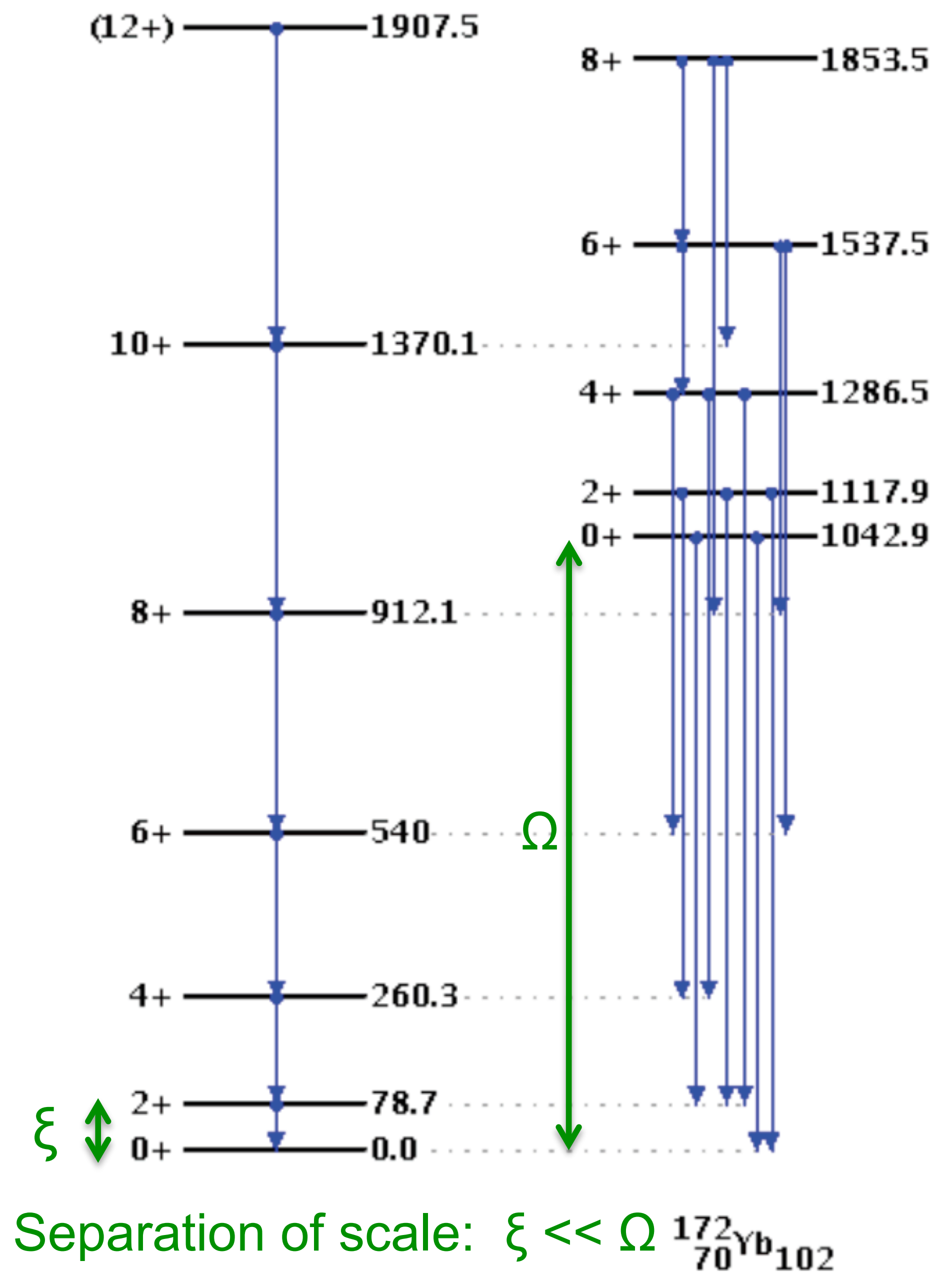
Effective theory!

Effective theory for deformed nuclei



Let us follow ideas by Weinberg, Leutwyler, …

1. Identify the relevant degrees of freedom for the resolution scale of interest:
   Quadrupole phonons
2. Identify the relevant symmetries of low-energy nuclear physics and investigate if and how they are broken:
   Spontaneously broken rotational symmetry
3. Construct the most general Lagrangian consistent with those symmetries and the symmetry breaking.
   Nonlinear realization of rotational symmetry
4. Design an organizational scheme (power counting) that can distinguish between more and less important contributions:
   Separation of scale between rotational and vibrational modes



Nonlinear realization of a symmetry – main idea

Nonlinear realization of (rotational) symmetry

Weinberg 1967; Coleman, Callan, Wess & Zumino 1969

Assume ground state is invariant only under rotations around the z-axis. Rotations of that state cannot be distinguished if they differ only by a rotation around the z-axis.
Nambu-Goldstone modes parameterize the coset SO(3)/SO(2) ~ S^2

Nambu-Goldstone modes:
Rotations that change the ground state:

$$\boxed{g(\alpha, \beta) = e^{-i\alpha \hat{J}_z} e^{-i\beta \hat{J}_y}}$$

Non-linear realization:
The angles α and β parameterize the two-sphere. Under rotations, they transform nonlinearly.

Effective theory – not an effective field theory:
The angles depend only on time $\alpha=\alpha(t)$, $\beta=\beta(t)$

Nonlinear realization of the rotational symmetry: Quantities with definite symmetry properties

1. E_x and E_y transform as the x and y-components of a vector under rotations.

$$\begin{aligned} E_x &= \dot{\alpha}\sin\beta \\ E_y &= -\dot{\beta} \end{aligned}$$

2. The "covariant derivative" D_t transforms as the z-component of a vector under rotations.

$$D_t \equiv \partial_t - iE_z J_z$$

$$E_z = -\dot{\alpha}\cos\beta$$

Any Lagrangian consisting of combinations of E_x, E_y, and D_t (acting on other fields) **that is formally invariant under SO(2)** (i.e. axially symmetric) **is indeed invariant under SO(3)**.

Weinberg (1967); Coleman, Wess, Zumino (1969); Callan, Coleman, Wess & Zumino (1969).
Pedagogical reviews: S. Weinberg, The Quantum Theory of Fields, Vol.II, chap. 19; C. P. Burgess, Physics Reports 330 (2000) 193; T. Brauner, arXiv:1001.5212.

Nambu-Goldstone modes

Lagrangian
$$L = \frac{C_0}{2}(\partial_t \vec{n}) \cdot (\partial_t \vec{n}) = \frac{C_0}{2}\left(\dot{\beta}^2 + \dot{\alpha}^2 \sin^2\beta\right)$$

Hamiltonian
$$\boxed{H = \frac{p_\beta^2}{2C_0} + \frac{p_\alpha^2}{2C_0 \sin^2\beta}}$$

Quantization
$$\begin{aligned} p_\beta^2 &= -\frac{1}{\sin\beta}\partial_\theta \sin\beta \partial_\beta \ , \\ p_\alpha &= -i\partial_\alpha \ . \end{aligned}$$

Spectrum
$$\boxed{\hat{H} Y_{lm}(\beta, \alpha) = \frac{l(l+1)}{2C_0} Y_{lm}(\beta, \alpha)}$$

Rotational bands are quantized Nambu-Goldstone modes.
Low-energy constant C_0 is moment of inertia and fit to data.

Nuclei with nonzero ground-state spins: Wess Zumino terms

A finite ground-state spin breaks time reversal invariance.
→ Consider terms that are first order in the time derivative
→ No such terms are invariant under rotations.
BUT: under rotations, E_z changes by a total derivative. Action remains essentially invariant (Wess-Zumino term)

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

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

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

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

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

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

Power counting and beyond leading order

Estimates
(naïve dimensional analysis)
$H_{LO} \sim \xi$

$$C_0 \sim \xi^{-1} ,$$
$$p_\beta \sim p_\alpha \sim q \sim \xi^0 ,$$
$$\dot\beta \sim \dot\alpha \sim E_{x,y,z} \sim \xi .$$

Lagrangian at NLO

$$L_{\rm NLO} = L_{\rm LO} + \frac{C_2}{4}\left(E_x^2 + E_y^2\right)^2$$

Power counting

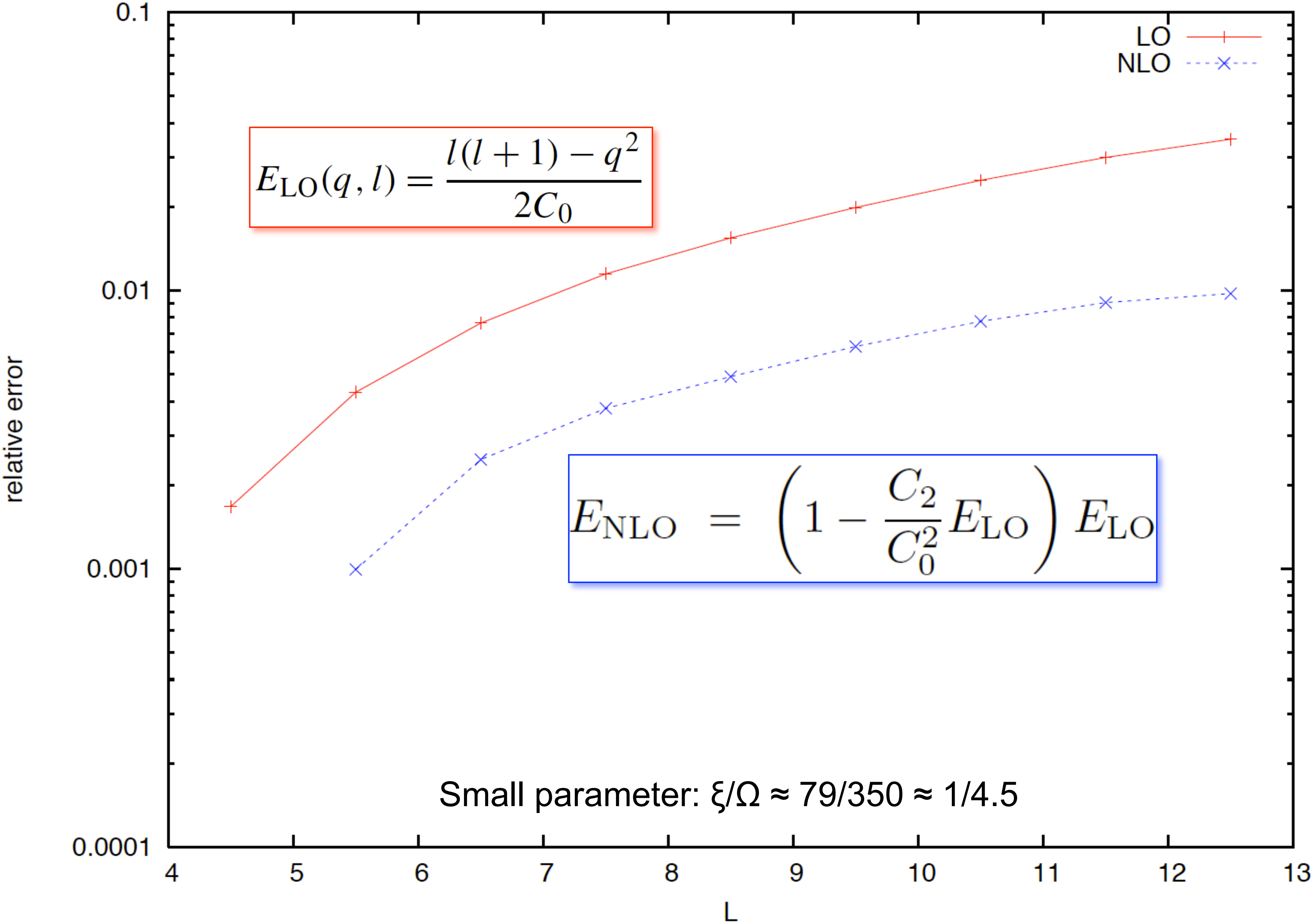
Main idea: higher-oder term due to neglected couplings between NG modes and vibrations. $[C_2/C_0]$= energy^{-2}

$$\frac{C_2}{C_0} \sim \Omega^{-2} \Longrightarrow \frac{C_2}{C_0}\left(E_x^2 + E_y^2\right) \sim \left(\frac{\xi}{\Omega}\right)^2 \ll 1$$

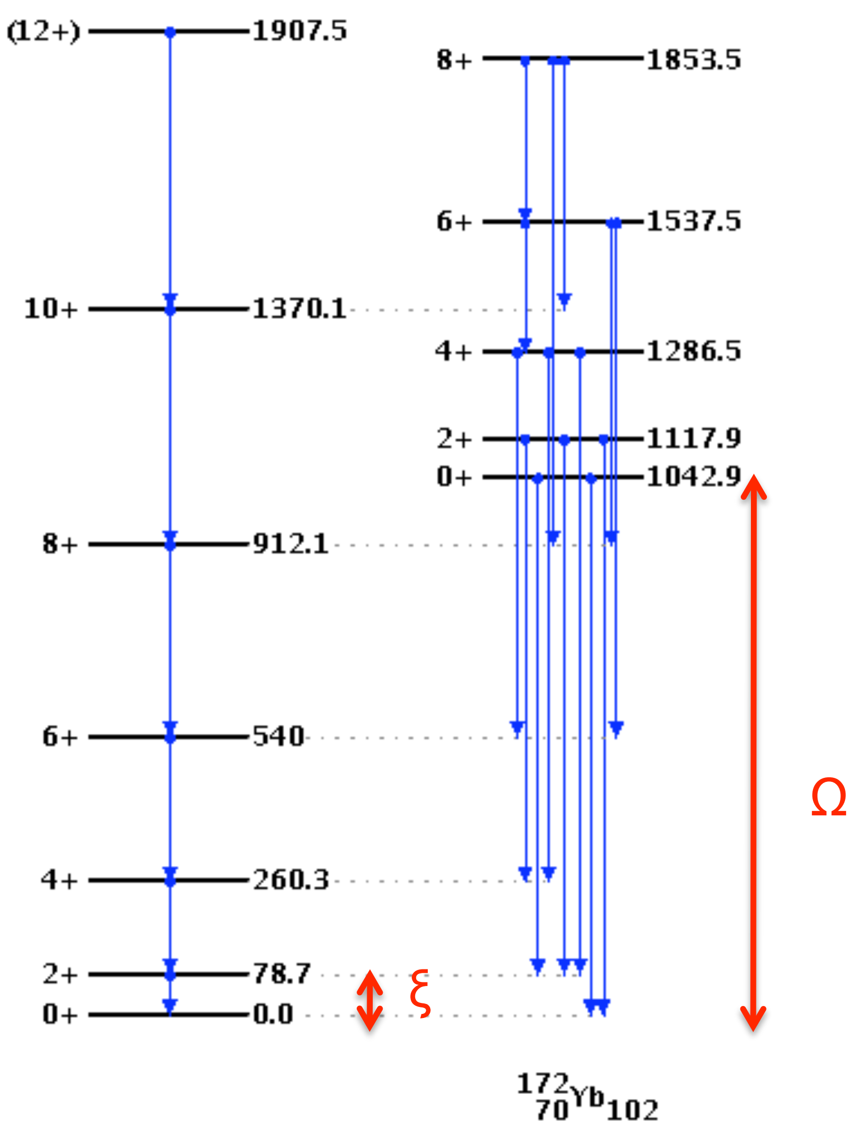
Spectrum: $AL(L+1) + B(L(L+1))^2$ for even-even nuclei. (Bohr & Mottelson)
In general:

$$\boxed{E_{\rm NLO} = \left(1 - \frac{C_2}{C_0^2} E_{\rm LO}\right) E_{\rm LO}}$$

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



Beyond NG modes: coupling to vibrations



Higher energetic degrees of freedom need to be included.

Quadrupole field exhibits spontaneous symmetry breaking.

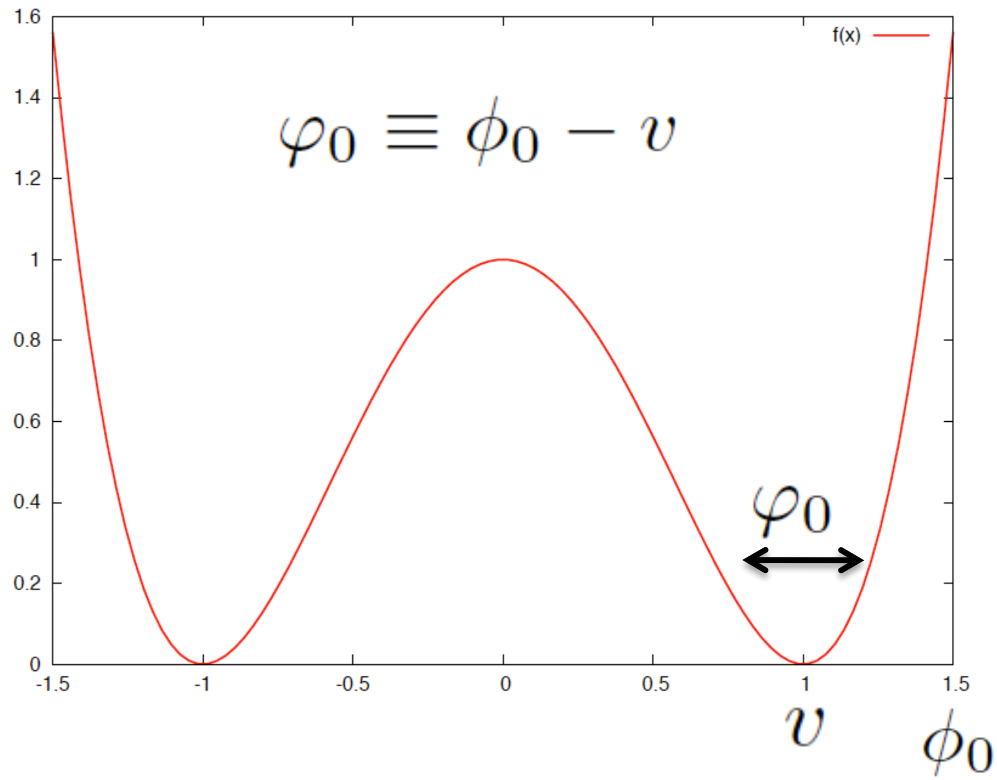
→5 DoF – 2NG = 3DoF

$$\phi = \begin{pmatrix} \phi_2 \\ 0 \\ \phi_0 \\ 0 \\ \phi_2^* \end{pmatrix}$$

Separation of scale: ξ << Ω

Couplings to vibrations: power counting

Low energy scale ξ
High energy scale Ω>>ξ



Dimensional analysis

$$
\begin{aligned}
v \sim \phi_0 &\sim \xi^{-1/2}\,, \\
\varphi_0 \sim \phi_2 &\sim \Omega^{-1/2}\,, \\
\dot\varphi_0 = \dot\phi_0 \sim \dot\phi_2 &\sim \Omega^{1/2}\,.
\end{aligned}
$$

Potential expanded around miniumum

$$V_2(\phi) = \frac{\omega_0^2}{2}(\phi_0 - v)^2 + \frac{\omega_2^2}{4}|\phi_2|^2$$

$$V = V_2 + \sum_{k+2l>2} v_{kl}\varphi_0^k|\phi_2|^{2l}$$

Power counting: large amplitudes φ_0≈ v restore rotational symmetry → breakdown of EFT

$$v_{kl}\varphi_0^k|\phi_2|^{2l} \sim \Omega\left(\frac{\xi}{\Omega}\right)^{l-1+k/2}$$

Main results: effective theory for deformed nuclei

[TP, Nucl. Phys. A 852, 36 (2011)]

• Odd-mass and odd-odd nuclei on equal footing with even-even nuclei

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

• Bohr Hamiltonian / general collective model recovered in next-to-leading order

$$\begin{aligned} E(n_0,n_2,m_l,l) &= \omega_0\left(n_0+\frac{1}{2}\right)+\frac{\omega_2}{2}(2n_2+|m_l|+1) \\ &+ \frac{1}{6v^2}\left(l(l+1)-(2m_l)^2\right) \end{aligned}$$

• **Novel terms** in Hamiltonian seen at next-to-next-to leading order

• Field-theoretical formulation under way.
• **First insights**: vibrations are true NG-modes (compare w/ spin waves); quantized rotations from finite system (no spontaneous symmetry breaking)
[TP and H. A. Weidenmüller, work in progress]

Summary & Outlook

- Model independent description of atomic nuclei under way!
- Inclusion of continuum effects → merger of structure and reactions; essential for computation of fragile halo states and weakly-bound nuclei
- Coupled-cluster method (imaginary time evolution) is a SRG
- Effective theory for deformed nuclei under development; treats nuclei with finite ground-state spins on same footing as even-even nuclei

Leading order ~O(Ω)

Lagrangian at leading order:

$$L_{\mathrm{LO}} = \frac{1}{2}\dot{\varphi_0}^2 + |\dot{\phi}_2|^2 - \frac{\omega_0^2}{2}\varphi_0^2 - \frac{\omega_2^2}{4}|\phi_2|^2$$

$$H_{\mathrm{LO}} = \frac{1}{2}p_0^2 + \frac{1}{4}\left(p_{2r}^2 + p_{2i}^2\right) + \frac{\omega_0^2}{2}\varphi_0^2 + \frac{\omega_2^2}{4}\left(\phi_{2r}^2 + \phi_{2i}^2\right)$$

Spectrum

$$E(n_0, n_2, m_l) = \omega_0\left(n_0 + \frac{1}{2}\right) + \frac{\omega_2}{2}(2n_2 + |m_l| + 1)$$

Leading order yields the band heads

Lagrangian as function of E_x, E_y, $D_t\varphi_0$, $D_t\phi_2$, φ_0, ϕ_2, needs to be formally invariant under SO(2) (axial symmetry only).

Next-to-leading order ~O(ξ)

Lagrangian
$$L_{\rm NLO} = L_{\rm LO} + \frac{3}{2}v^2\left(E_x^2 + E_y^2\right) - 4E_z {\rm Im}\left(\dot{\phi}_2\phi_2^*\right) - \sum_{k+2l=3,4} v_{kl}\varphi_0^k|\phi_2|^{2l} \,.$$

Hamiltonian (kinetic energy)

$$H_{\rm NLO} = H_{\rm LO} + \frac{1}{6v^2}\left(p_\beta^2 + \frac{1}{\sin^2\beta}\left[p_\alpha^2 + 2p_\alpha l_z\cos\beta\right]\right)$$

Spectrum: a rotational band on every vibrational band head

$$\boxed{\begin{aligned} E(n_0,n_2,m_l,l) \;=\; & \omega_0\left(n_0+\frac{1}{2}\right) + \frac{\omega_2}{2}\left(2n_2+|m_l|+1\right) \\ & + \frac{1}{6v^2}\left(l(l+1)-(2m_l)^2\right) \end{aligned}}$$

Corrections ~ξ of band heads due to anharmonicities in the potential neglected.

In next-to-leading order, the results of the rotational-vibrational model are reproduced.