Computations of medium-mass nuclei, nuclear interactions and saturation

Thomas Papenbrock

and Oak Ridge National Laboratory

Reactions and Structure of Exotic Nuclei

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Menu

- Development of interactions from chiral effective field theory

with A. Ekström, B. Carlsson, C. Forssén, G. Hagen, M. Hjorth-Jensen, G. R. Jansen, P. Navrátil, W. Nazarewicz, K. Wendt

- Extrapolations in finite model spaces

with R. J. Furnstahl, G. Hagen, Sushant More, K. Wendt

- Effective (field) theory for deformed nuclei

with E. A. (Toño) Coello Pérez and H. A. Weidenmüller

Energy scales and relevant degrees of freedom

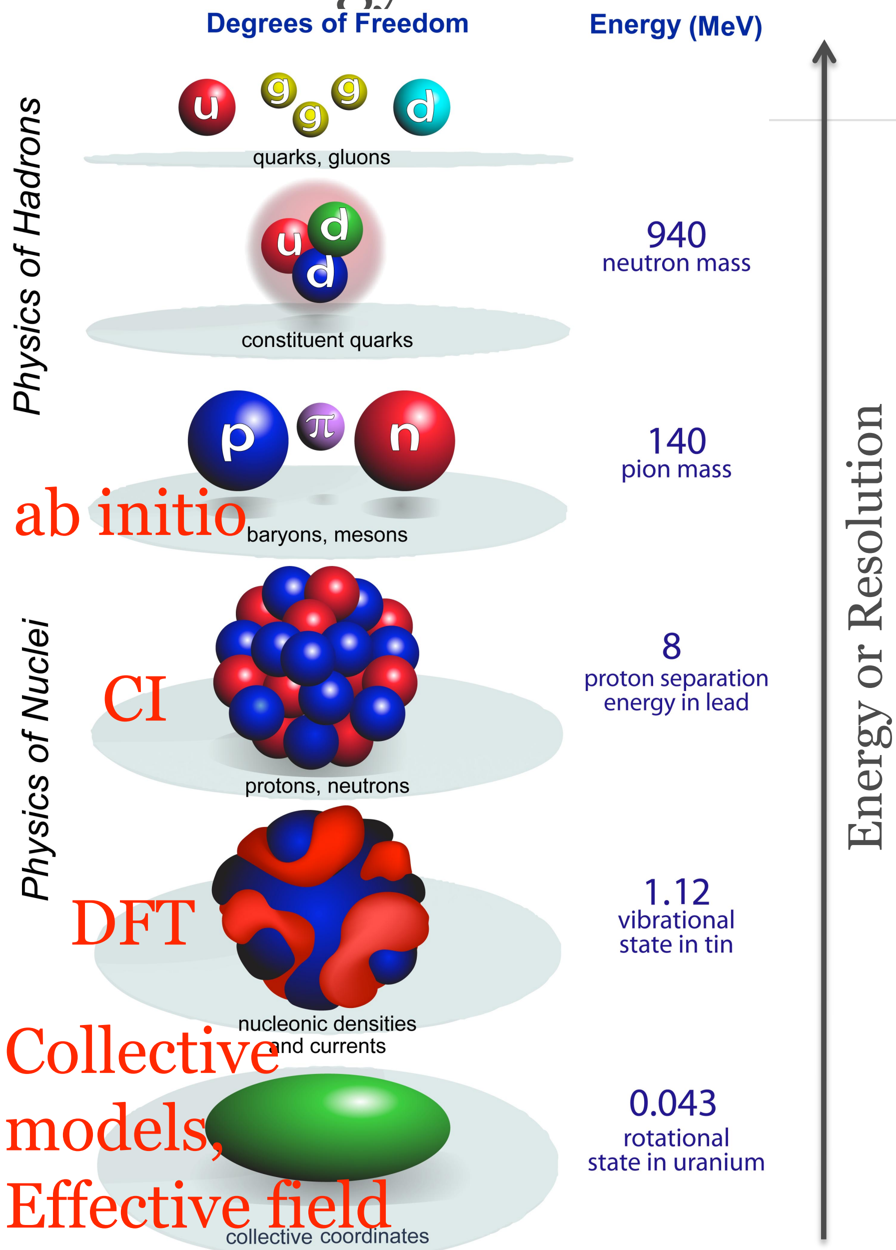

Fig.: Bertsch, Dean, Nazarewicz, SciDAC review (2007)

Chiral symmetry is broken

Pion is Nambu-Goldstone boson

Tool: Chiral effective field

Effective theories provide us with model independent approaches to atomic nuclei

Key: Separation of scales

Rotations are low lying degrees of freedom

Tool: Effective field theory for deformed nuclei

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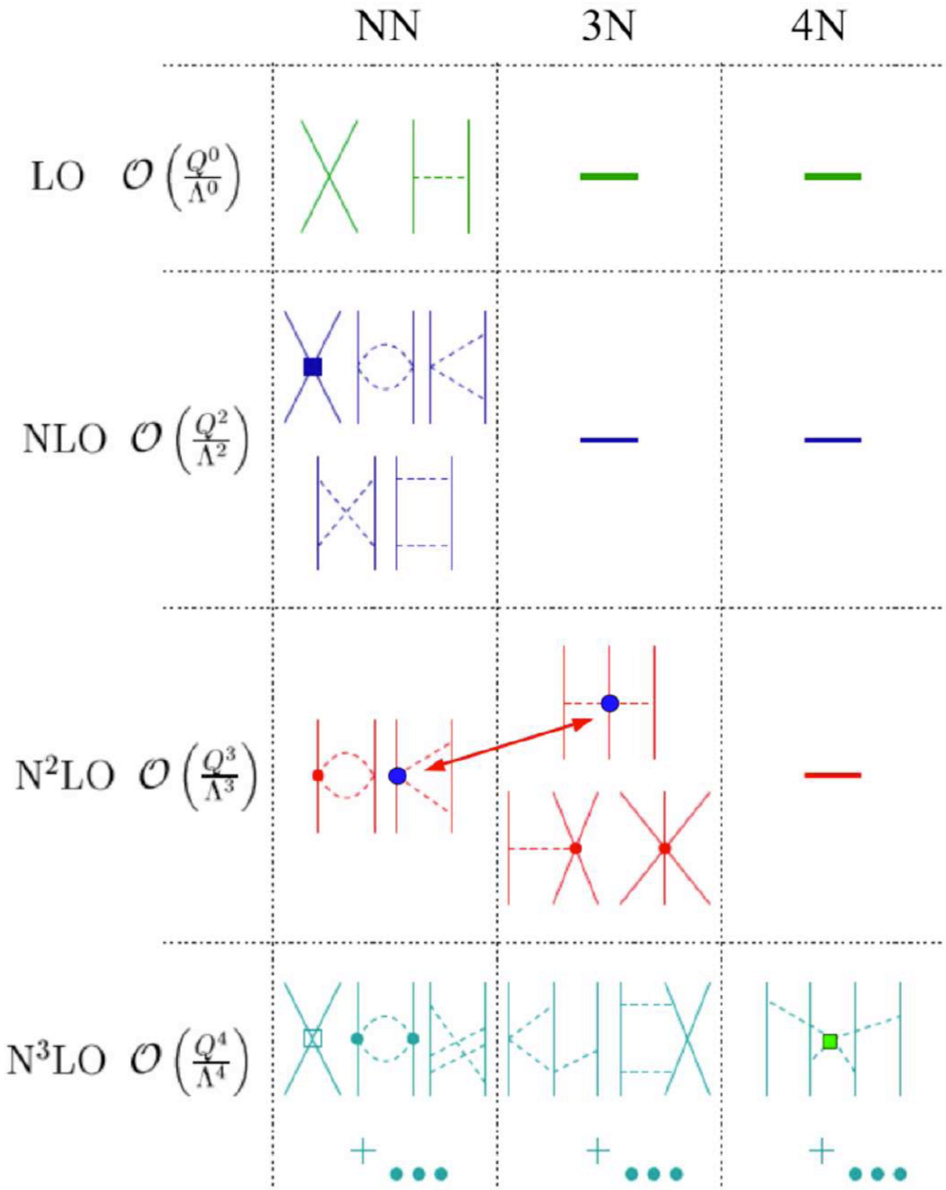
Nuclear forces from chiral effective field theory

[Weinberg; van Kolck; Epelbaum, Gloeckle, Meissner; Entem & Machleidt; …]



Usual approach to interaction

- Subsequent optimization of *NN* force and *NNN* forces
- Low energy constants from fit of *NN* data, A=3,4 nuclei.

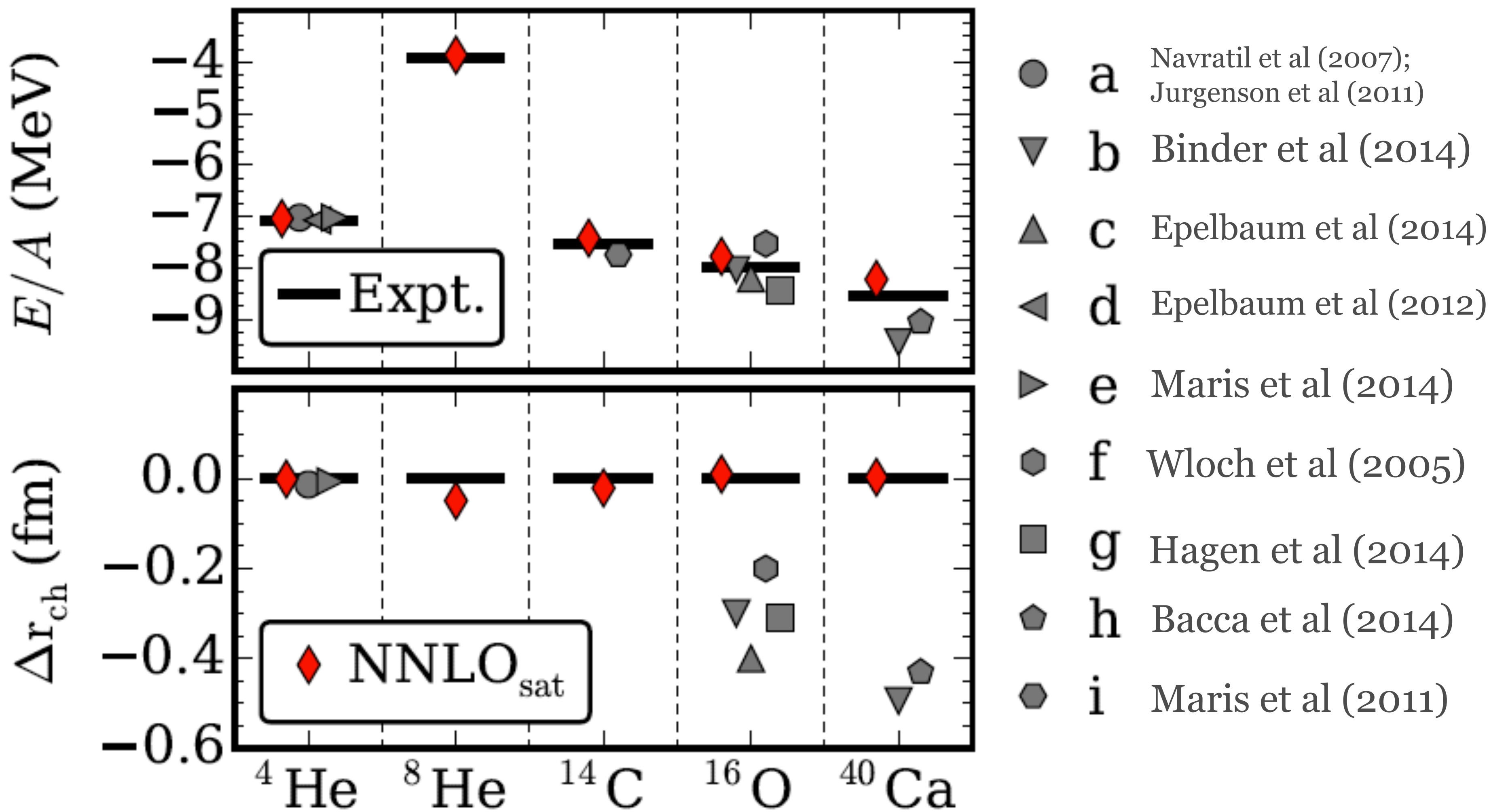
Many-body solvers

Over the past decade, frontier pushed to medium-mass nuclei (Coupled clusters, Green's functions, Gorkov method, In-Medium SRG, Lattice EFT, …)

Result

Interactions from chiral EFT exhibit deficient saturation properties. This limits meaningful computations in medium-mass nuclei.

Chiral interactions fail to saturate accurately: too much binding and too small radii



A. Ekström, G. Jansen, K. Wendt et al, arXiv:1502.04682 (2015)

Chiral interaction NNLO_{sat}

- Simultaneous optimization of *NN* and *NNN* forces at NNLO
- Optimization includes (Λ=450 MeV, nonlocal regulators)
  - nucleon-nucleon scattering data (up to 35 MeV laboratory energy)
  - binding energies and radii of ^{2}H, ^{3}H, ^{3}He, ^{4}He, ^{14}C, ^{16}O
  - ground-state energies of ^{22,24,25}O

TABLE I. The values of the LECs for the NNLO_{sat} interaction. The c_i, $\tilde{C}_i$, and C_i are in units of GeV^{-1}, 10^4 GeV^{-2}, and 10^4 GeV^{-4}, respectively.

LEC	Value	LEC	Value	LEC	Value
c_1	-1.12	c_3	-3.93	c_4	3.77
$\tilde{C}^{pp}_{^1S_0}$	-0.16	$\tilde{C}^{np}_{^1S_0}$	-0.16	$\tilde{C}^{nn}_{^1S_0}$	-0.16
$C_{^1S_0}$	2.54	$C_{^3S_1}$	1.00	$\tilde{C}_{^3S_1}$	-0.18
$C_{^1P_1}$	0.56	$C_{^3P_0}$	1.40	$C_{^3P_1}$	-1.14
$C_{^3S_1-^3D_1}$	0.60	$C_{^3P_2}$	-0.80	c_D	0.82
c_E	-0.04				

Low-energy coefficients within range of other chiral interactions.

A. Ekström, G. Jansen, K. Wendt et al, arXiv:1502.04682 (2015)

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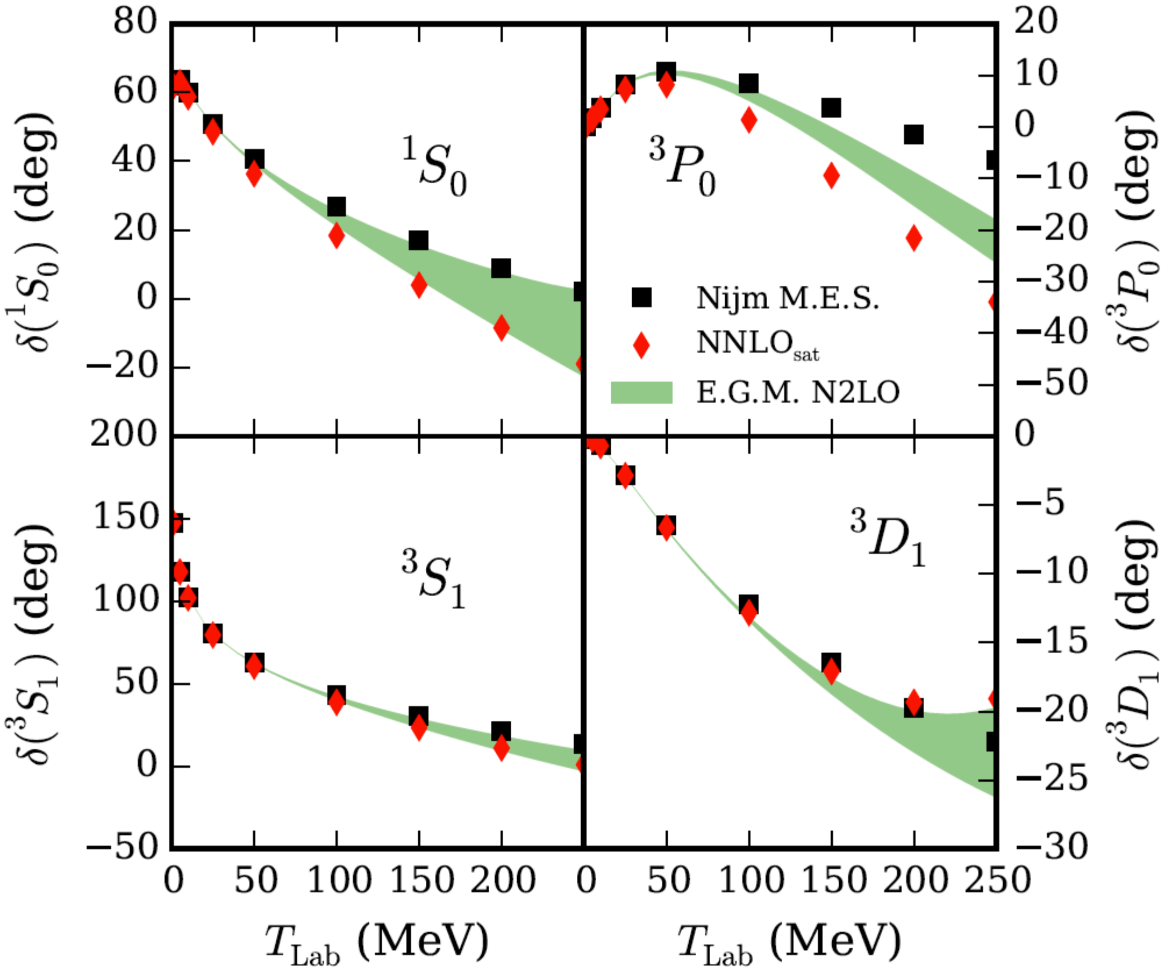
Results in *NN* sector

	NNLO$_{\mathrm{sat}}$	N^{3}LO$_{\mathrm{EM}}$ [47]	Exp.
a_{pp}^C	-7.8258	-7.8188	$-7.8196(26)$
r_{pp}^C	2.855	2.795	2.790(14)
a_{nn}	-18.929	-18.900	$-18.9(4)$
r_{nn}	2.911	2.838	2.75(11)
a_{np}	-23.728	-23.732	$-23.740(20)$
r_{np}	2.798	2.725	2.77(5)
E_D	2.22457	2.22458	2.224566
r_D	1.978	1.975	1.97535(85)
Q_D	0.270	0.275	0.2859(3)

Results for nuclei employed in optimization

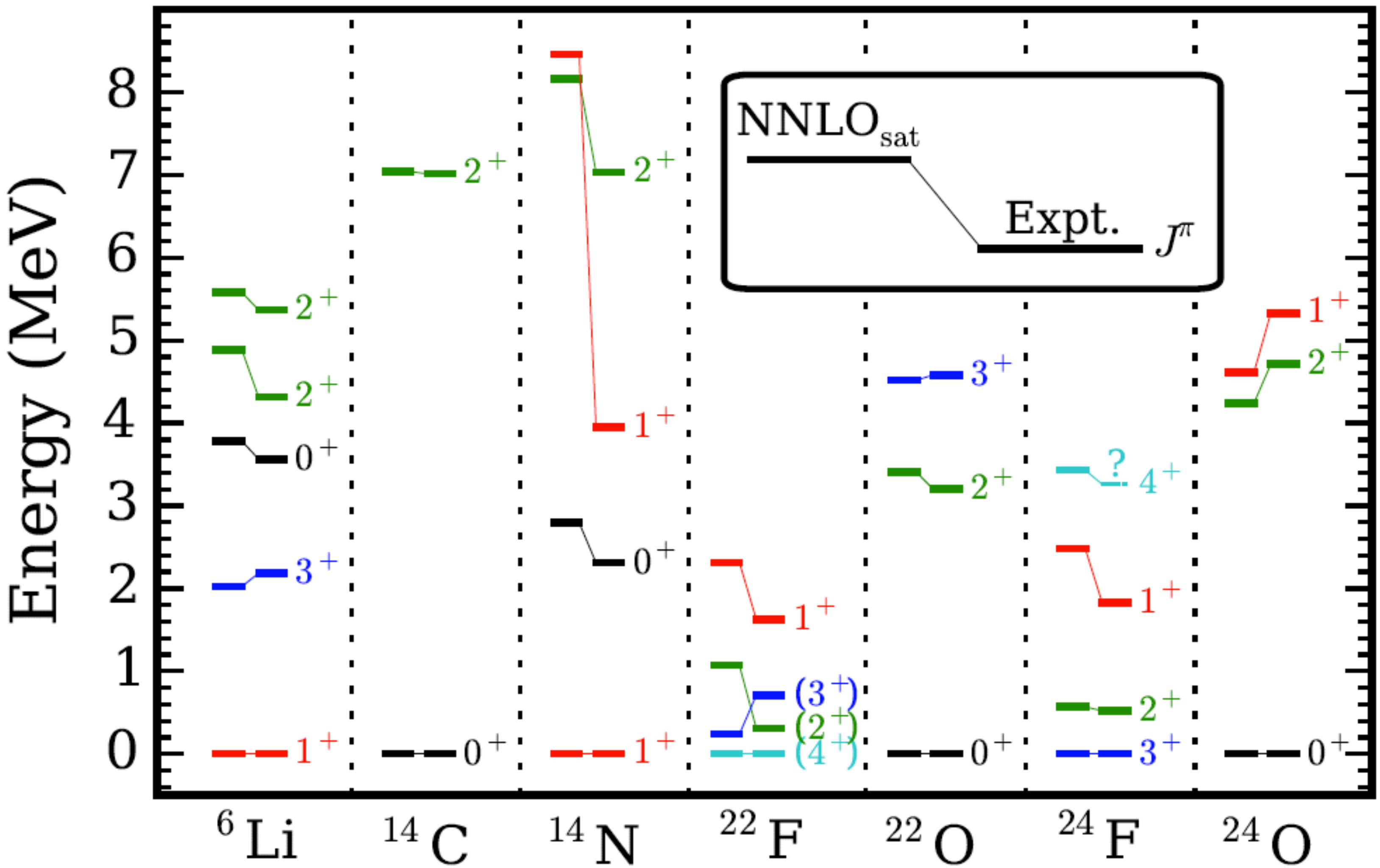
	E_{gs}	Exp.	r_{ch}	Exp.
^{3}H	8.52	8.482	1.78	1.7591(363)
^{3}He	7.76	7.718	1.99	1.9661(30)
^{4}He	28.43	28.296	1.70	1.6755(28)
^{14}C	103.6	105.285	2.48	2.5025(87)
^{16}O	124.4	127.619	2.71	2.6991(52)
^{22}O	160.5	162.028(57)		
^{24}O	167.8	168.96(12)		
^{25}O	167.1	168.18(10)		

NN phase shifts



Above 35 MeV, deviations probably at limit of one would expect at NNLO.

NNLO$_{sat}$ spectra



Other deficiencies: ^{17,18}O ($s_{1/2}$ and $d_{3/2}$ too low, 2^+ too low)

Overall NNLOsat spectra comparable to other chiral interactions

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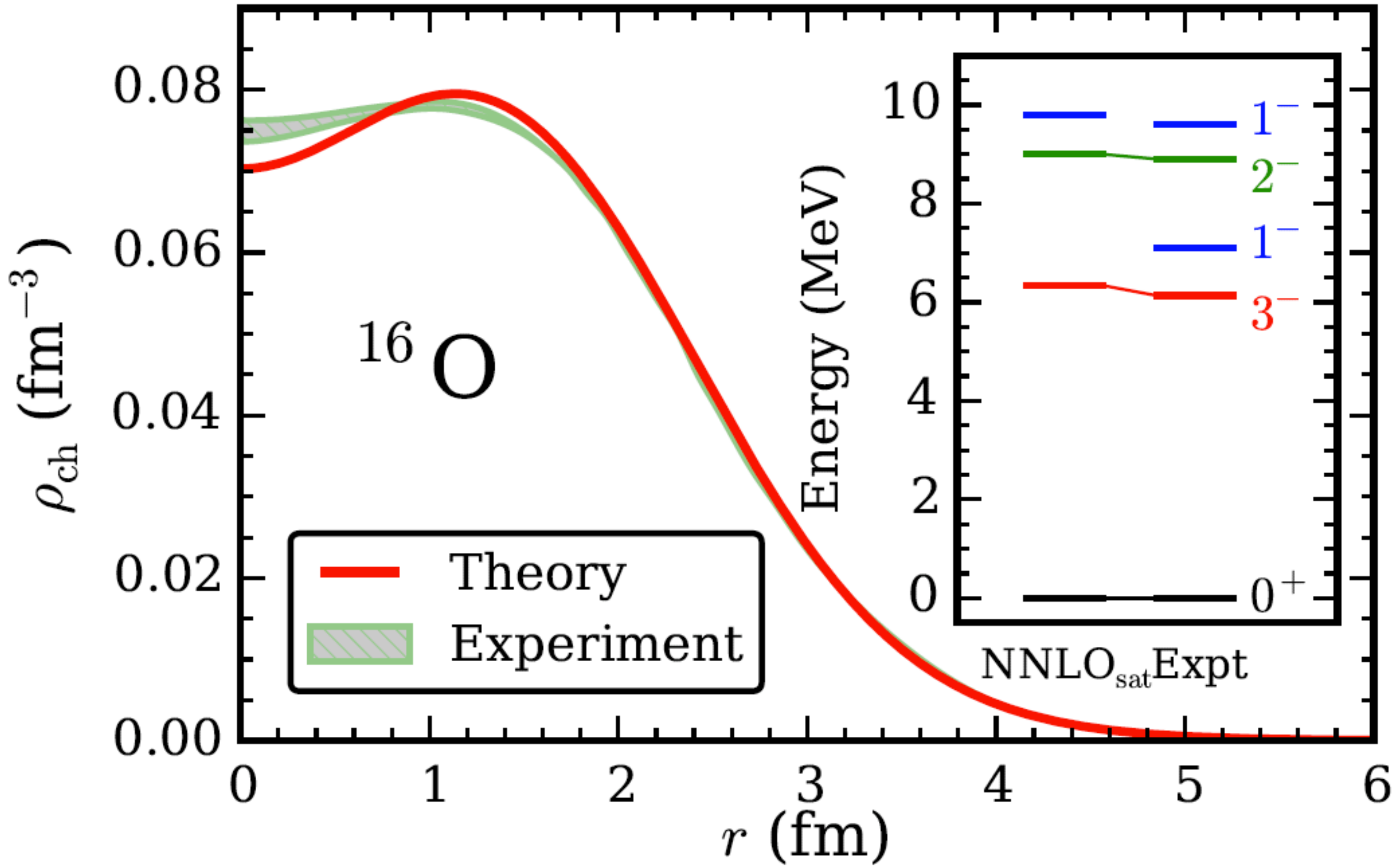
Charge density and excitations of ^{16}O



A. Ekström, G. Jansen, K. Wendt et al, arXiv:1502.04682 (2015)

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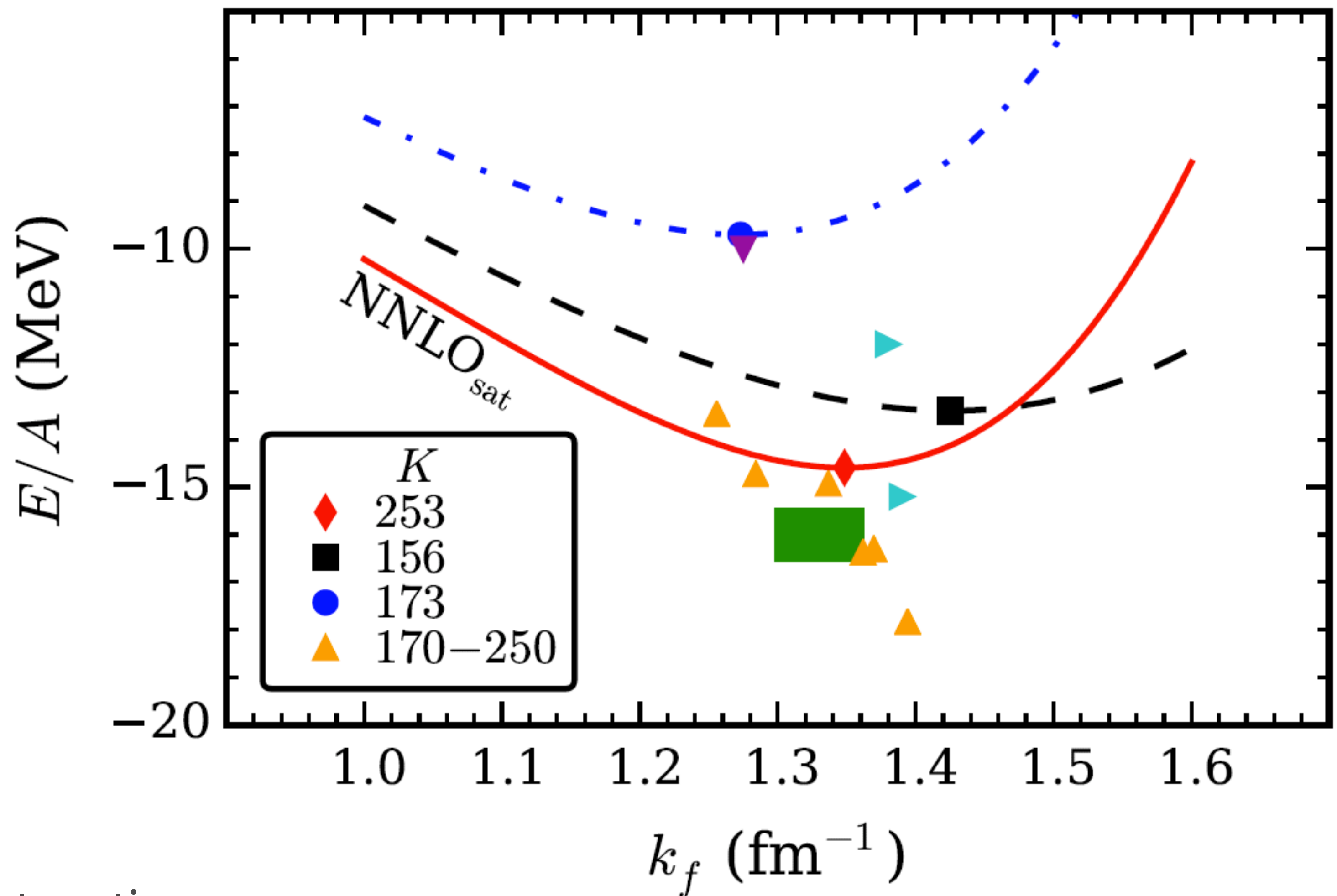
Nuclear matter from NNLO_{sat}



Other interactions:
Hagen et al (2014); Carbone et al (2013);
Coraggio et al 2014; Hebeler et al 2011.

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Intermission

- Chiral interaction NNLO_{sat}
  - Simultaneous optimization of *NN* and *NNN*
  - Radii and binding energies of selected *p* and *sd* shell nuclei employed in optimization

- Spectra of *p* and *sd* shell nuclei comparable to other chiral interactions
- Radii and binding energy much improved
- Promising also for calcium isotopes

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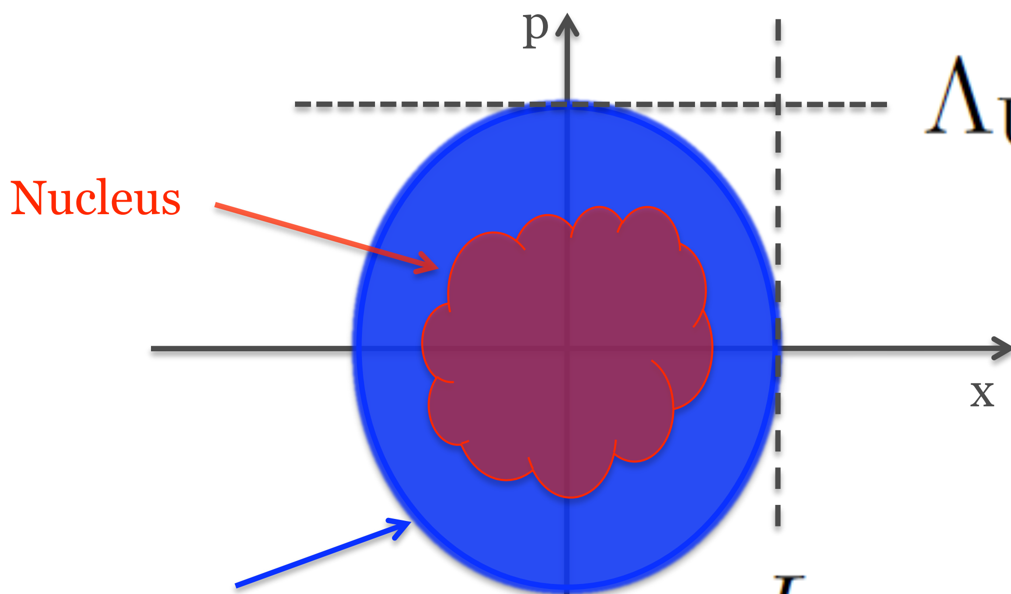
Convergence in finite oscillator spaces

What is the equivalent of Lüscher's formula for the harmonic oscillator basis?
[Lüscher, Comm. Math. Phys. 104, 177 (1986)]

Convergence in momentum space (UV) and in position space (IR) needed
[Stetcu *et al.*, PLB (2007); Hagen *et al.*, PRC (2010); Jurgenson *et al.*, PRC (2011); Coon *et al.*, PRC (2012); König *et al.*, PRC (2014)]



$$\Lambda_{\mathrm{UV}} \approx \sqrt{2N}/b$$

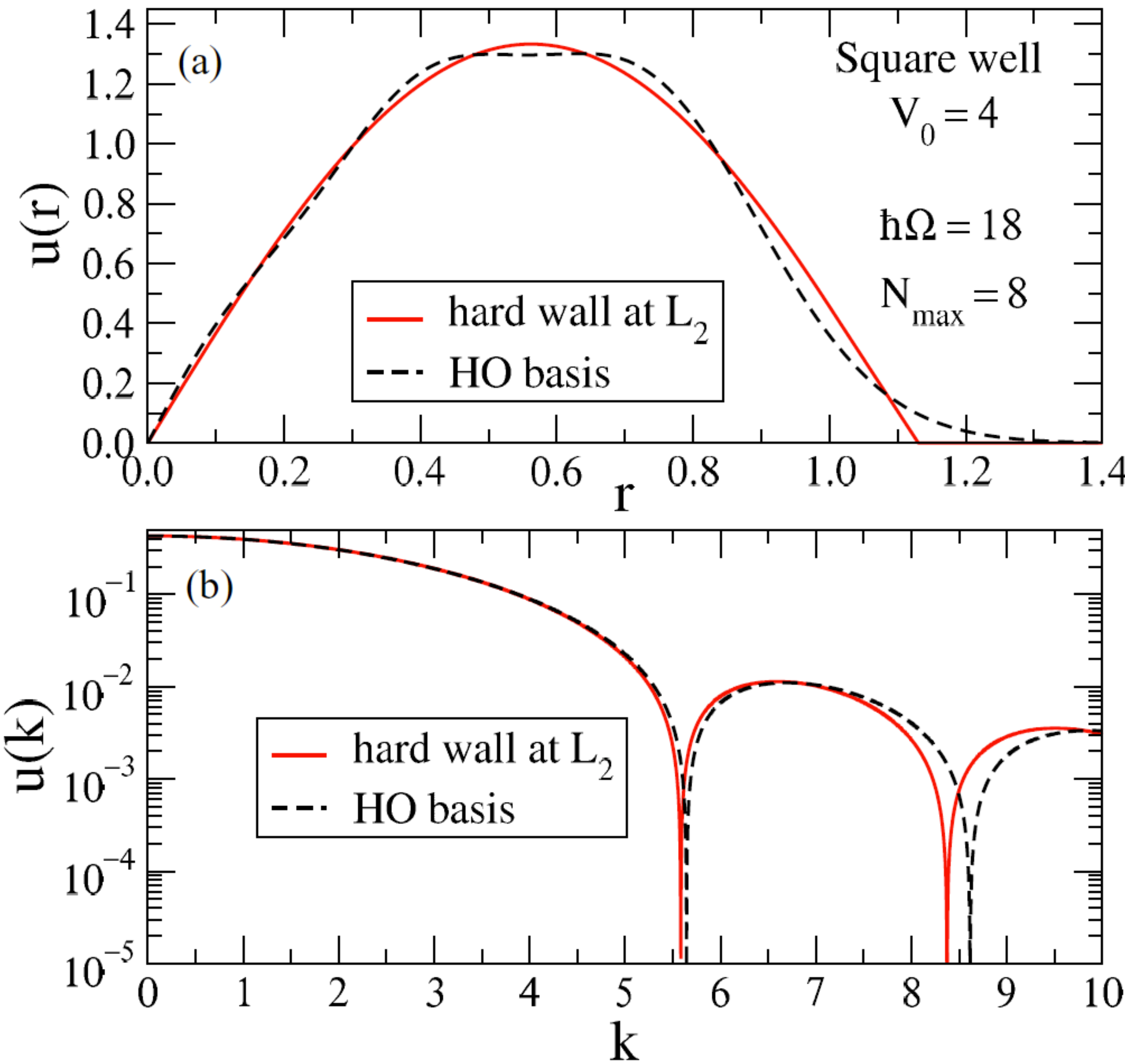
Phase space covered by
oscillator basis with (N, b)

$$L \approx \sqrt{2N}b$$

Nucleus needs to "fit" into basis:

- Nuclear radius $R < L$
- cutoff of interaction $\Lambda < \Lambda_{\mathrm{UV}}$

For long wave lengths, a finite HO basis resembles a spherical box



ground wave functions in position space

$(\pi/L_2)^2$ is the lowest eigenvalue of the operator p^2.

$$L_2 = \sqrt{2(N + 3/2 + 2)}b$$

Fourier transforms differ only at large momentum

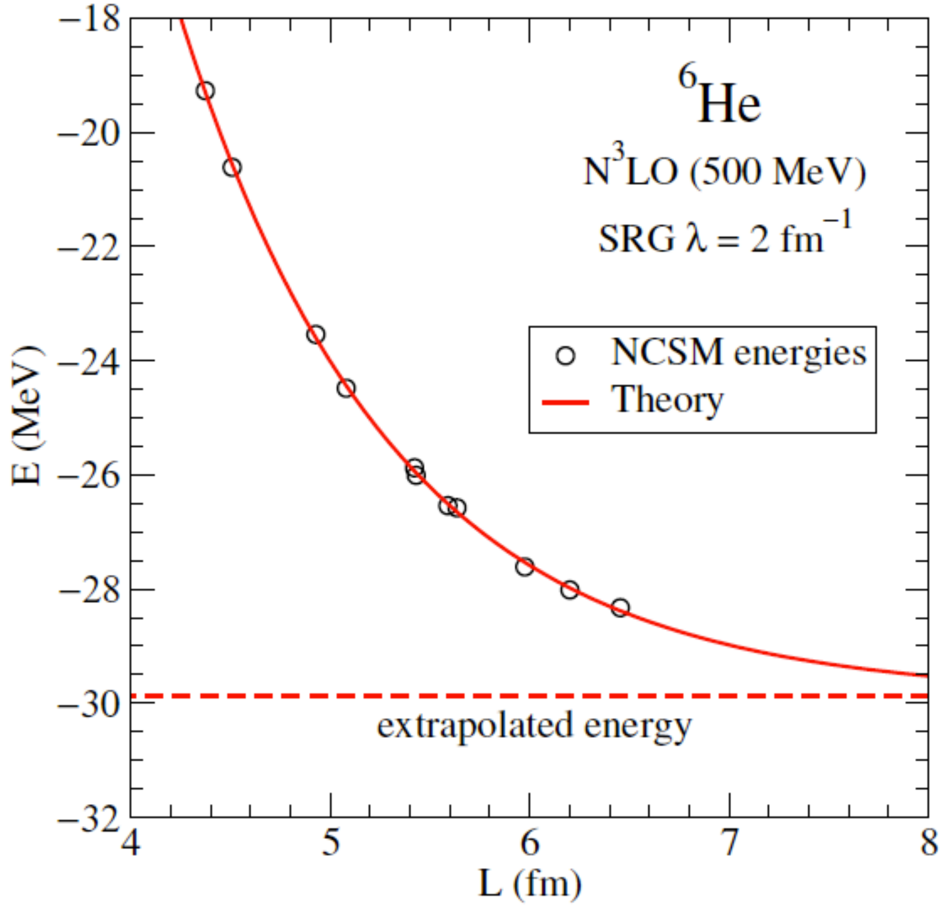
The difference between the HO basis and a box of size L_2 can not be resolved at low momentum.

Extrapolations in finite Hilbert spaces

$$u_E(r) \xrightarrow{r \gg R} A_E(e^{-k_E r} + \alpha_E e^{+k_E r})$$

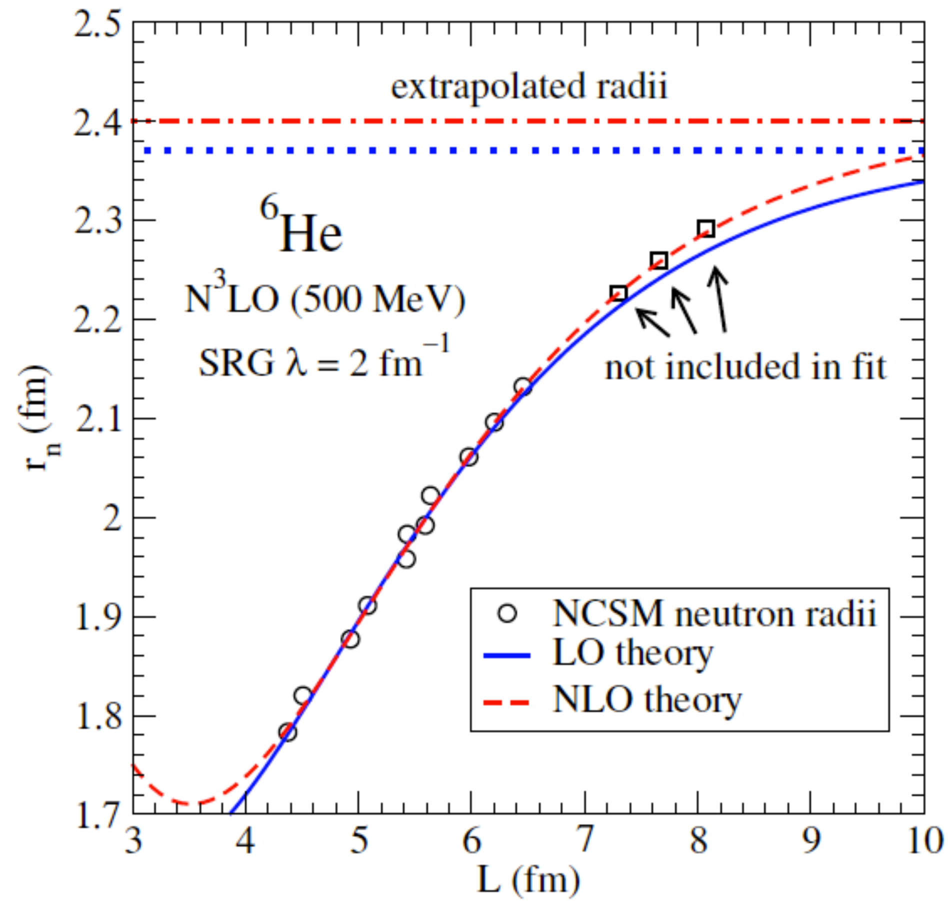
Ground-state energy

$$E_L = E_\infty + a_0 e^{-2k_\infty L}$$



Radius

$$\langle r^2 \rangle_L \approx \langle r^2 \rangle_\infty [1 - (c_0 \beta^3 + c_1 \beta) e^{-\beta}]$$
$$\beta \equiv 2k_\infty L$$



What (precisely) is the IR length L?

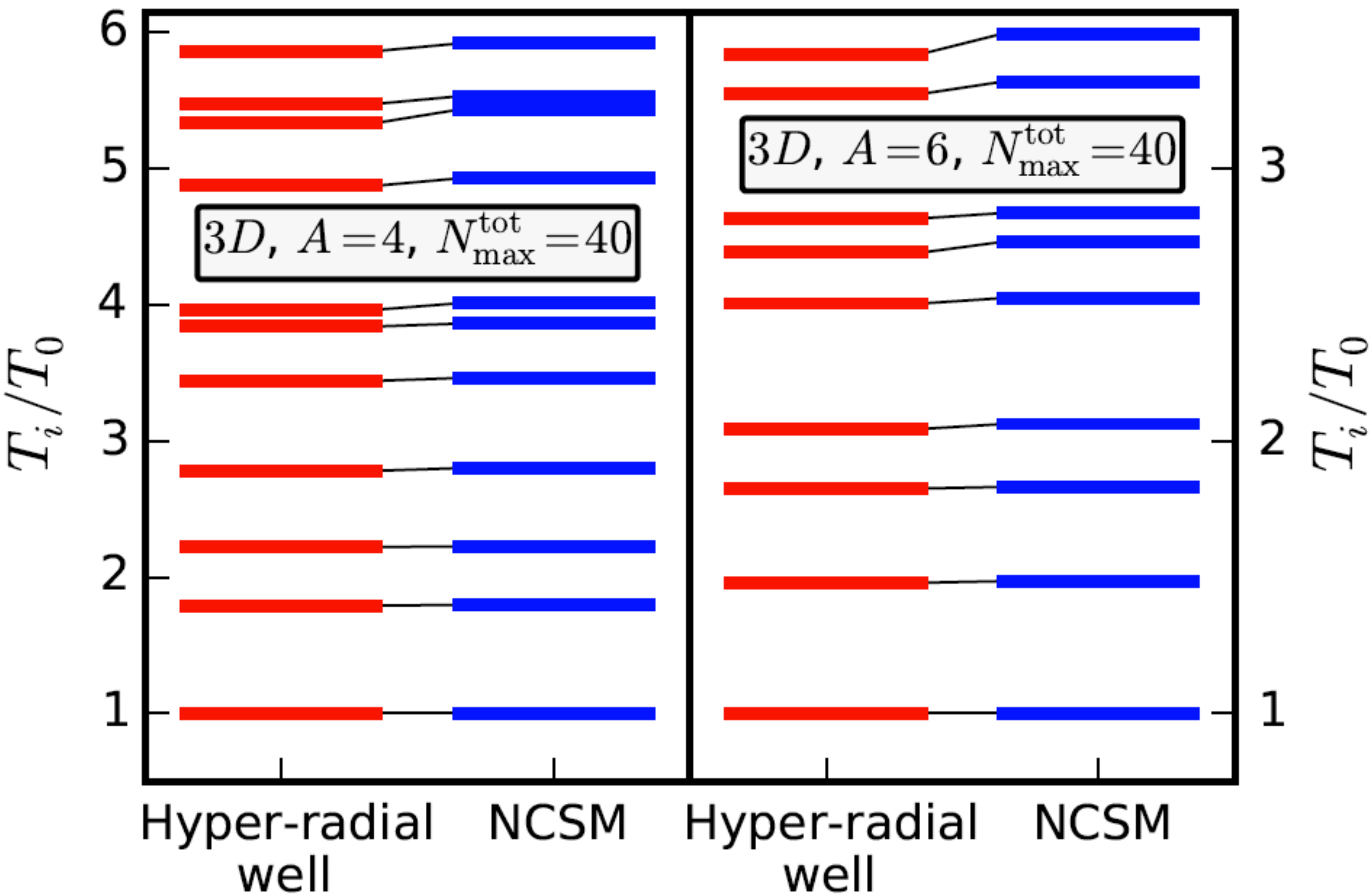
Key idea: compute eigenvalues of kinetic energy and compare with *corresponding* (hyper)spherical cavity to find L.

What is the corresponding cavity?

Single particle	***A* particles (product space)**	***A* particles in No-core shell model**
Diagonalize $T_{kin}=p^2$	Diagonalize *A*-body T_{kin}	Diagonalize *A*-body T_{kin}
3D spherical cavity	*A* fermions in 3D cavity	*3(A-1)* hyper-radial cavity
$L_2 = \sqrt{2(N+3/2+2)}b$	$L_{\rm eff} = \left(\frac{\sum_{nl}\nu_{nl}a_{l,n}^2}{\sum_{nl}\nu_{nl}\kappa_{l,n}^2}\right)^{1/2}$	$L_{\rm eff} = b\frac{X_{1,\mathcal{L}}}{\sqrt{T_{1,\mathcal{L}}(N_{\rm max}^{\rm tot})}}$
More, Ekström, Furnstahl, Hagen, TP, PRC 87, 044326 (2013)	Furnstahl, Hagen, TP, Wendt, J. Phys. G 42, 034032 (2015)	Wendt, Forssén, TP, Sääf, in preparation

For precise a value of UV cutoff, see [König, Bogner, Furnstahl, More, TP (2014)]

IR physics of NCSM equivalent to hyper-radial well



K. Wendt, C. Forssén, TP, D. Sääf, in preparation

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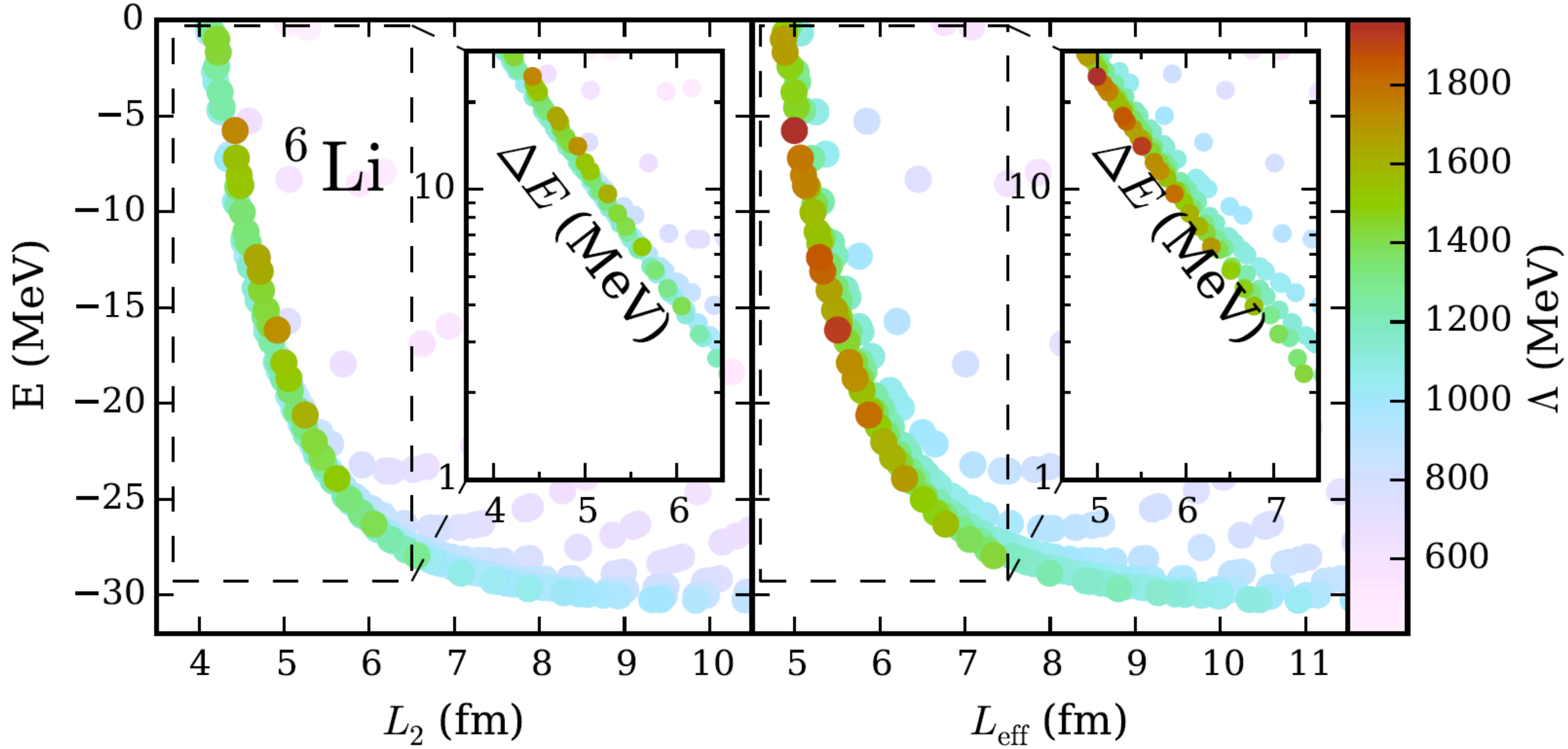
IR length L_{eff} for the NCSM



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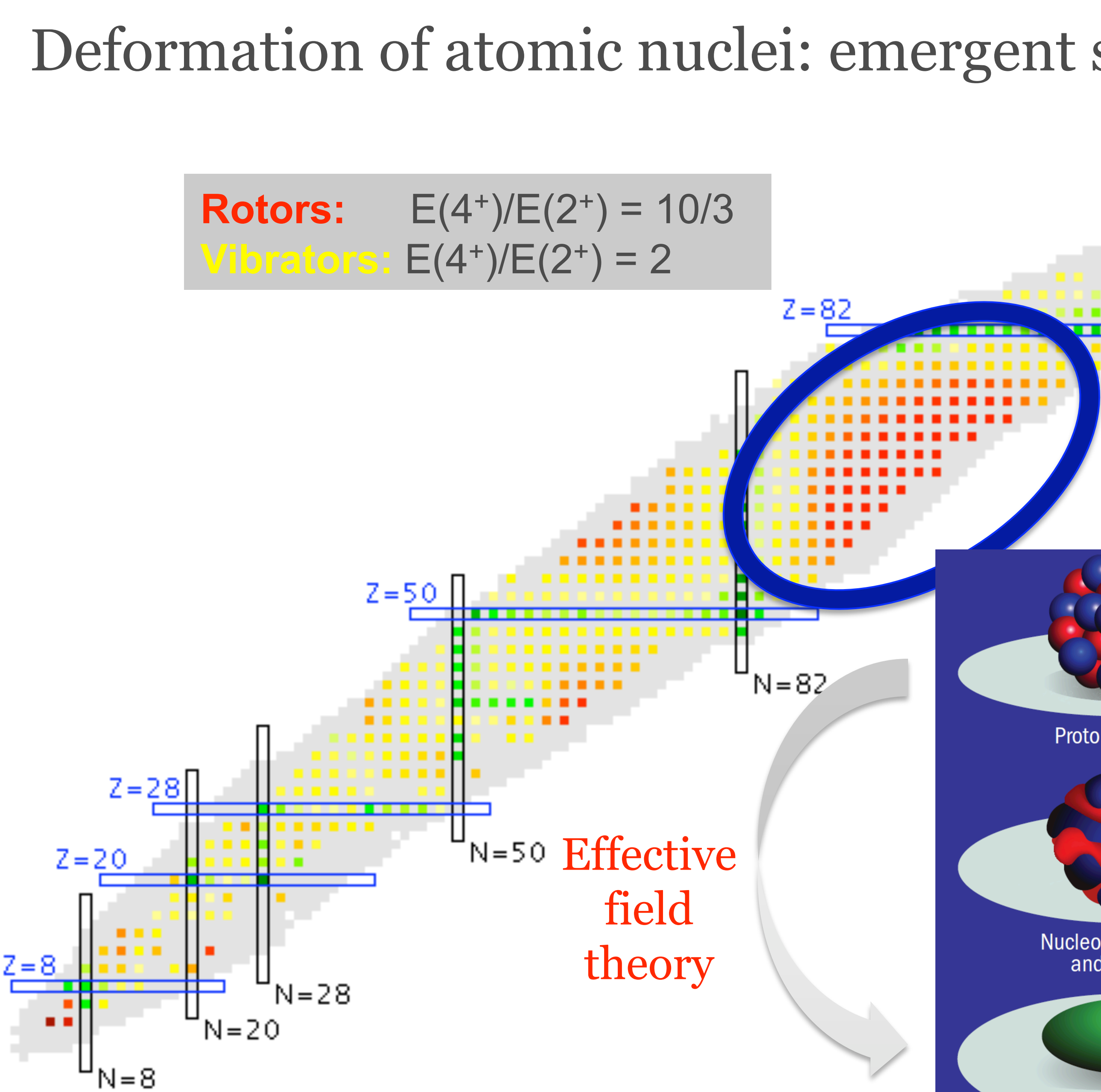
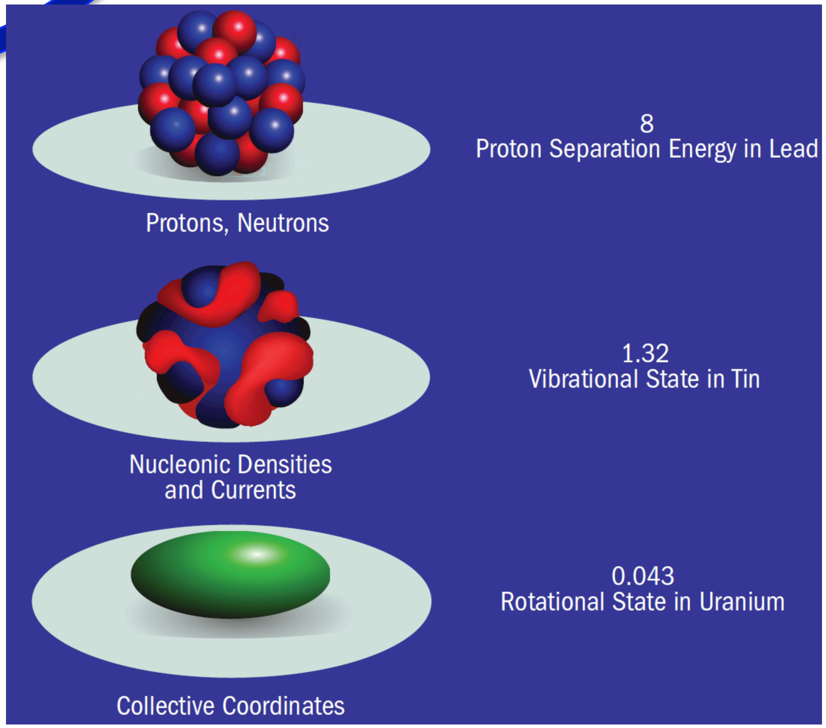
Deformation of atomic nuclei: emergent symmetry breaking

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

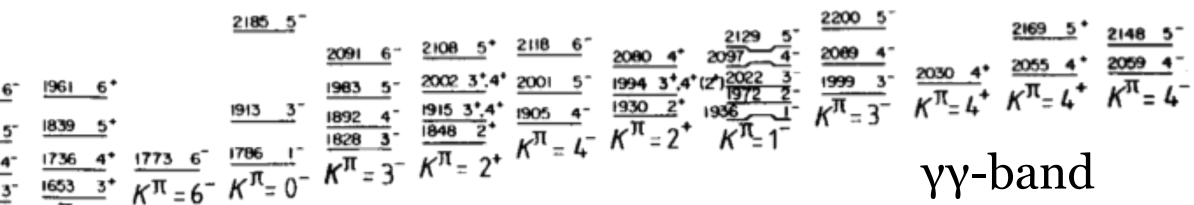


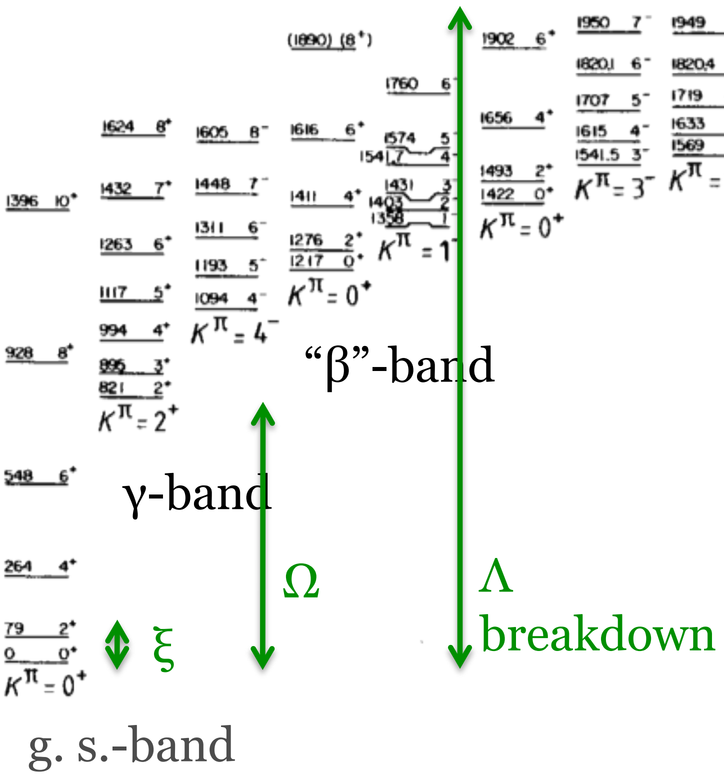
Effective field theory



Electromagnetic transitions in deformed nuclei

“Complete” spectrum of ^{168}Er [Davidson *et al.*, J. Phys. G 7, 455 (1981)]





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

Key features of geometric collective model

✓ Rotational bands on top of vibrational band heads
✓ Strong in-band E2 transitions
✓ Weaker inter-band E2 transitions
✓ Spectra are reproduced rather well

✗ Inter-band transitions are factors 2-10 too strong [Garrett, J. Phys. G 27 (2001) R1; Rowe & Wood “Fundamentals of Nuclear Models” (2010)]

Consistent coupling of EM fields addresses this problem

Some results from the EFT approach

• Quantized vibrations are Nambu-Goldstone modes of emergent breaking of SO(3) symmetry in finite systems [TP & Weidenmüller 2014]

• Adiabatic Bohr Hamiltonian reproduced at NLO [TP 2011]

• NNLO corrections differ from Bohr Hamiltonian; yield small changes in moments of inertia proportional to number of vibrational quanta [Zhang and TP 2013]

• Gauging of EFT yields correct description of weak inter-band transitions and theoretical uncertainty estimates [E. A. Coello Pérez and TP 2015]

Effective theory of ground-state rotational band equivalent to particle on a sphere because the coset SO(3)/SO(2) ~ S^2 is the two-sphere.

Gauging $\hat{\mathbf{I}} \rightarrow \hat{\mathbf{I}} - q\mathbf{e}_r \times \mathbf{A}$ instead of using quadrupole operator. Non-minimal couplings enter at higher order.

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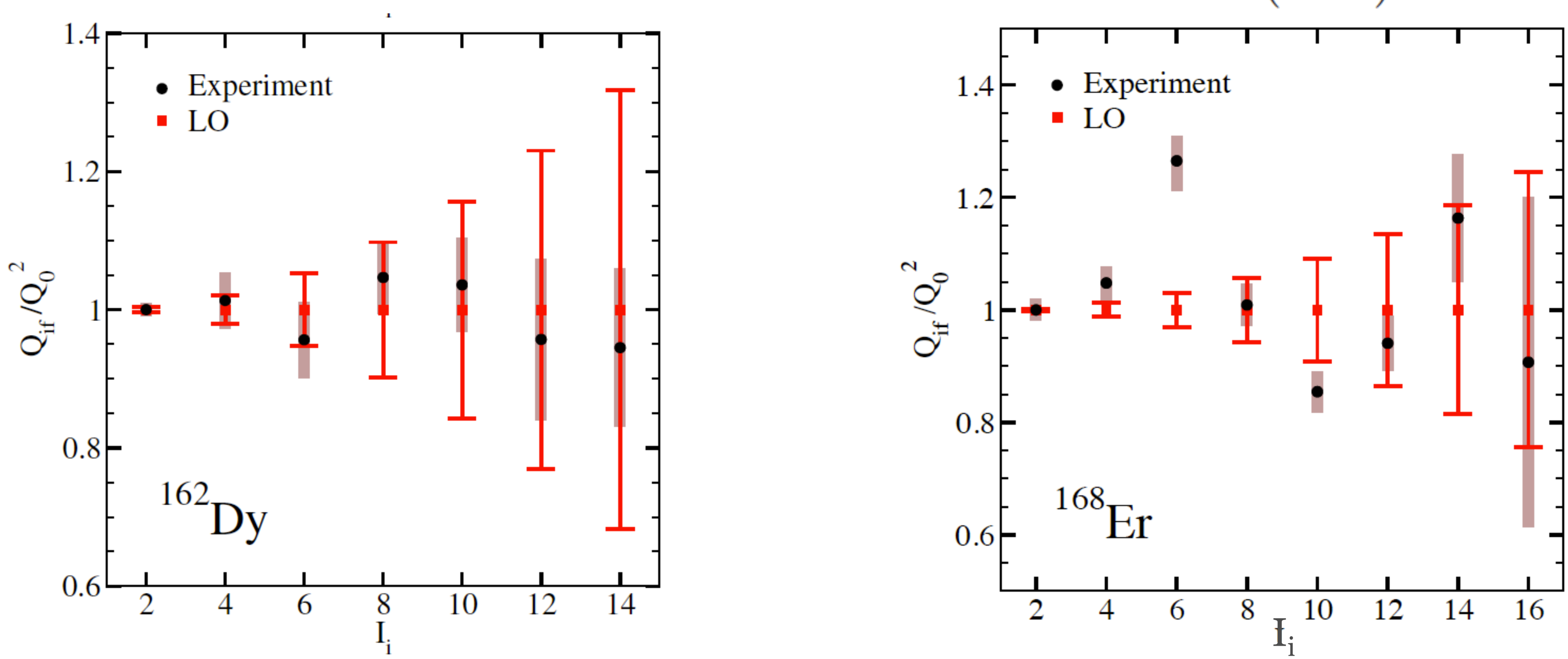
Quadrupole transitions in well-deformed nuclei

Transitions $I_i \rightarrow I_i - 2$ in ground-state band; result as [Mikhailov (1964,1966)]

$$B(E2, i \to f) = \frac{(aqR)^2}{60}\left(C^{I_f 0}_{I_i 020}\right)^2\left[1 + \frac{b}{a} I_i(I_i - 1)\right] \qquad Q_{if} \equiv \frac{B(E2, i \to f)}{\left(C^{I_f 0}_{I_i 020}\right)^2}$$

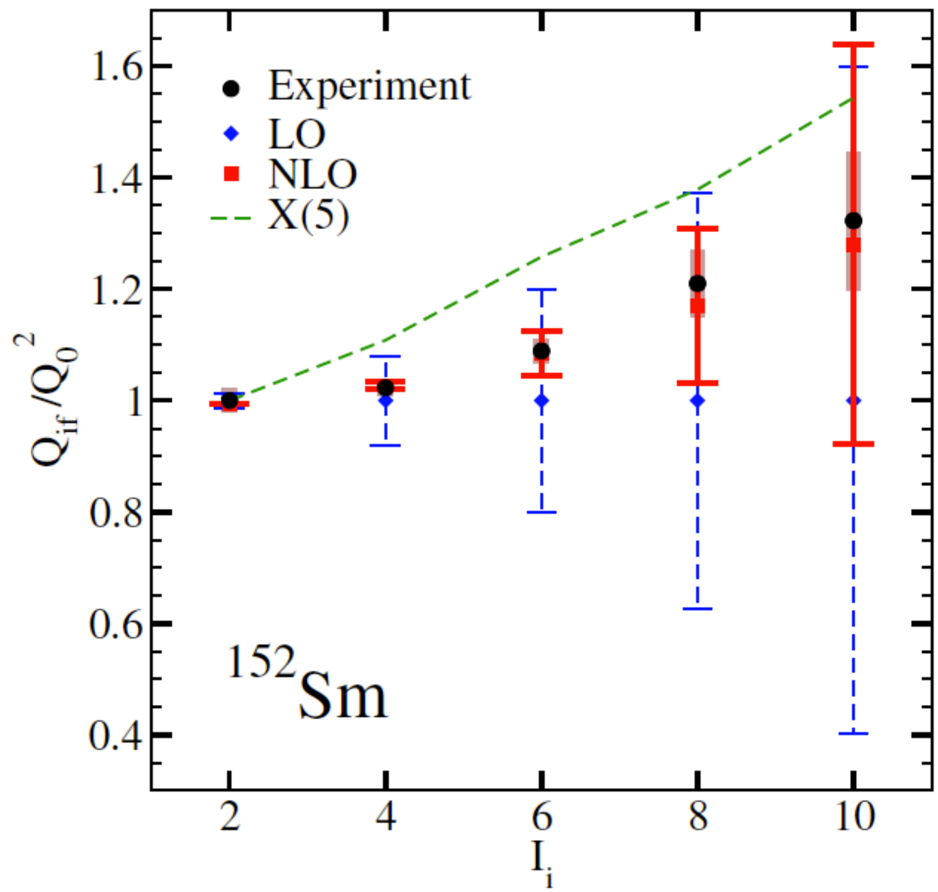


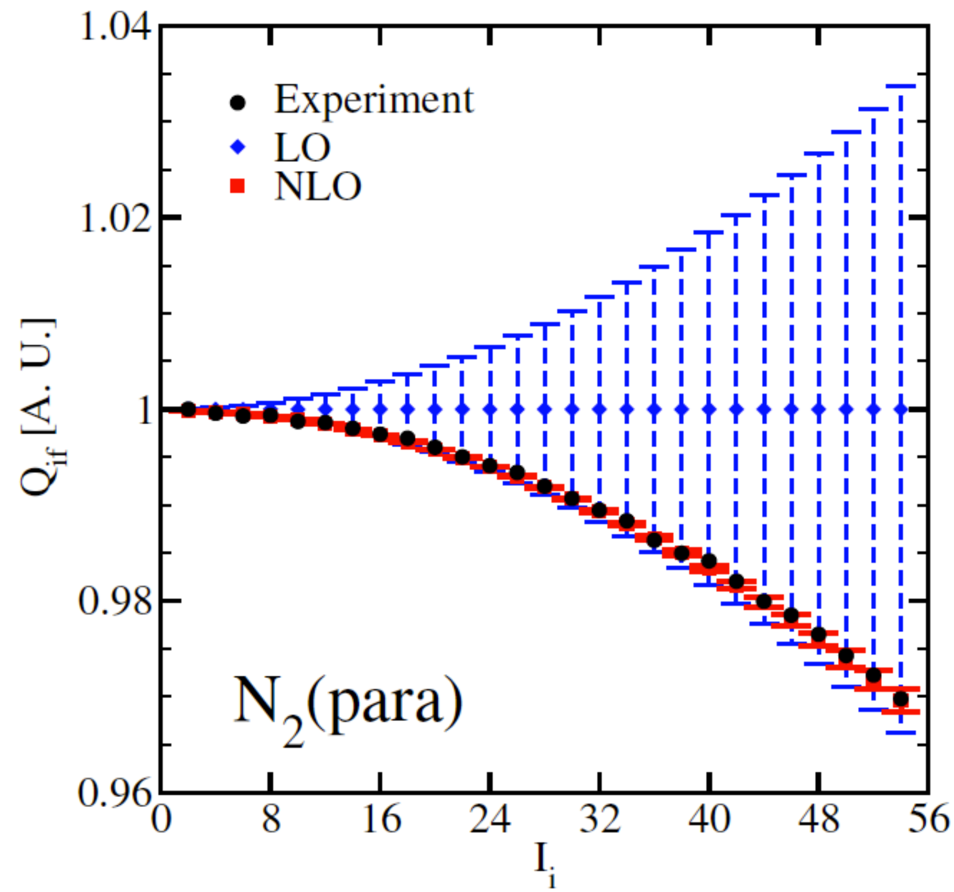
Rigid rotor has constant Q_{if}. More precise data needed for comparison at NLO.

E. A. Coello Pérez and TP, arXiv:1502.04405 (2015)

Quadrupole transitions in ^{152}Sm and N_2

Transitions $I_i \rightarrow I_i - 2$ in ground-state band





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^{154}Sm

$i \to f$	$B(E2)_{\text{exp}}$	$B(E2)_{\text{ET}}$	$B(E2)_{\text{CBS}}$	$B(E2)_{\text{BH}}$
$2_g^+ \to 0_g^+$	0.863(5)	0.863[a]	0.853	0.863
$4_g^+ \to 2_g^+$	1.201(29)	1.233(41)	1.231	1.234
$6_g^+ \to 4_g^+$	1.417(39)	1.358(101)	1.378	1.355
$8_g^+ \to 6_g^+$	1.564(83)	1.421(189)	1.471	1.424
$2_\gamma^+ \to 0_g^+$	0.0093(10)	0.0110(28)		0.0492
$2_\gamma^+ \to 2_g^+$	0.0157(15)	0.0157[a]		0.0703
$2_\gamma^+ \to 4_g^+$	0.0018(2)	0.0008(2)		0.0050
$2_\beta^+ \to 0_g^+$	0.0016(2)	0.0025(6)	0.0024	0.0319
$2_\beta^+ \to 2_g^+$	0.0035(4)	0.0035[a]	0.0069	0.0456
$2_\beta^+ \to 4_g^+$	0.0065(7)	0.0063(16)	0.0348	0.0821

In-band transitions are LO, inter-band transitions are NLO. Effective theory is more complicated than Bohr Hamiltonian both in Hamiltonian and E2 transition operator. Approach correctly predicts strengths of inter-band transitions with natural LECs.

E. A. Coello Pérez and TP, arXiv:1502.04405 (2015)

Summary

NNLOsat from simultaneous optimization of *NN* and *NNN* forces with input from p shell and sd shell nuclei

Improved understanding of finite model spaces via precise identification of IR length

Developed EFT for heavy deformed nuclei; correctly describes weak inter-band transitions

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