Open-shell nuclei from coupled-cluster theory

Gustav R. Jansen[1,2]

gustav.jansen@utk.edu

[1]University of Tennessee, Knoxville

[2]Oak Ridge National Laboratory

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- Andreas Ekström (UiO, MSU)
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SciDAC Scientific Discovery through Advanced Computing

NUCLEI Nuclear Computational Low-Energy Initiative

Outline

- Coupled cluster theory.
- Two-particles attached EOMCC.
- Shell evolution in oxygen isotopes.
- ^{26}F with 2PA-EOMCC.
- Shell evolution in calcium isotopes.
- NNLO (POUNDerS)

The nuclear manybody problem

Need to solve the Schrödinger equation

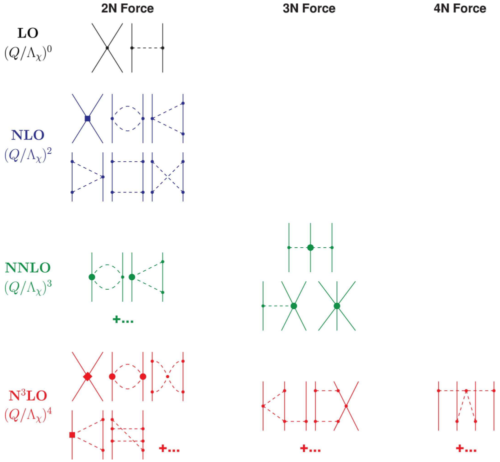
$$\hat{\mathrm{H}}|\Psi\rangle = \left(\hat{\mathrm{T}} + \hat{\mathrm{V}}_1 + \hat{\mathrm{V}}_2 + \hat{\mathrm{V}}_3 \ldots\right)|\Psi\rangle = \mathrm{E}|\Psi\rangle$$

Two ingredients

1. The nuclear interaction.
2. A method to solve the many body problem.

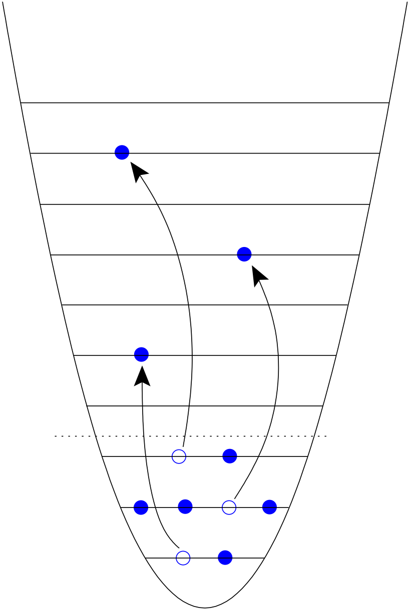
Chiral effective field theory

D. R. Entem and R. Machleidt, Phys. Rev. C 68, 041001 (2003)



- Direct link to QCD.
- Perturbative expansion in momentum.
- Chiral symmetry is spontaneously and explicitly broken.
- The hierarchy of nuclear forces unfolds automatically.

Finite basis expansion

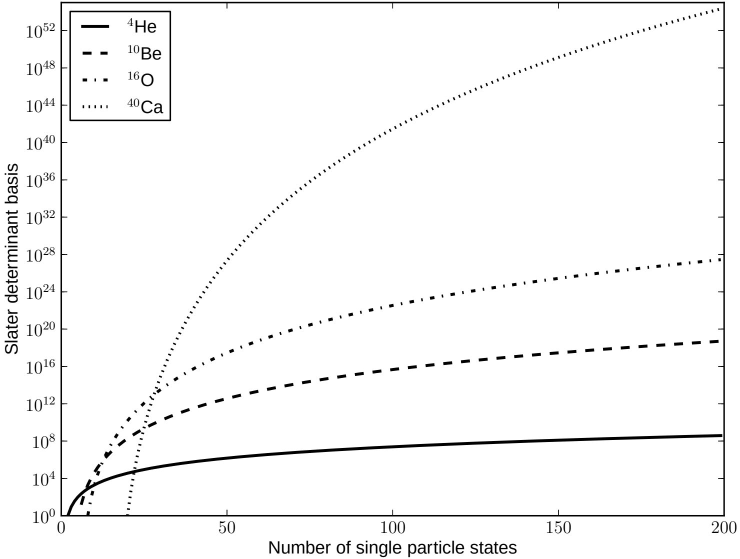


- The wavefunction is expanded in Slater determinants

$$|\Psi\rangle = \sum_i^D c_i |\Phi_i\rangle.$$

- The number of possible Slater determinants is $\binom{n}{A}$, where n is the number of single particle states and A is the number of nucleons.

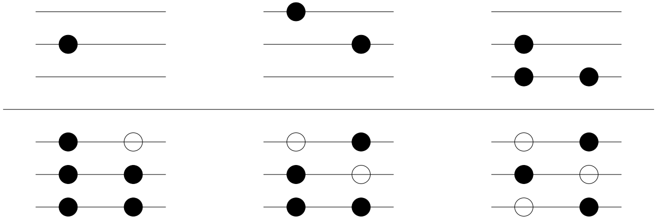
Curse of dimensionality



Coupled-cluster summary

Reduction of the number of degrees of freedom

$$\hat{T} = \hat{T}_1 + \hat{T}_2 + \ldots + \hat{T}_A$$
$$= \sum_{ia} t_i^a \left\{ a_a^\dagger a_i \right\} + \sum_{ijab} t_{ij}^{ab} \left\{ a_a^\dagger a_b^\dagger a_j a_i \right\} + \ldots +$$
$$\sum_{\substack{i_1,\ldots i_A \\ a_1,\ldots a_A}} t_{i_1,\ldots i_A}^{a_1,\ldots a_A} a_{a_1}^\dagger \ldots a_{a_A}^\dagger a_{i_A} \ldots a_{i_1}$$



Coupled-cluster summary

Exponential ansatz

$$|\Psi\rangle \approx |\Psi_{CC}\rangle = e^{\hat{\mathrm{T}}}|\Phi_0\rangle = \left(\sum_{n=1}^{\infty} \frac{1}{n!}\hat{\mathrm{T}}^n\right)|\Phi_0\rangle,$$

Include terms like

$$e^{\hat{\mathrm{T}}} \leftarrow \frac{1}{6}\hat{\mathrm{T}}_1^3 + \frac{1}{2}\hat{\mathrm{T}}_1\hat{\mathrm{T}}_2 + \frac{1}{A!}\hat{\mathrm{T}}_1^A$$

Coupled-cluster summary

Similarity transformed Hamiltonian

$$\bar{\mathrm{H}} = e^{-\hat{\mathrm{T}}}\hat{\mathrm{H}}_N e^{\hat{\mathrm{T}}}$$

$$\begin{pmatrix}
\langle\Phi_0|\bar{\mathrm{H}}|\Phi_0\rangle & \dots & \langle\Phi_0|\bar{\mathrm{H}}|\Phi_{i_1,\dots i_A}^{a_1,\dots a_A}\rangle \\
\langle\Phi_i^a|\bar{\mathrm{H}}|\Phi_0\rangle & \dots & \langle\Phi_i^a|\bar{\mathrm{H}}|\Phi_{i_1,\dots i_A}^{a_1,\dots a_A}\rangle \\
\langle\Phi_{ij}^{ab}|\bar{\mathrm{H}}|\Phi_0\rangle & \dots & \langle\Phi_{ij}^{ab}|\bar{\mathrm{H}}|\Phi_{i_1,\dots i_A}^{a_1,\dots a_A}\rangle \\
\langle\Phi_{ijk}^{abc}|\bar{\mathrm{H}}|\Phi_0\rangle & \dots & \langle\Phi_{ijk}^{abc}|\bar{\mathrm{H}}|\Phi_{i_1,\dots i_A}^{a_1,\dots a_A}\rangle \\
\vdots & \ddots & \vdots \\
\langle\Phi_{i_1,\dots i_A}^{a_1,\dots a_A}|\bar{\mathrm{H}}|\Phi_0\rangle & \dots & \langle\Phi_{i_1,\dots i_A}^{a_1,\dots a_A}|\bar{\mathrm{H}}|\Phi_{i_1,\dots i_A}^{a_1,\dots a_A}\rangle
\end{pmatrix}$$

Coupled-cluster summary

Similarity transformed Hamiltonian

CCS

$$\begin{pmatrix} E_{\mathrm{CCS}} & \dots & \langle \Phi_0 | \bar{\mathrm{H}} | \Phi_{i_1,\dots i_A}^{a_1,\dots a_A} \rangle \\ 0 & \dots & \langle \Phi_i^a | \bar{\mathrm{H}} | \Phi_{i_1,\dots i_A}^{a_1,\dots a_A} \rangle \\ \langle \Phi_{ij}^{ab} | \bar{\mathrm{H}} | \Phi_0 \rangle & \dots & \langle \Phi_{ij}^{ab} | \bar{\mathrm{H}} | \Phi_{i_1,\dots i_A}^{a_1,\dots a_A} \rangle \\ \langle \Phi_{ijk}^{abc} | \bar{\mathrm{H}} | \Phi_0 \rangle & \dots & \langle \Phi_{ijk}^{abc} | \bar{\mathrm{H}} | \Phi_{i_1,\dots i_A}^{a_1,\dots a_A} \rangle \\ \vdots & \ddots & \vdots \\ \langle \Phi_{i_1,\dots i_A}^{a_1,\dots a_A} | \bar{\mathrm{H}} | \Phi_0 \rangle & \dots & \langle \Phi_{i_1,\dots i_A}^{a_1,\dots a_A} | \bar{\mathrm{H}} | \Phi_{i_1,\dots i_A}^{a_1,\dots a_A} \rangle \end{pmatrix}$$

Coupled-cluster summary

Similarity transformed Hamiltonian

CCSD

$$\begin{pmatrix} E_{\mathrm{CCSD}} & \dots & \langle\Phi_0|\bar{\mathrm{H}}|\Phi_{i_1,\dots i_A}^{a_1,\dots a_A}\rangle \\ 0 & \dots & \langle\Phi_i^a|\bar{\mathrm{H}}|\Phi_{i_1,\dots i_A}^{a_1,\dots a_A}\rangle \\ 0 & \dots & \langle\Phi_{ij}^{ab}|\bar{\mathrm{H}}|\Phi_{i_1,\dots i_A}^{a_1,\dots a_A}\rangle \\ \langle\Phi_{ijk}^{abc}|\bar{\mathrm{H}}|\Phi_0\rangle & \dots & \langle\Phi_{ijk}^{abc}|\bar{\mathrm{H}}|\Phi_{i_1,\dots i_A}^{a_1,\dots a_A}\rangle \\ \vdots & \ddots & \vdots \\ \langle\Phi_{i_1,\dots i_A}^{a_1,\dots a_A}|\bar{\mathrm{H}}|\Phi_0\rangle & \dots & \langle\Phi_{i_1,\dots i_A}^{a_1,\dots a_A}|\bar{\mathrm{H}}|\Phi_{i_1,\dots i_A}^{a_1,\dots a_A}\rangle \end{pmatrix}$$

Coupled-cluster summary

Similarity transformed Hamiltonian

CCSDT

$$\begin{pmatrix} E_{\mathrm{CCSDT}} & \dots & \langle \Phi_0 | \bar{\mathrm{H}} | \Phi_{i_1,\dots i_A}^{a_1,\dots a_A} \rangle \\ 0 & \dots & \langle \Phi_i^a | \bar{\mathrm{H}} | \Phi_{i_1,\dots i_A}^{a_1,\dots a_A} \rangle \\ 0 & \dots & \langle \Phi_{ij}^{ab} | \bar{\mathrm{H}} | \Phi_{i_1,\dots i_A}^{a_1,\dots a_A} \rangle \\ 0 & \dots & \langle \Phi_{ijk}^{abc} | \bar{\mathrm{H}} | \Phi_{i_1,\dots i_A}^{a_1,\dots a_A} \rangle \\ \vdots & \ddots & \vdots \\ \langle \Phi_{i_1,\dots i_A}^{a_1,\dots a_A} | \bar{\mathrm{H}} | \Phi_0 \rangle & \dots & \langle \Phi_{i_1,\dots i_A}^{a_1,\dots a_A} | \bar{\mathrm{H}} | \Phi_{i_1,\dots i_A}^{a_1,\dots a_A} \rangle \end{pmatrix}$$

Coupled-cluster summary

Similarity transformed Hamiltonian

FCI

$$\begin{pmatrix}
E & \dots & \langle\Phi_0|\bar{\mathrm{H}}|\Phi_{i_1,\dots i_A}^{a_1,\dots a_A}\rangle \\
0 & \dots & \langle\Phi_i^a|\bar{\mathrm{H}}|\Phi_{i_1,\dots i_A}^{a_1,\dots a_A}\rangle \\
0 & \dots & \langle\Phi_{ij}^{ab}|\bar{\mathrm{H}}|\Phi_{i_1,\dots i_A}^{a_1,\dots a_A}\rangle \\
0 & \dots & \langle\Phi_{ijk}^{abc}|\bar{\mathrm{H}}|\Phi_{i_1,\dots i_A}^{a_1,\dots a_A}\rangle \\
\vdots & \ddots & \vdots \\
0 & \dots & \langle\Phi_{i_1,\dots i_A}^{a_1,\dots a_A}|\bar{\mathrm{H}}|\Phi_{i_1,\dots i_A}^{a_1,\dots a_A}\rangle
\end{pmatrix}$$

Excited states using EOM-CC

Eigenvalues of $\bar{\mathrm{H}} = e^{-\hat{\mathrm{T}}}\hat{\mathrm{H}}e^{\hat{\mathrm{T}}} - \langle\Phi_0|\hat{\mathrm{H}}|\Phi_0\rangle$

$$\left(\bar{\mathrm{H}}\hat{\mathrm{R}}\right)_c = \omega\hat{\mathrm{R}}$$

Properties of $\bar{\mathrm{H}}$.

- Non-symmetric (non-hermetian) operator.
- For CCSD and a twobody hamiltonian - six-body operator.
- The matrix representation is very sparse.
- Generally too large to store and diagonalize exactly.

Efficient implementation of $\left(\bar{\mathrm{H}}\hat{\mathrm{R}}\right)_C$ *is key.*

Two particles attached (2PA-EOM-CCSD)

Why?

- Access to additional isotopes.
- Possibility of effective interactions for shell model.

Two particles attached (2PA-EOM-CCSD)

Eigenvalue problem

$$\left(\bar{\mathrm{H}}\hat{\mathrm{R}}\right)_c = \omega\hat{\mathrm{R}}$$

2PA-EOM-CCSD(2p0h)

$$\hat{\mathrm{R}} = \hat{\mathrm{R}}_2 = \frac{1}{2}\sum_{a,b} r^{ab} a_a^\dagger a_b^\dagger$$

2PA-EOM-CCSD(3p1h)

$$\hat{\mathrm{R}} = \hat{\mathrm{R}}_2 + \hat{\mathrm{R}}_3 = \frac{1}{2}\sum_{a,b} r^{ab} a_a^\dagger a_b^\dagger + \frac{1}{6}\sum_{a,b,c,i} r_i^{abc} a_a^\dagger a_b^\dagger a_c^\dagger a_i$$

Testcase - ^{6}He

GRJ, M. Hjorth-Jensen, G. Hagen, and T. Papenbrock,
Phys. Rev. C 83, 054306, 2011

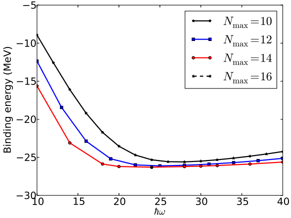
	0_1^+	2_1^+	0^+ $\langle J \rangle$	2_1^+ $\langle J \rangle$
CCSD	-22.732	-20.905	0.78	2
CCSDT-1	-24.617	-21.586	0.25	2
CCSDT	-24.530	-21.786	0.01	2
2PA-EOM-CCSD(2p-0h)	-21.185	-18.996	0	2
2PA-EOM-CCSD(3p-1h)	-24.543	-21.634	0	2
FCI	-24.853	-21.994	0	2

Table : Energies (in MeV) for the ground state and first excited state of ^{6}He and the expectation value of the total angular momentum, calculated with coupled-cluster methods truncated at the 2-particle-2-hole (CCSD) level, 3-particle-3-hole (CCSDT) and a hybrid (CCSDT-1) where the 3-particle-3-hole amplitudes are treated perturbatively.

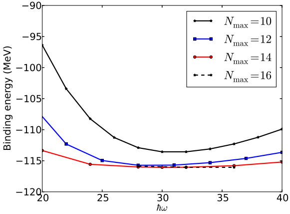
Convergence

GRJ, arXiv:1207.7099 (2012)

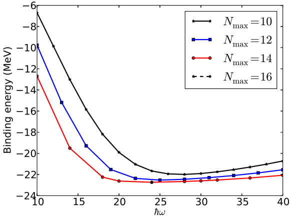
^{6}Li (1+)



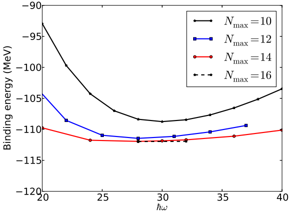
^{18}O (0+)



^{6}Li (3+)

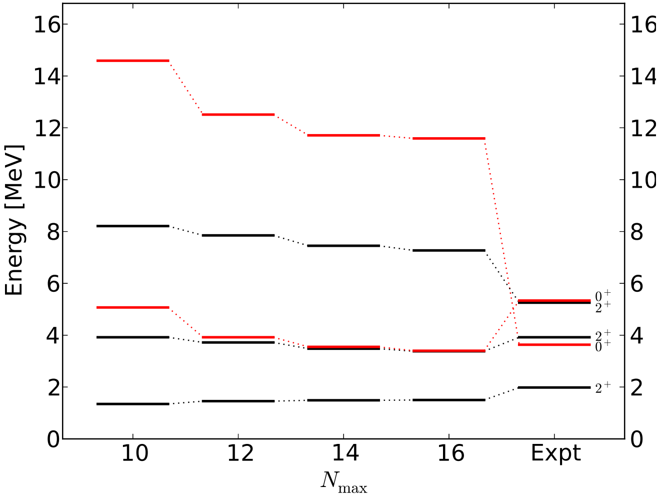


^{18}O (3+)

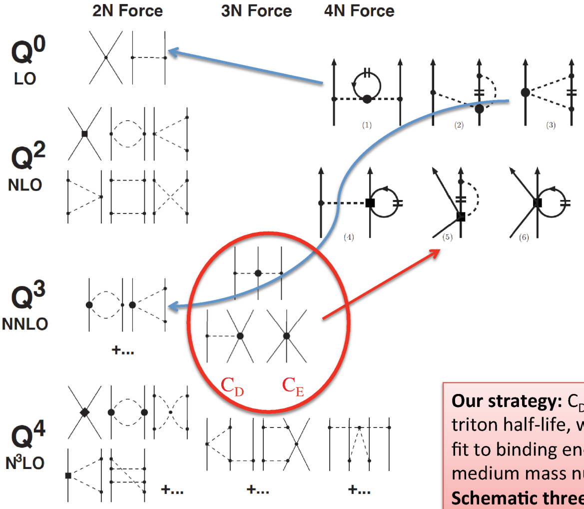


4p-2h states in ^{18}O

GRJ, arXiv:1207.7099 (2012)



Density dependent chiral threebody force



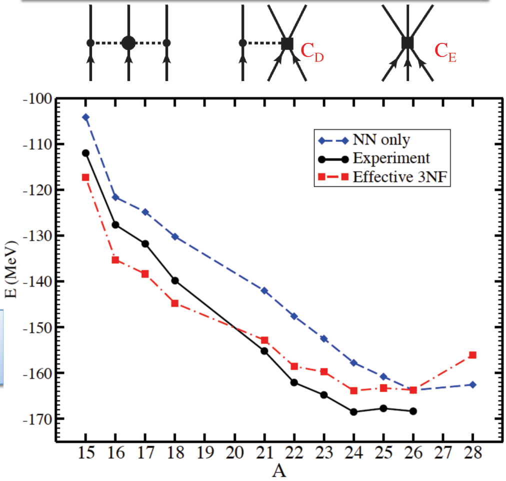
Integrating over the third leg in infinite nuclear matter and derive density dependent corrections to the nucleon-nucleon interaction.
J. W. Holt N. Kaiser and W. Weise. Phys.Rev.C 79, 054331 (2009)
K. Hebeler and A. Schwenk (2010)

Our strategy: C_D is given by fit to triton half-life, we fix C_E and k_F from fit to binding energy in selected medium mass nuclei:
Schematic three-nucleon forces

Oxygen isotopes from chiral interaction

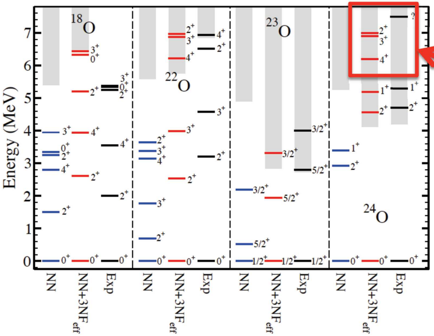
- Inclusion of effective 3NF places dripline at ^{25}O.
- Overall the odd-even staggering in the neutron rich oxygen is well reproduced.
- We find ^{26}O to unbound with respect to ^{24}O by ~100keV, agreement with **E. Lunderberg et al., Phys. Rev. Lett. 108 (2012) 142503**
- We find ^{28}O to be unbound with a resonance width of ~2MeV

Chiral three-nucleon force at order N2LO. k_f=1.05fm^{-1}, C_D = 0.2, C_E = 0.71 (k_f and c_E fitted to to the binding Energy of ^{16}O and ^{22}O).



G. Hagen, M. Hjorth-Jensen, G. R. Jansen, R. Machleidt, T. Papenbrock, Phys. Rev. Lett. 108, 242501 (2012).

Oxygen isotopes from chiral interaction



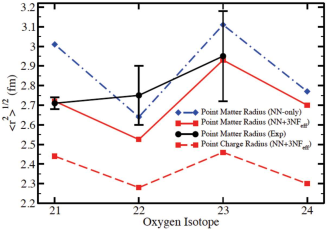
The effects of three-nucleon forces decompress the spectra and brings it in good agreement with experiment.

We find several states ($4^+,3^+,2^+$) near the observed peak at ~7.5MeV in ^{24}O
C. R. Hoffman et al Phys. Rev. C **83**, 031303 (2011)

Excited states in ^{24}O computed with EOM-CCSD and compared to experiment

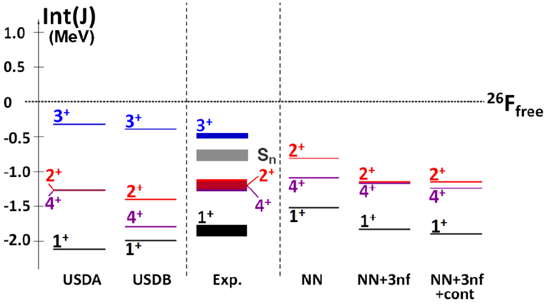
J^π	2_1^+	1_1^+	4_1^+	3_1^+	2_2^+	1_2^+
E_{CC}	4.56	5.2	6.2	6.9	7.0	8.4
E_{Exp}	4.7(1)	5.33(10)				
Γ_{CC}	0.03	0.04	0.005	0.01	0.04	0.56
Γ_{Exp}	$0.05^{+0.21}_{-0.05}$	$0.03^{+0.12}_{-0.03}$				

Matter and charge radii for $^{21-24}O$
Computed from intrinsic densities and
Compared to experiment.



Threebody forces in ^{26}F

A. Lepailleur *et al.*, Phys. Rev. Lett. 110, 082502 (2013)

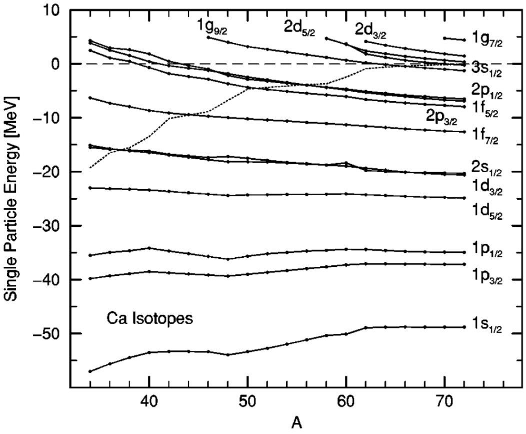


Technical details

- Chiral interaction at N^{3}LO.
- Identical threebody force as established in the oxygen chain.
- 17 major harmonic oscillator shells with a Gamow-Hartree-Fock basis for $\nu s_{1/2}$ and $\nu d_{3/2}$
- CCSD with triples corrections (Λ-CCSD(T)) for ^{24}O, with 2PA-EOMCC.
- $^{26}\mathrm{F}_{free} = B(^{25}\mathrm{O}) + B(^{25}\mathrm{F}) - B(^{24}\mathrm{O})$

Threebody forces are crucial for correct levelspacing.

Evolution of single particle energies



Technical details

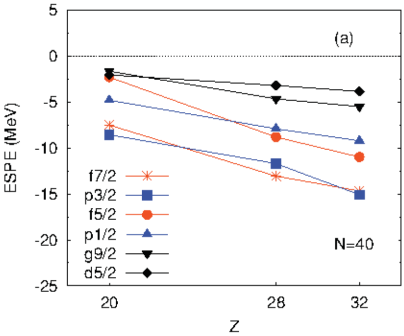
- J. Meng, H. Toki, J. Y. Zeng, S. Q. Zhang and S. -G. Zhou, PRC 65 041302(R) (2002).
- Relativistic mean-field including continuum effects.

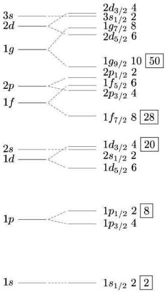
Main features

- Bunching of single-particle energies outside the *pf*-shell.
- No shell-gap in ^{60}Ca - ^{70}Ca.
- Large deformations and no shell-closure.
- Continuum effects responsible for bound ^{60}Ca - ^{72}Ca.

Evolution of single particle energies

S. M. Lenzi, F. Nowacki, A. Poves and K. Sieja, PRC 82 054301 (2010)



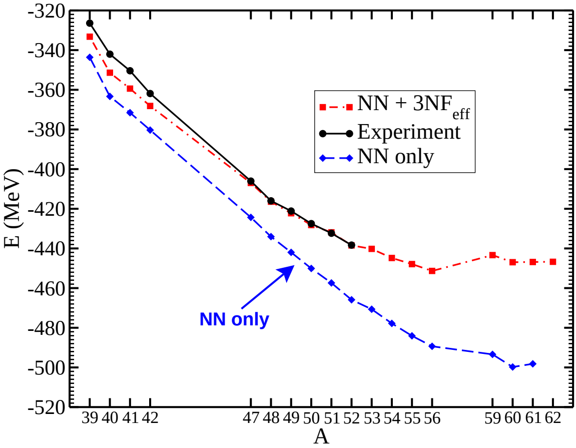


Main features

- Shell-model calculation in the *pf*-shell including $0g_{9/2}$ and $2d_{5/2}$ for neutrons.
- Inversion of the $0g_{9/2}$ and the $2d_{5/2}$ single particle states in ^{60}Ca.
- Bunching of levels including the $0f_{5/2}$ state indicates no shell-closure.

Binding energies in calcium isotopes

G. Hagen, M. Hjorth-Jensen, GRJ, R. Machleidt, and T. Papenbrock,
PRL109 032502 (2012)



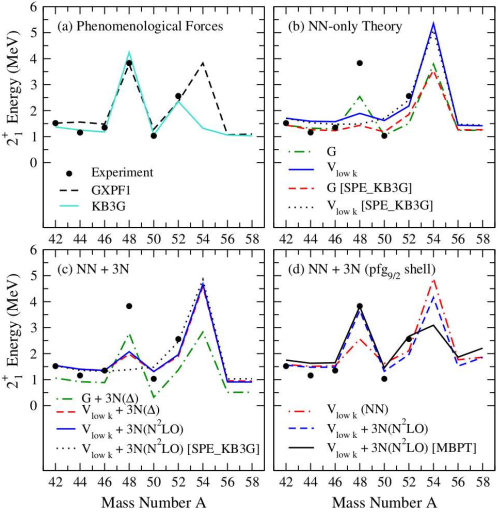
Technical details

- Chiral interaction at N^3LO.
- Density dependent three body force with $k_F = 0.95\text{fm}^{-1}$, $c_D = -0.2$ and $c_E = 0.735$. $N_{max} = 18$ and $\hbar\omega = 26$ MeV.
- Mass of ^{51}Ca and ^{52}Ca from A. T. Gallant *et al.*, PRL 109, 032506 (2012)

Main features

- Total binding energies agree well with experimental masses.
- ^{60}Ca is not magic.
- Three nucleon force is repulsive.

Shell evolution in neutron rich calcium isotopes.



Details

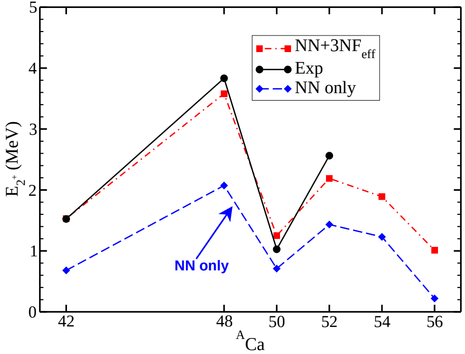
- J. D. Holt, T. Otsuka, A. Schwenk and T. Suzuki, J Phys G39 085111 (2012)..
- $J^{\pi} = 2^{+}$ systematics in even calcium isotopes.

Main features

- Threebody forces needed to make ^{48}Ca magic.
- Different models have ^{54}Ca magic, semi magic and not magic at all.

$J^\pi = 2^+$ systematics in even calcium isotopes

G. Hagen, M. Hjorth-Jensen, GRJ, R. Machleidt, and T. Papenbrock, PRL109 032502 (2012)



	^{48}Ca	^{52}Ca	^{54}Ca
E_{2^+}(CC)	3.58	2.19	1.89
E_{2^+}(Exp)	3.83	2.56	n.a.
E_{4^+}/E_{2^+}(CC)	1.17	1.80	2.36
E_{4^+}/E_{2^+}(Exp)	1.17	n.a.	n.a.
S_n(CC)	9.45	6.59	4.59
S_n(Exp)	9.95	6.0*	4.0†

Technical details

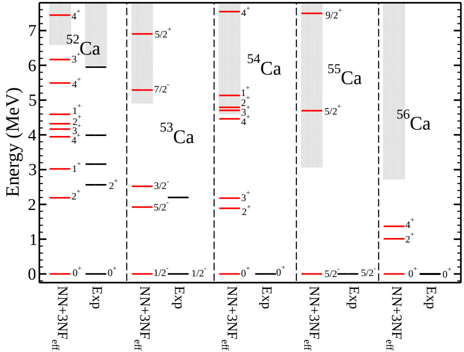
- Chiral interaction at N^{3}LO.
- Density dependent three body force with $k_F = 0.95\text{fm}^{-1}$, $c_D = -0.2$ and $c_E = 0.735$. $N_{max} = 18$ and $\hbar\omega = 26$ MeV.

Main features

- Good agreement between theory and experiment.
- Shell closure in ^{48}Ca.
- Sub-shell closure in ^{52}Ca.
- Predict weak sub-shell closure in ^{54}Ca.

Spectra in calcium isotopes

G. Hagen, M. Hjorth-Jensen, GRJ, R. Machleidt, and T. Papenbrock,
PRL109 032502 (2012)



	^{53}Ca		^{55}Ca		^{61}Ca	
J^π	Re[E]	Γ	Re[E]	Γ	Re[E]	Γ
$5/2^+$	1.99	1.97	1.63	1.33	1.14	0.62
$9/2^+$	4.75	0.28	4.43	0.23	2.19	0.02

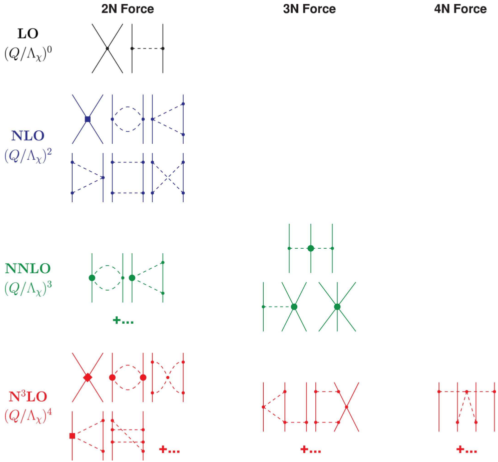
Technical details

- Chiral interaction at N^3LO.
- Density dependent three body force with $k_F = 0.95\text{fm}^{-1}$, $c_D = -0.2$ and $c_E = 0.735$. $N_{max} = 18$ and $\hbar\omega = 26$ MeV.
- Continuum included for selected weakly bound and resonant states.

Main features

- Inversion of $g_{9/2}$ and $d_{5/2}$.
- $1/2^+$ groundstate in ^{61}Ca.
- Continuum effects are crucial.

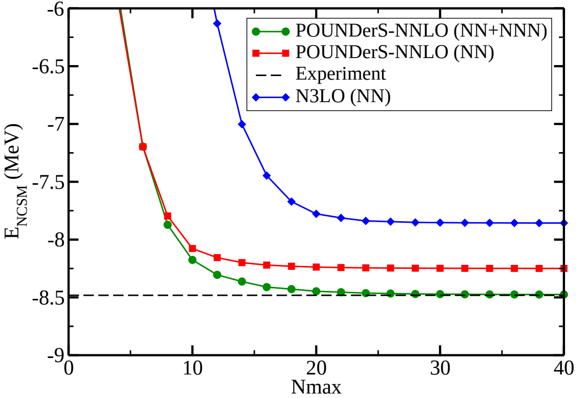
NNLO (POUNDerS)



- Want to derive consistent forces.
- All contributions at a given order are evaluated.
- Currently NNLO.
- Apply numerical optimization algorithms to find the optimal parameters.

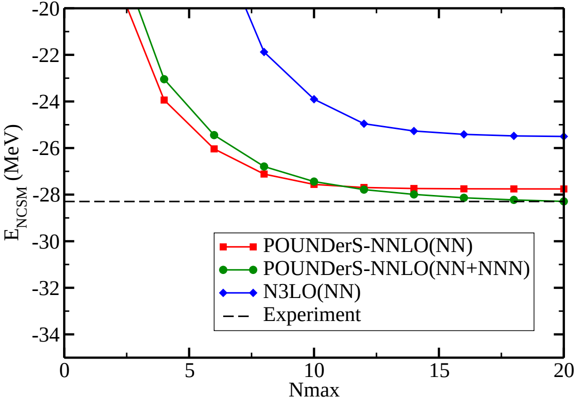
Triton binding energy

A. Ekström, Baardsen, Forssén, Hagen, Hjorth-Jensen, GRJ, Machleidt, Nazarewicz, Papenbrock, Sarich, Wild, arXiv:1303.4674 (2013)



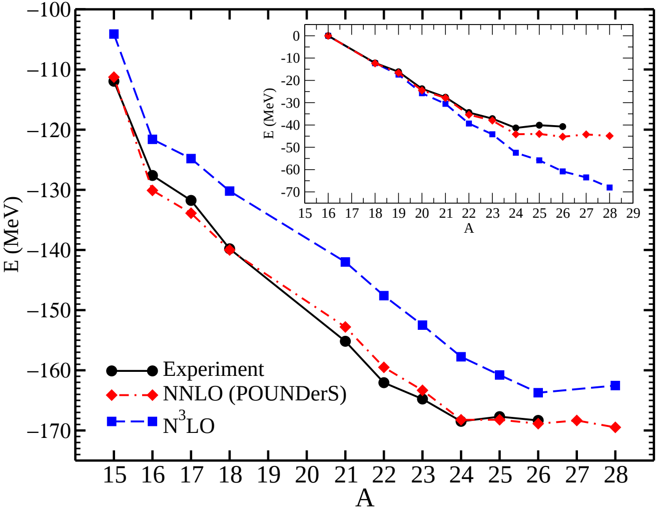
^{4}He binding energy

A. Ekström, Baardsen, Forssén, Hagen, Hjorth-Jensen, GRJ, Machleidt, Nazarewicz, Papenbrock, Sarich, Wild, arXiv:1303.4674 (2013)



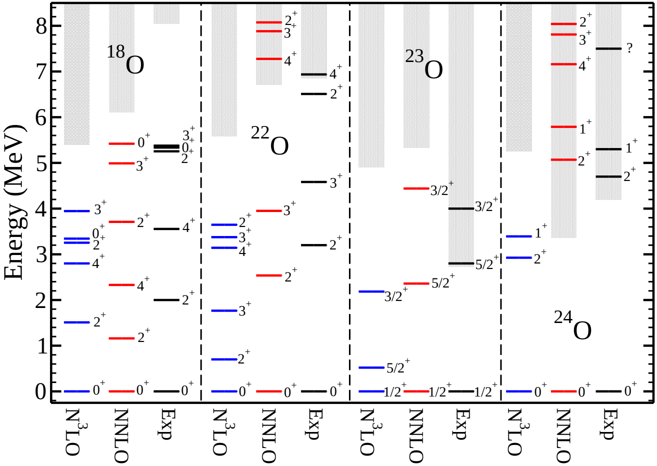
Oxygen isotopes with NNLO (POUNDerS)

A. Ekström, Baardsen, Forssén, Hagen, Hjorth-Jensen, GRJ, Machleidt, Nazarewicz, Papenbrock, Sarich, Wild, arXiv:1303.4674 (2013)



Oxygen spectra with NNLO (POUNDerS)

A. Ekström, Baardsen, Forssén, Hagen, Hjorth-Jensen, GRJ, Machleidt, Nazarewicz, Papenbrock, Sarich, Wild, arXiv:1303.4674 (2013)



$J^\pi = 2^+$ systematics with NNLO (POUNDerS)

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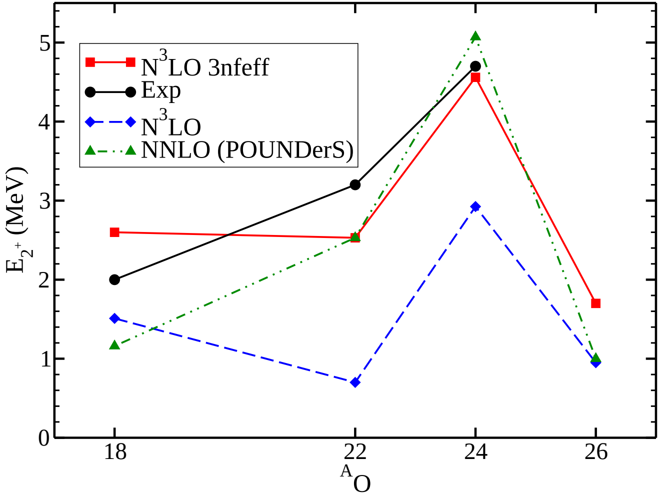

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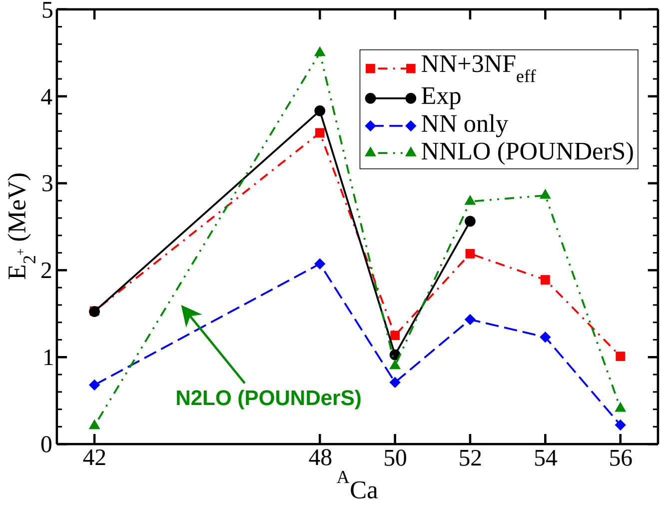

Calcium isotopes with NNLO (POUNDerS)

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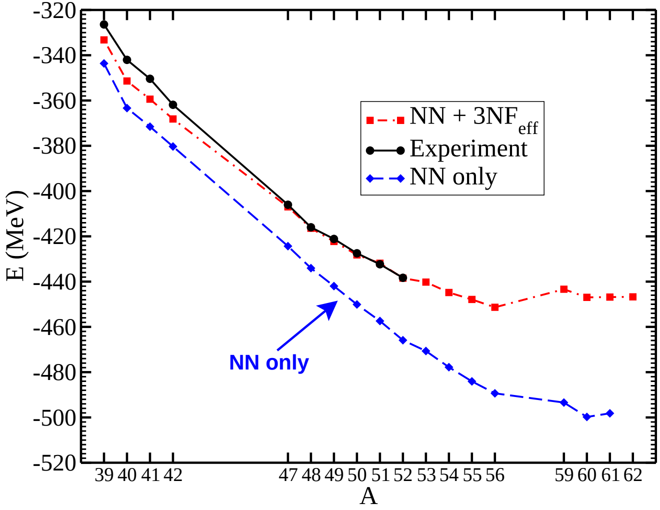

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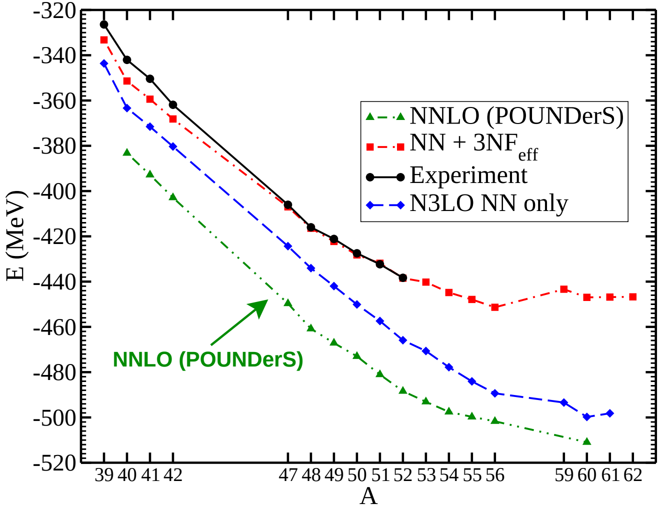

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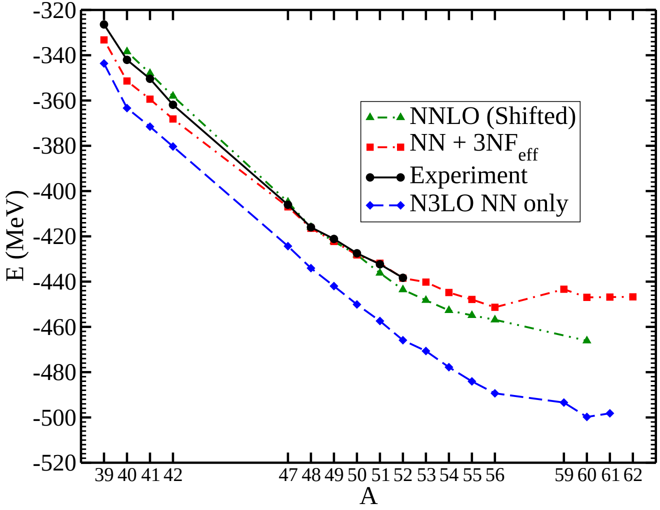

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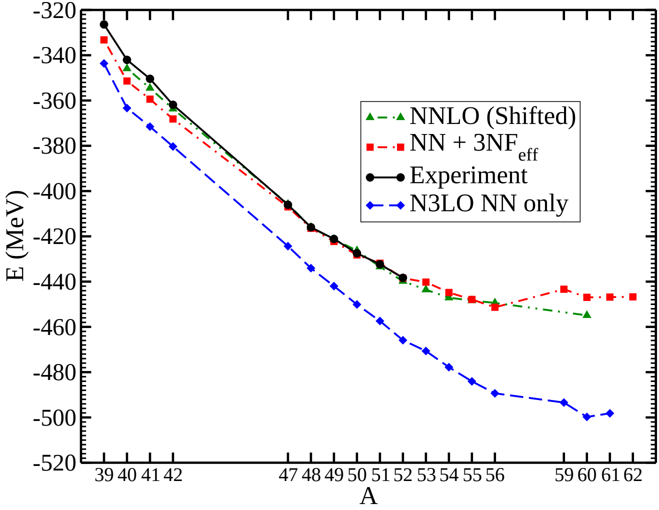

Questions?

Gustav R. Jansen
gustav.jansen@utk.edu

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