Ab Initio Nuclear Structure Theory

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National Nuclear Physics Summer School
SUNY Stony Brook
July 2013

I. Realistic NN & NNN Interactions and their range of validity

- Overview of these lectures
- Short historical review
- Review of NN+NNN interactions - emphasis on Chiral EFT
- Alternative NN interaction from inverse scattering – JISP16

Overall plan for the 3 lecture series by Prof. James P. Vary

1. Realistic NN & NNN Interactions and their range of validity

Short historical review
Review of NN+NNN interactions - emphasis on Chiral EFT
Alternative NN interaction from inverse scattering – JISP16

2. IR/UV Regulators and Renormalization Methods

IR and UV properties of the Harmonic Oscillator (HO)
IR and UV properties of NN interactions
Okubo-Lee-Suzuki (OLS) renormalization scheme in the HO basis
Similarity Renormalization Group (SRG) method

3. Recent results in light nuclei with ab initio no core methods

Overview of ab initio approaches (GFMC, CC, NCSM, NCFC)
Applications to light nuclei – importance of NNN
Applications to nuclear reactions – deferred due to time limits
Applications to non-perturbative solution of quantum field theory
Conclusions and outlook

Overarching Problem

Main hypothesis

If the Standard Model is correct, we should be able to accurately describe all nuclear processes

Long-term goal

Use all fundamental interactions including yet-to-be-discovered interactions to describe and predict experimental and astrophysical phenomena

Fundamental questions of nuclear physics => discovery potential

- What controls nuclear saturation?
- How shell and collective properties emerge from the underlying theory?
- What are the properties of nuclei with extreme neutron/proton ratios?
- Can we predict useful cross sections that cannot be measured?
- Can nuclei provide precision tests of the fundamental laws of nature?
- Can we solve QCD to describe hadronic structures and interactions?

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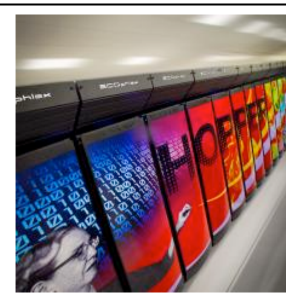


+ K-super.
+ Blue Waters
+ Lomonosov
+ Tachyon-II

ab initio nuclear theory - building bridges

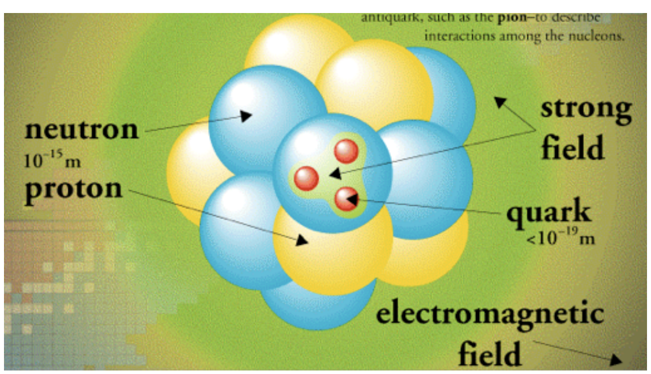
Standard Model (QCD + Electroweak)

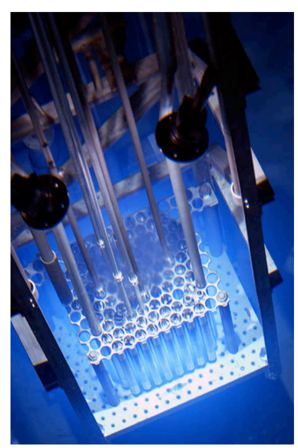
NN + NNN interactions & effective EW operators

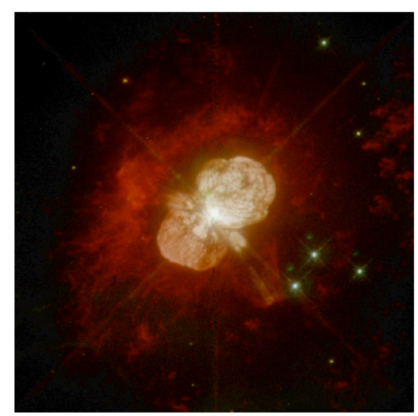
quantum many-body theory

describe/predict experimental data

UPDATE







A (very) brief history of NN interactions

- 1935 – Yukawa (meson theory)
- 1957 – Gammel and Thaler (full theory of OPE)
- 1960’s – non-relativistic OBEP (pions, scalar mesons)
  Bryan-Scott potential (1969)
- 1970’s – fully relativistic OBEPs -- 2-pion exchange
  Stony Brook, Paris, Bonn
- 1980’s – Nijmegen potentials (1978)
- 1990’s – Nijmegen II, Bonn potentials
- 1990’s – AV18 + 3-body (NNN) potentials
- 2000’s – chiral EFT potentials (2-body and 3-body)

χ^2 / dof ~ 10 in 1960’s; ~ 2 in 1980’s ; ~1 in 1990’s….

OPE = One Pion Exchange	AV18 = Argonne V18 (18 operators)
OBEP = One Boson Exchange Potential	EFT = Effective Field Theory

Can we “derive” the NN interaction from QCD?

- What is the role of confinement?
- If derivation is successful, is this the full story?
- What about probing nuclei at ever higher energies & densities?

=> Need a perspective on derivations of interactions

All interactions are "effective" until the ultimate theory unifying all forces in nature is attained.

Thus, even the Standard Model, incorporating QCD,
is an effective theory valid below the Planck scale
$\lambda < 10^{19}$ GeV/c

The "bare" NN interaction, usually with derived quantities,
is thus an effective interaction valid up to some scale, typically
the scale of the known NN phase shifts and Deuteron properties
$\lambda \sim 600$ MeV/c ($3.0\ \mathrm{fm}^{-1}$)

Effective NN interactions can be further renormalized to lower scales
and this can enhance convergence of the many-body applications
$\lambda \sim 300$ MeV/c ($1.5\ \mathrm{fm}^{-1}$)

"Consistent" NNN and higher-body forces, as well as electroweak
currents, are those valid to the same scale as their corresponding
NN partner, and obtained in the same renormalization scheme.

ab initio renormalization schemes

SRG: Similarity Renormalization Group
OLS: Okubo-Lee-Suzuki
Vlowk: V with low k scale limit
UCOM: Unitary Correlation Operator Method
and there are more!

Realistic NN & NNN interactions
High quality fits to 2- & 3- body data

Need
Consistent
EW operators

Meson-exchange

NN: AV18, CD-Bonn, Nijmegen, . . .
NNN: Tucson-Melbourne, UIX, IL7, . . .

Need
Improved NNN

Chiral EFT (Idaho)

NN: N3LO
NNN: N2LO
4N: predicted & needed for consistent N3LO

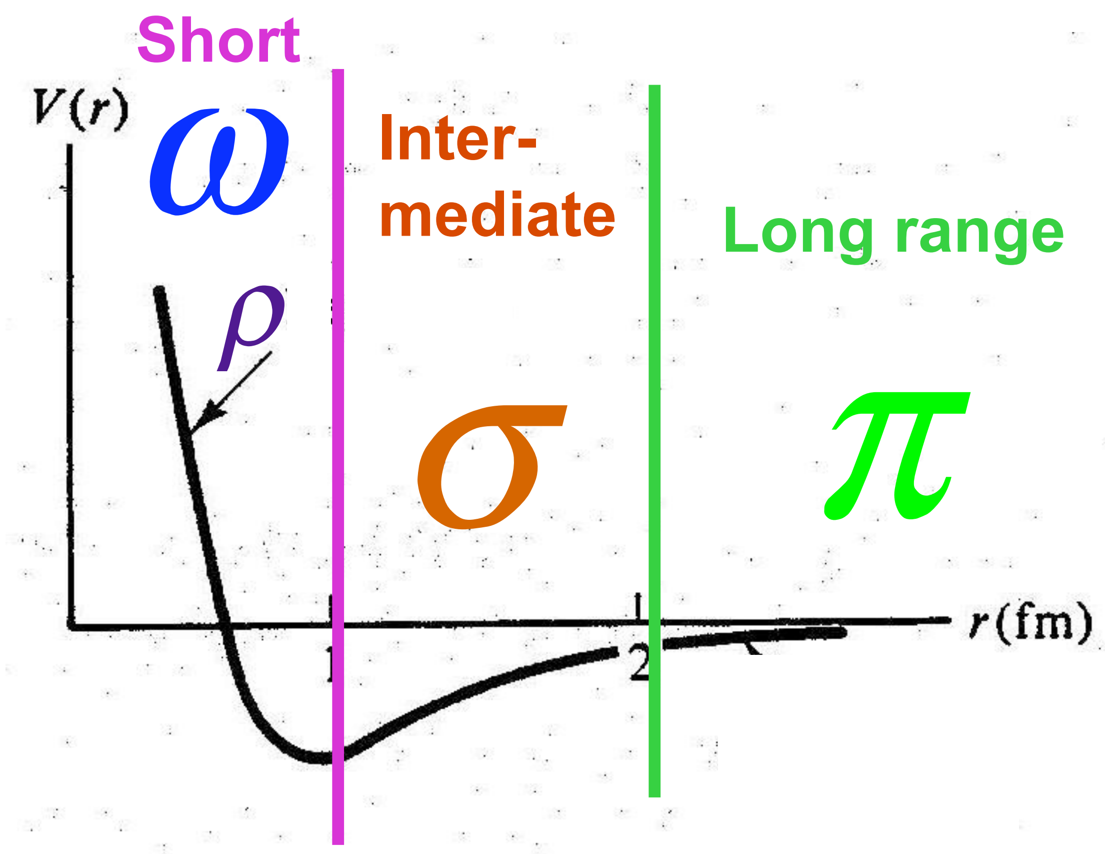
Need
Fully derived/coded
NNN(N3LO)

Inverse Scattering

NN: JISP16

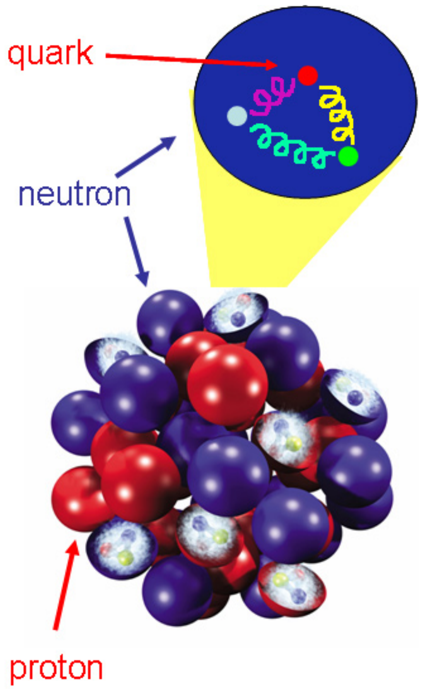
Need
JISP40
Consistent NNN

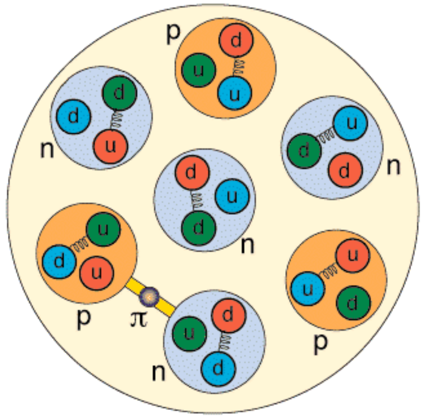
While Chiral EFT is a theory based on an expansion in a momentum scale parameter, meson-exchange models are based on arguments for coordinate space roles of massive meson exchanges.

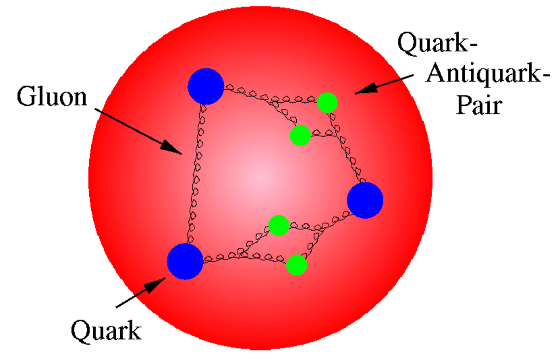


Adapted from R. Machleidt NTSE-2013

Effective Field Theory







Interplay between nucleonic and subnucleonic (quarks and gluons) degrees of freedom in few-body nuclear system!

Starting point is an effective chiral πN Lagrangian:

$$L_{\pi N} = L_{\pi N}^{(1)} + L_{\pi N}^{(2)} + L_{\pi N}^{(3)} + \ldots$$

- Obeys QCD symmetries (spin, isospin, chiral symmetry breaking)
- Develops a low-momentum interaction suitable for nuclei
- Should some day be connected directly to QCD?

The heavy baryon (HB) formulation of χ**PT**:

$$L_{\pi N}^{(1)} = \overline{N}(iD_0 - \frac{g_A}{2}\vec{\sigma}\bullet\vec{u})N \approx \overline{N}[i\partial_0 - \frac{1}{4f_\pi^2}\tau\bullet(\pi\times\partial_0\pi) - \frac{g_A}{2f_\pi}\tau\bullet(\vec{\sigma}\bullet\nabla)\pi]N + \ldots$$

Effective Field Theory

$$L_{\pi N}^{(2)} = L_{\pi N,fix}^{(2)} + L_{\pi N,ct}^{(2)}$$

$$L_{\pi N,fix}^{(2)} = \overline{N}[\frac{1}{2M_N}\vec{D}\cdot\vec{D} + i\frac{g_A}{4M_N}\{\vec{\sigma}\cdot\vec{D},u_0\}]N$$

$$L_{\pi N,ct}^{(2)} = \overline{N}[2c_1 m_\pi^2(U+U^+) + (c_2 - \frac{g_A^2}{8M_N})u_0^2 + c_3 u_\mu u^\mu + \frac{i}{2}(c_4 + \frac{1}{4M_N})\vec{\sigma}.(\vec{u}\times\vec{u})]N$$

Where (D, U, u_μ) are quantities defined in terms of the pion field

Chiral symmetry of QCD (m_u & m_d->0), spontaneously broken with pion as the Goldstone boson

❖ Systematic low-momentum expansion in (Q/Λ; Λ ~ 1 GeV; Q ≤ 135 MeV [c=1])
   - •Power-counting
   - •Chiral perturbation theory (χPT)

❖ Describe pion-pion, pion-nucleon and inter-nucleon interactions at low energies
   - Nucleon-nucleon sector - S. Weinberg (1991)
   - Worked out by van Kolck, Kaiser, Meissner, Epelbaum, Machleidt…

For more details see:
V. Bernard, N. Kaiser and U.G. Meissner, *Int. J. Mod. Phys. E4, 193 (1995)*;
D.R. Entem and R. Machleidt, Phys.Lett. B524 93 (2002); arXiv 0108057

Can we obtain NN (and NNN) interactions directly from Lattice QCD?

N. Ishii, S. Aoki and T. Hatsuda,
``The Nuclear Force from Lattice QCD,''
Phys. Rev. Lett. 99, 022001 (2007)

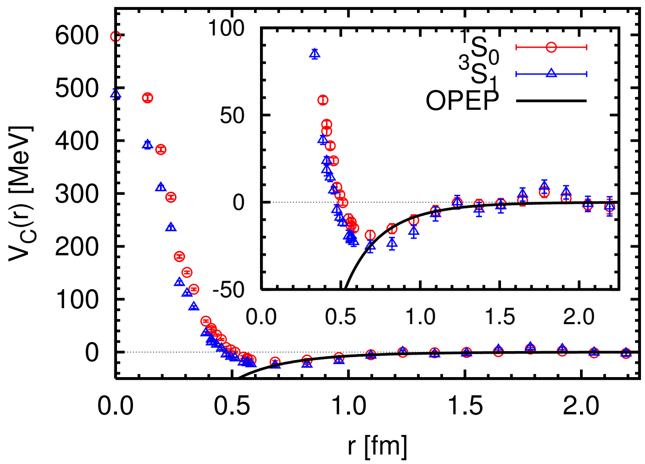


FIG. 3: The lattice QCD result of the central (effective central) part of the NN potential $V_C(r)$ ($V_C^{\rm eff}(r)$) in the $^1S_0$ ($^3S_1$) channel for $m_\pi/m_\rho = 0.595$. The inset shows its enlargement. The solid lines correspond to the one-pion exchange potential (OPEP) given in Eq.(5).

S. R. Beane, W. Detmold, K. Orginos & M. J. Savage,
``Nuclear Physics from Lattice QCD,''
Prog. Part. Nucl. Phys. 66, 1 (2011);
See Silas Beane, NNPSS2013-Lecture 3 for extrapns.

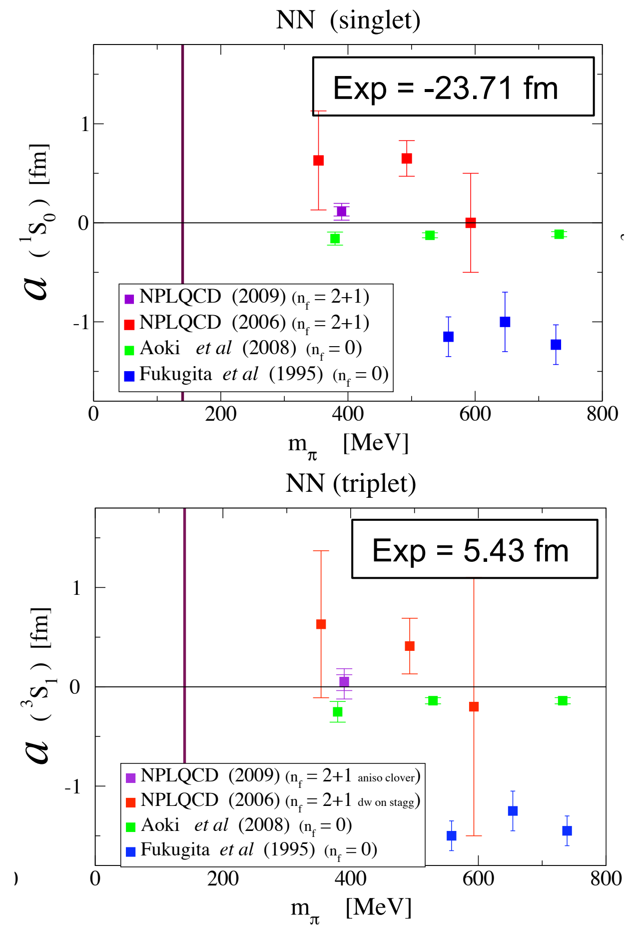


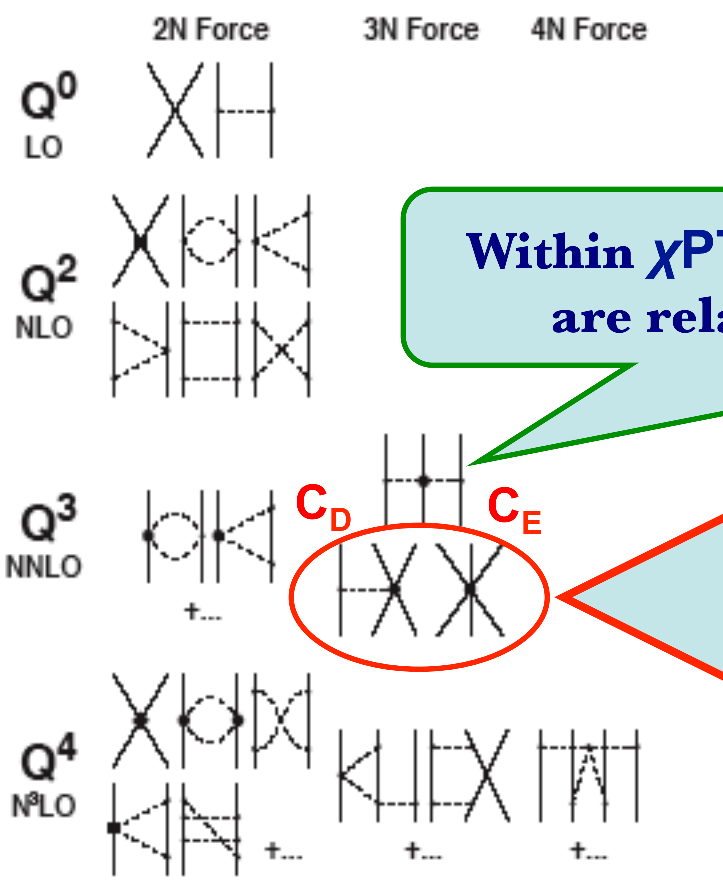
Fig. 14 NN scattering lengths in quenched Lattice QCD. Vertical lines correspond to the physical pion mass.

Effective Nucleon Interaction
(Chiral Perturbation Theory)

Chiral perturbation theory (χPT) allows for controlled power series expansion

Expansion parameter : $\left(\frac{Q}{\Lambda_\chi}\right)^\upsilon$, Q – momentum transfer,

$\Lambda_\chi \approx 1\ GeV$, χ - symmetry breaking scale



R. Machleidt, D. R. Entem, nucl-th/0503025

Within χPT 2π-NNN Low Energy Constants (LEC) are related to the NN-interaction LECs $\{c_i\}$.

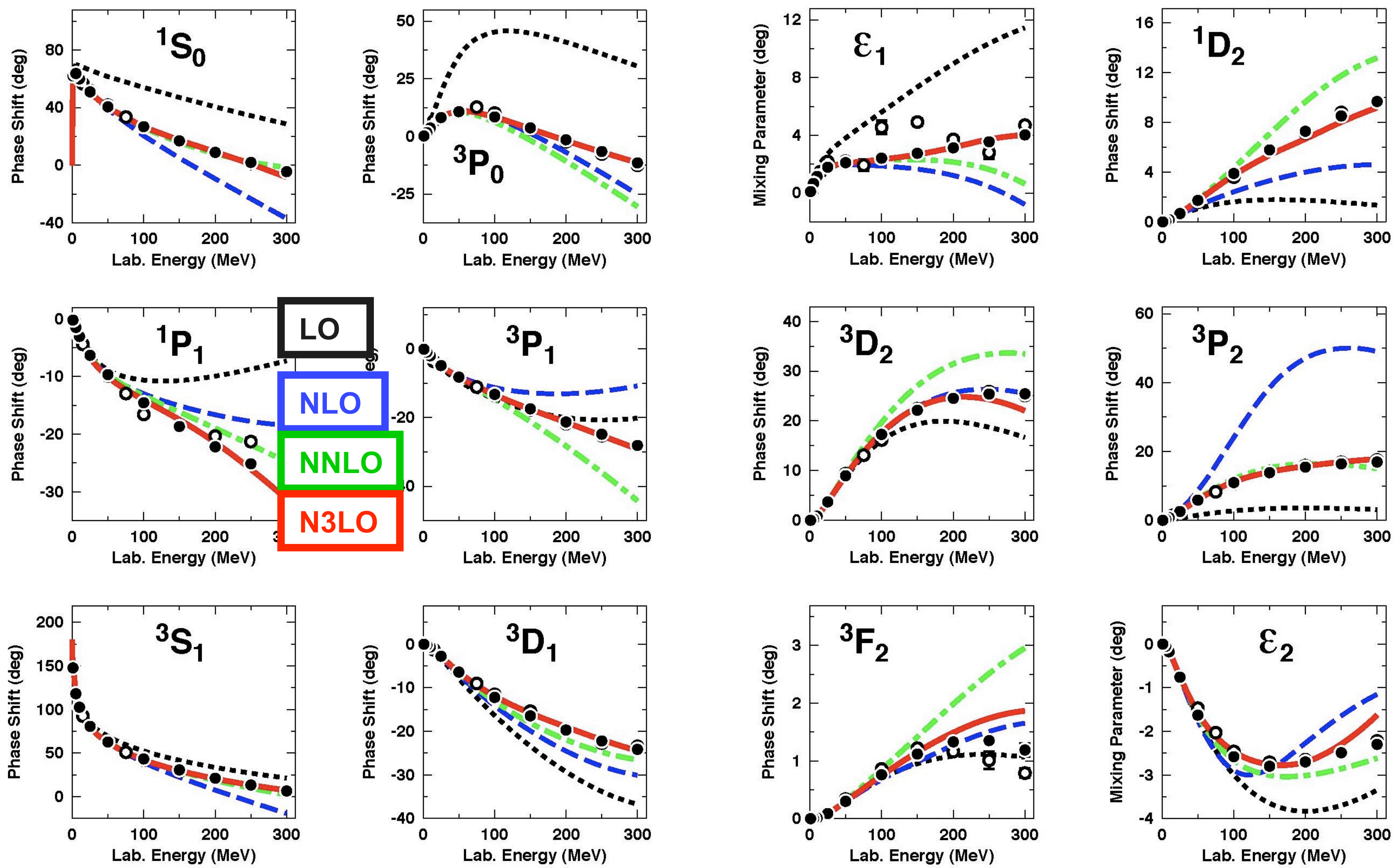
Terms suggested within the
Chiral Perturbation Theory

Regularization is essential, which is also implicit within the Harmonic Oscillator (HO) wave function basis (see below)

D.R. Entem and R. Machleidt, Phys Rev C68, 041001(R) (2003)

NN phase shifts up to 300 MeV

Red Line: N3LO Potential by Entem & Machleidt, PRC 68, 041001 (2003).
Green dash-dotted line: NNLO Potential, and
blue dashed line: NLO Potential
by Epelbaum et al., Eur. Phys. J. A19, 401 (2004).



R. Machleidt, NTSE 2013

PRL 110, 192502 (2013) PHYSICAL REVIEW LETTERS week ending 10 MAY 2013

Optimized Chiral Nucleon-Nucleon Interaction at Next-to-Next-to-Leading Order

A. Ekström,[1,2] G. Baardsen,[1] C. Forssén,[3] G. Hagen,[4,5] M. Hjorth-Jensen,[1,2,6] G. R. Jansen,[4,5] R. Machleidt,[7]
W. Nazarewicz,[5,4,8] T. Papenbrock,[5,4] J. Sarich,[9] and S. M. Wild[9]

Bin (MeV)	# of data	N^3LO	NNLO	NLO	AV18
0–100	1058	1.05	1.00	4.5	0.95
100–190	501	1.08	1.87	100	1.10
190–290	843	1.15	6.09	180	1.11
0–290	2402	1.10	2.95	86	1.04

N3LO Potential by Entem & Machleidt, PRC 68, 041001 (2003).
NNLO and NLO Potentials by Epelbaum et al., Eur. Phys. J. A19, 401 (2004).

Phenomenological NN interaction: JISP16

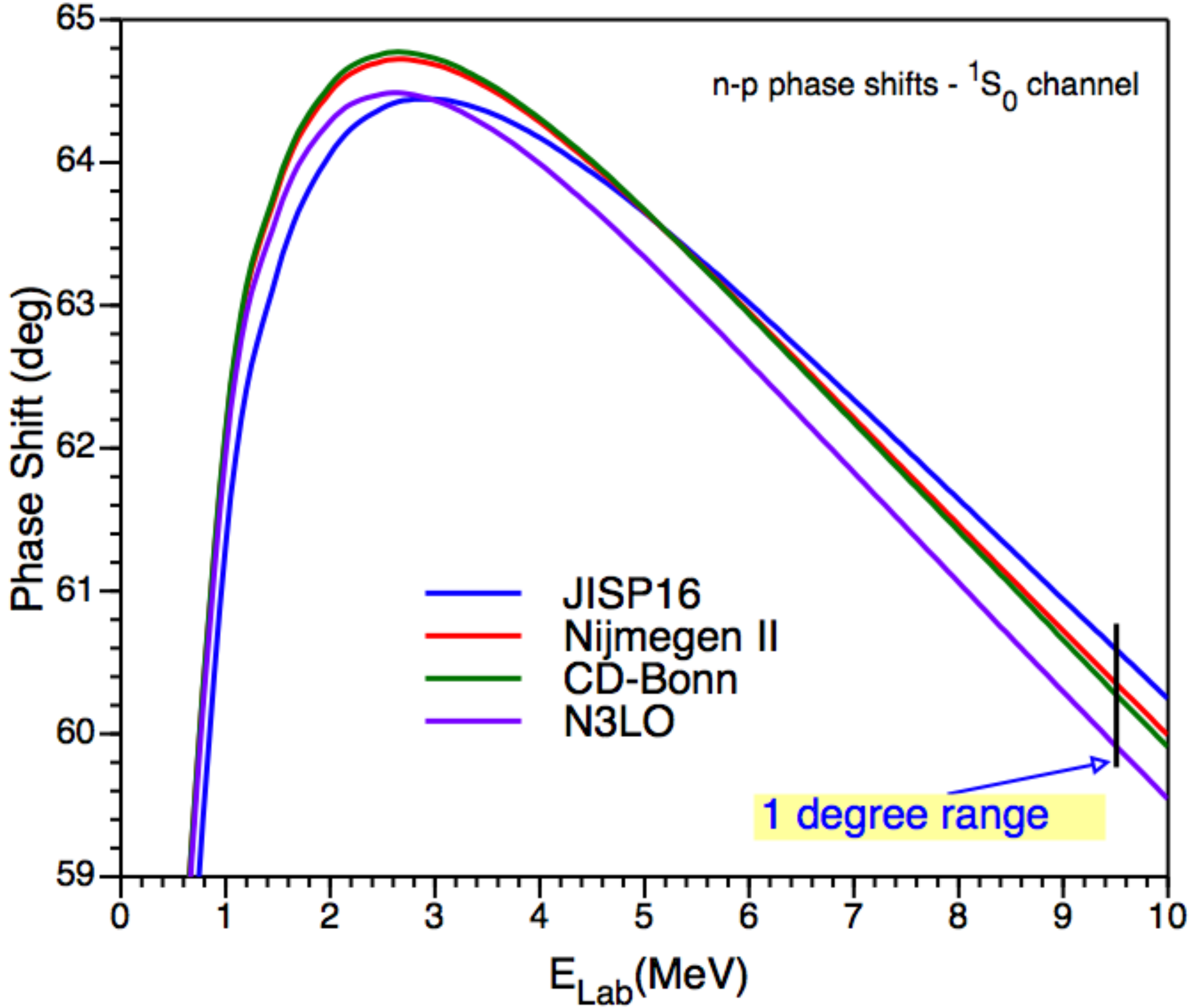
J-matrix **I**nverse **S**cattering **P**otential tuned up to ^{16}O

A. M. Shirokov, J. P. Vary, A. I. Mazur and T. A. Weber Phys. Letts. B 644, 33 (2007)

- Finite rank separable potential in HO representation for each partial wave
- Fitted to available NN scattering data and Deuteron properties
- Use unitary transformation to tune off-shell interaction to
  - binding energy of ^{3}He
  - low-lying spectrum of ^{6}Li (JISP6 precursor of JISP16)
  - binding energy of ^{16}O
- Good fit to a range of light nuclear properties
- Very soft potential compared to other NN potentials
- Non-local potential (by construction)
- Details, including JISP16 subroutine, available at

http://nuclear.physics.iastate.edu/

$$\langle k | V^{ll'SJ}_{JISP16} | k' \rangle = \sum_{nn'}^{n_{max}} \langle k | nl \rangle A^{SJ}_{nl\,n'l'} \langle n'l' | k' \rangle = \sum_{n,n'}^{n_{max}} A^{SJ}_{nl\,n'l'} R_{nl}(k) R_{n'l'}(k')$$



n-p phase shifts - $^1S_0$ channel
JISP16
Nijmegen II
CD-Bonn
N3LO
1 degree range
Phase Shift (deg)
E_{Lab}(MeV)
65
64
63
62
61
60
59
0
1
2
3
4
5
6
7
8
9
10

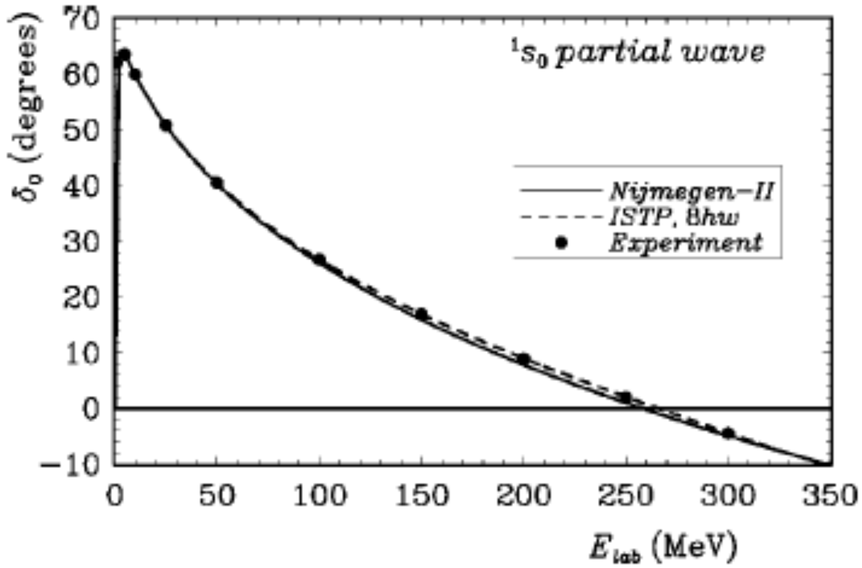


FIG. 1. $^1s_0$ np scattering phase shifts. Filled circles—experimental data of Ref. [3]; solid line—realistic meson exchange Nijmegen-II potential (See Ref. [3]) phase shifts; dashed line—ISTP phase shifts.

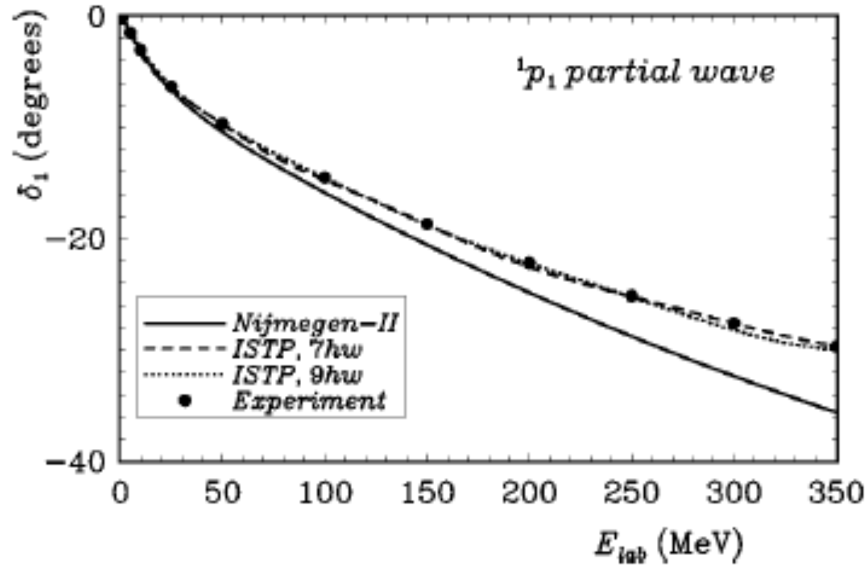


FIG. 3. $^1p_1$ np scattering phase shifts. Filled circles—experimental data of Ref. [3]; solid line—realistic meson exchange Nijmegen-II potential (See Ref. [3]) phase shifts; dashed line—$7\hbar\omega$ ISTP phase shifts; dotted line—$9\hbar\omega$ ISTP phase shifts.

Adapted from A.M. Shirokov, et al., Phys Rev C70, 044005 (2004)

Reference web sites:

"Nijmegen" phase shifts	http://nn-online.org/
"SAID" phase shifts	http://gwdac.phys.gwu.edu/

$^1S_0$ np scattering lengths and effective ranges (in fm)

	Experiment	Nijmegen II[5] eff EM?	Argonne V18[2] withEM/noEM	N3LO[5] eff EM	JISP16 no EM
a_{np}	-23.74 ± 0.020[1]	-23.738	-23.732 / -23.084	-23.732	-22.442[3]
	-23.749 ± 0.008[2]				-22.448[4]
r_{np}	2.77 ± 0.05[1]	2.670	2.697 / 2.703	2.725	2.597[3]
	2.81 ± 0.05[2]				2.586[4]

References:

1. C. Downum, J.R. Stone, T. Barnes, E.S. Swanson and I. Vidanya, arXiv:1001.3320v1.
2. R.B. Wiringa, V.G.J. Stoks and R. Schiavilla, Phys. Rev. C 51, 38 (1995).
3. Using effective range expansion and Schroedinger solutions at T(lab) = 0.05 & 0.10 MeV
4. Analytic extraction from J-matrix scattering amplitude for JISP16 (A. Mazur provided)
5. Provided by Ruprecht Machleidt in email of 2/20/10

Table 3
deuteron property predictions in comparison with the ones obtained with various realistic potentials

Potential	E_d, MeV	d state probability, %	rms radius, fm	Q, fm^2	As. norm. const. $\mathcal{A}_s$, fm$^{-1/2}$	$\eta = \frac{\mathcal{A}_d}{\mathcal{A}_s}$
JISP6 /JISP16	−2.224575	4.1360	1.9647	0.2915	0.8629	0.0252
Nijmegen-II	−2.224575	5.635	1.968	0.2707	0.8845	0.0252
AV18	−2.224575	5.76	1.967	0.270	0.8850	0.0250
CD–Bonn	−2.224575	4.85	1.966	0.270	0.8846	0.0256
Nature	−2.224575(9)	–	1.971(6)	0.2859(3)	0.8846(9)	0.0256(4)

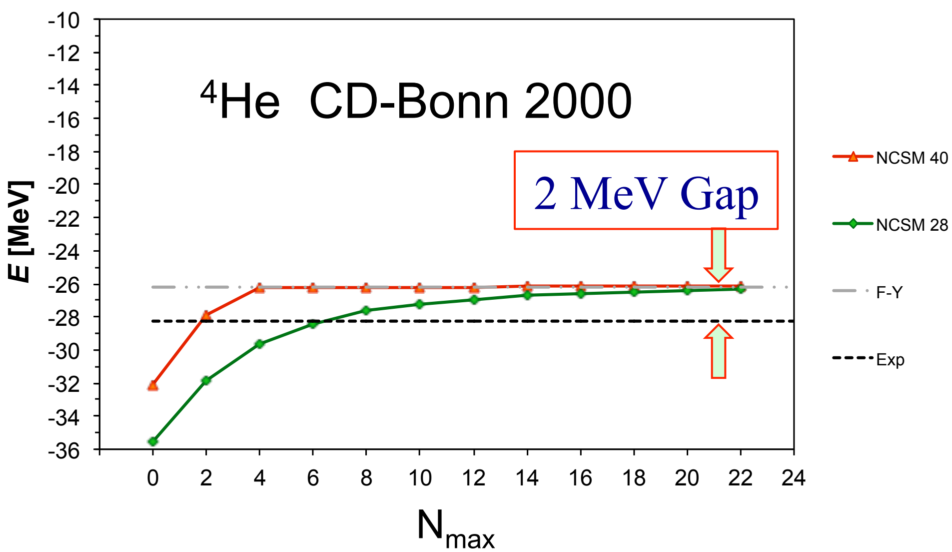
Table 4
The binding energies of ^{3}H, ^{3}He, ^{4}He, ^{6}He and ^{6}Li nuclei obtained with JISP6 in NCSM with $\hbar\omega = 15$ MeV in comparison with the results obtained with modern $NN + NNN$ interaction models in various approaches

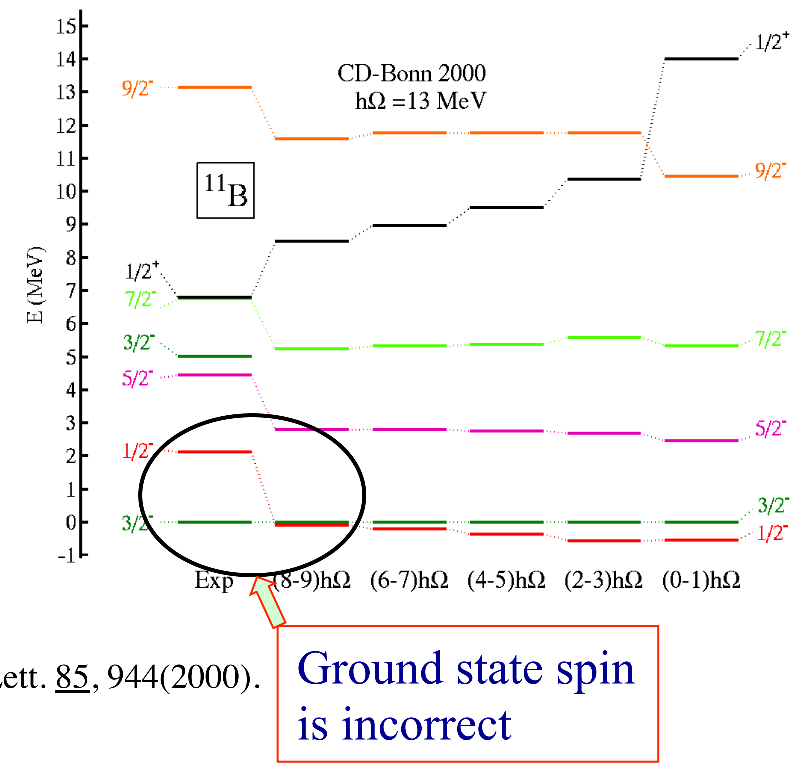
Potential and model	^{3}H	^{3}He	^{4}He	^{6}He	^{6}Li
JISP6, NCSM	8.461(5)	7.751(3)	28.611(41)	29.24(17)	31.48(27)
CD-Bonn+TM, Faddeev [17]	8.480	7.734	29.15		
AV18+TM, Faddeev [17]	8.476	7.756	28.84		
AV18 + TM′, Faddeev [17]	8.444	7.728	28.36		
NijmI+TM, Faddeev [17]	8.392	7.720	28.60		
NijmII+TM, Faddeev [17]	8.386	7.720	28.54		
AV18+UIX, Faddeev [17]	8.478	7.760	28.50		
AV18+UIX, GFMC [8]	8.46(1)	7.71(1)	28.33(2)	28.1(1)	31.1(1)
AV18+IL2, GFMC [8]	8.43(1)	7.67(1)	28.37(3)	29.4(1)	32.3(1)
AV8'+TM', NCSM [18]				28.189	31.036
Nature	8.48	7.72	28.30	29.269	31.995
JISP16, NCSM-2013*	8.369(1)#	7.668(5)#	28.299(1)#	28.8(1)*	31.49(6)*

#P. Maris, J.P. Vary and A.M. Shirokov, Phys. Rev. C79, 014308 (2009)
*P. Maris and J.P. Vary, Int. J. Mod. Phys. E., (in press).

Comments on need for NNN potentials

- Binding energies of A=3-4 nuclei can be calculated exactly in non-relativistic QM (NRQM). Realistic local NN potentials underbind A=3 by ~500keV and A=4 by 2-4 MeV. Compared to total interaction energy, <GS| V |GS>, these are 2-6% effects.
- Nearly exact results for 5<A<16 nuclei these days indicate spin-sensitive observables (splitting of spin-orbit partners in odd nuclei, ground state spin of ^{10}B, magnetic transitions, neutrino cross sections, etc.) require more than realistic local NN potential.





References:
A. Nogga, H. Kamada and W. Gloeckle, Phys. Rev. Lett. 85, 944(2000).
J.L. Friar, et al., Phys. Rev. C 59, 53(1999).
B.S. Pudliner, et al., Phys. Rev. Lett. 74, 4396(1995).
D.R. Entem, et al., Phys. Rev. C 68, 064001 (2002).

Chiral 3N Force

Δ-less

LO
$(Q/\Lambda_\chi)^0$

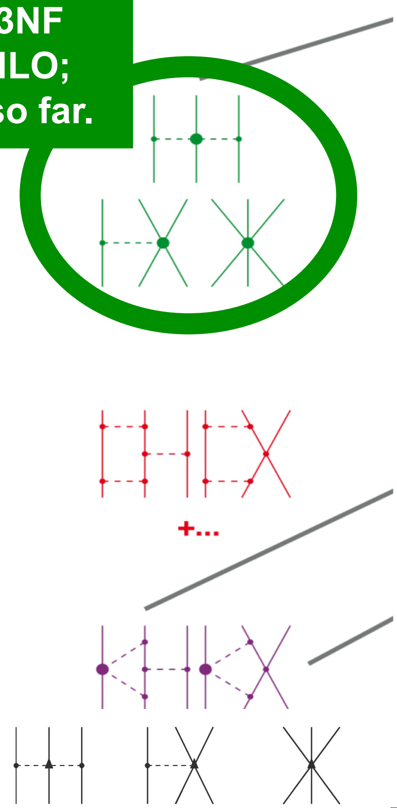
NLO
$(Q/\Lambda_\chi)^2$

The 3NF at NNLO; used so far.

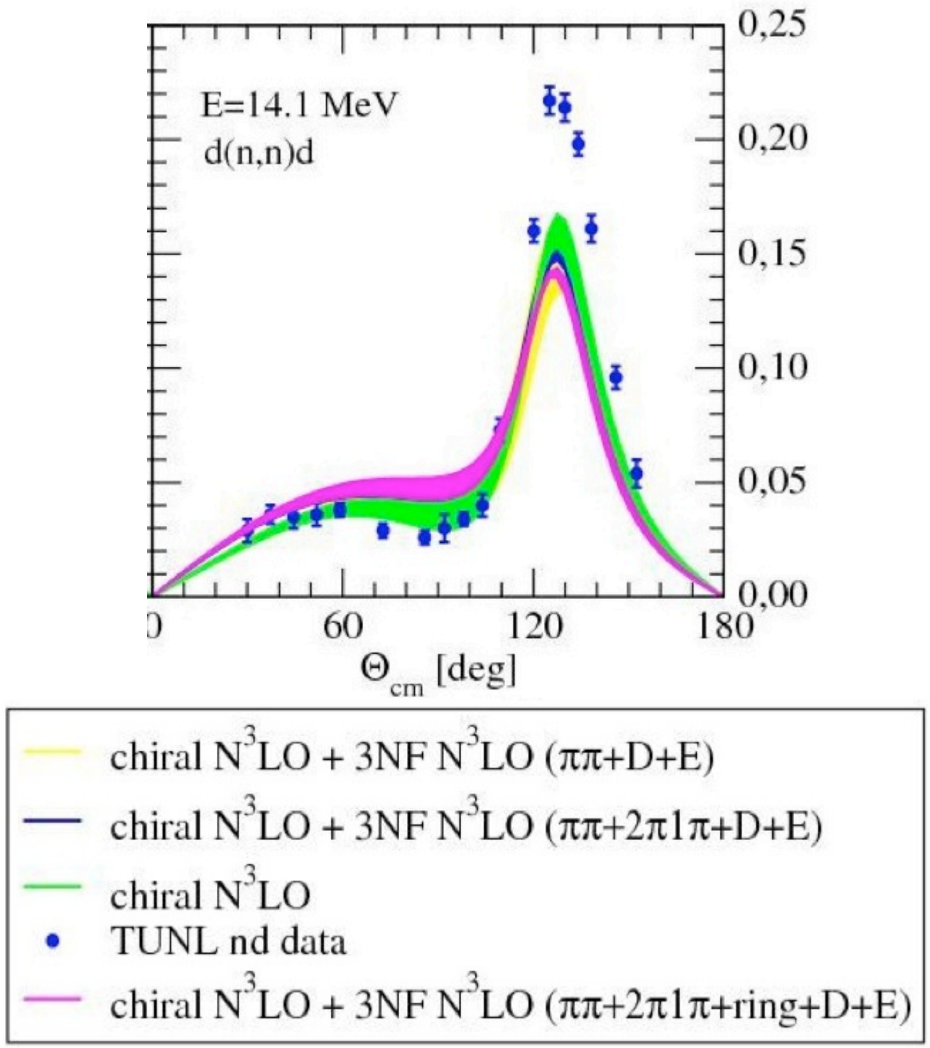
NNLO
$(Q/\Lambda_\chi)^3$

N^{3}LO
$(Q/\Lambda_\chi)^4$

N^{4}LO
$(Q/\Lambda_\chi)^5$



N-d A_y calculations by Witala et al.

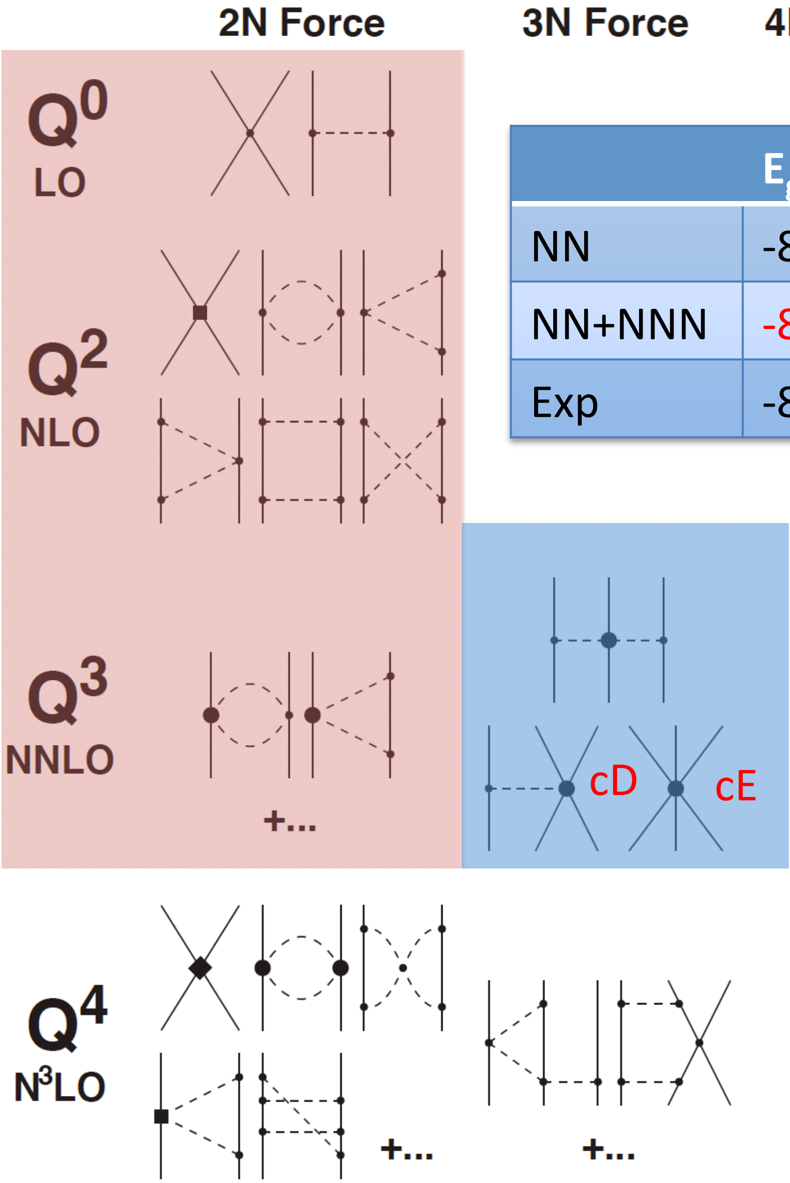


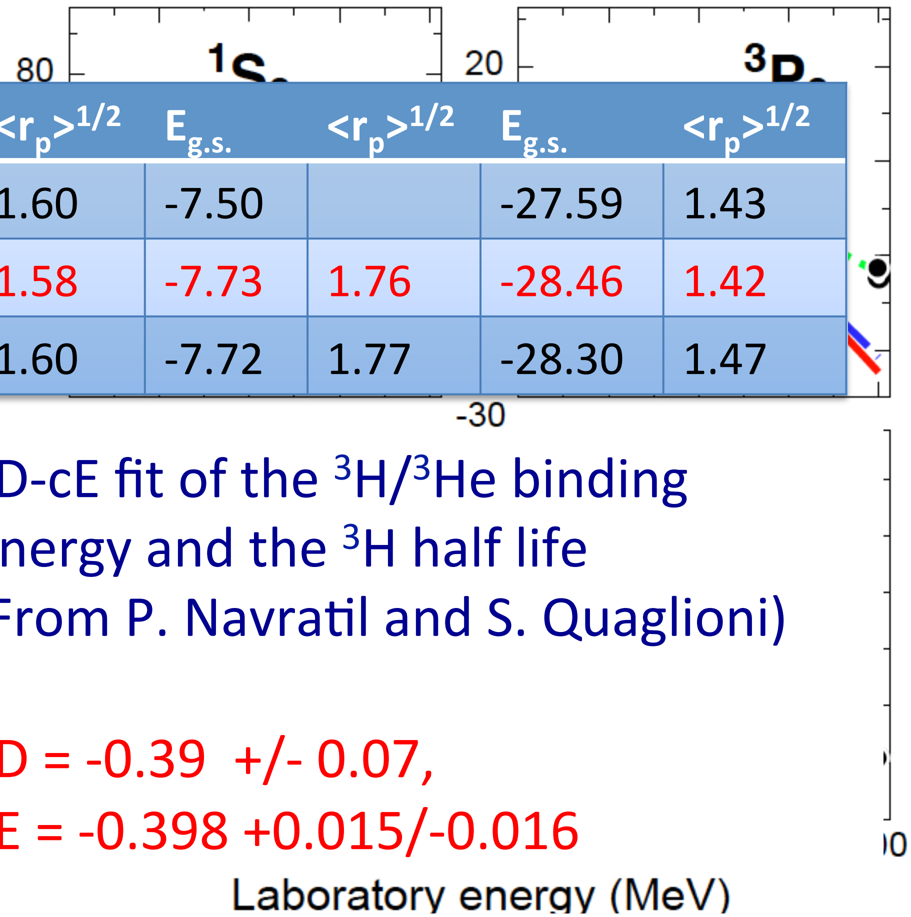
The Ay puzzle suggests re-examination of the current status of chiral EFT:

- Is there a need to better tune the LEC's?
- Do we need to go to N4LO to resolve it?
- Is there an alternative scheme, such as the Delta-full theory, that is better?

Optimization of Chiral interactions at NNLO

A. Ekström et al, Phys. Rev. Lett. 110, 192502 (2013)





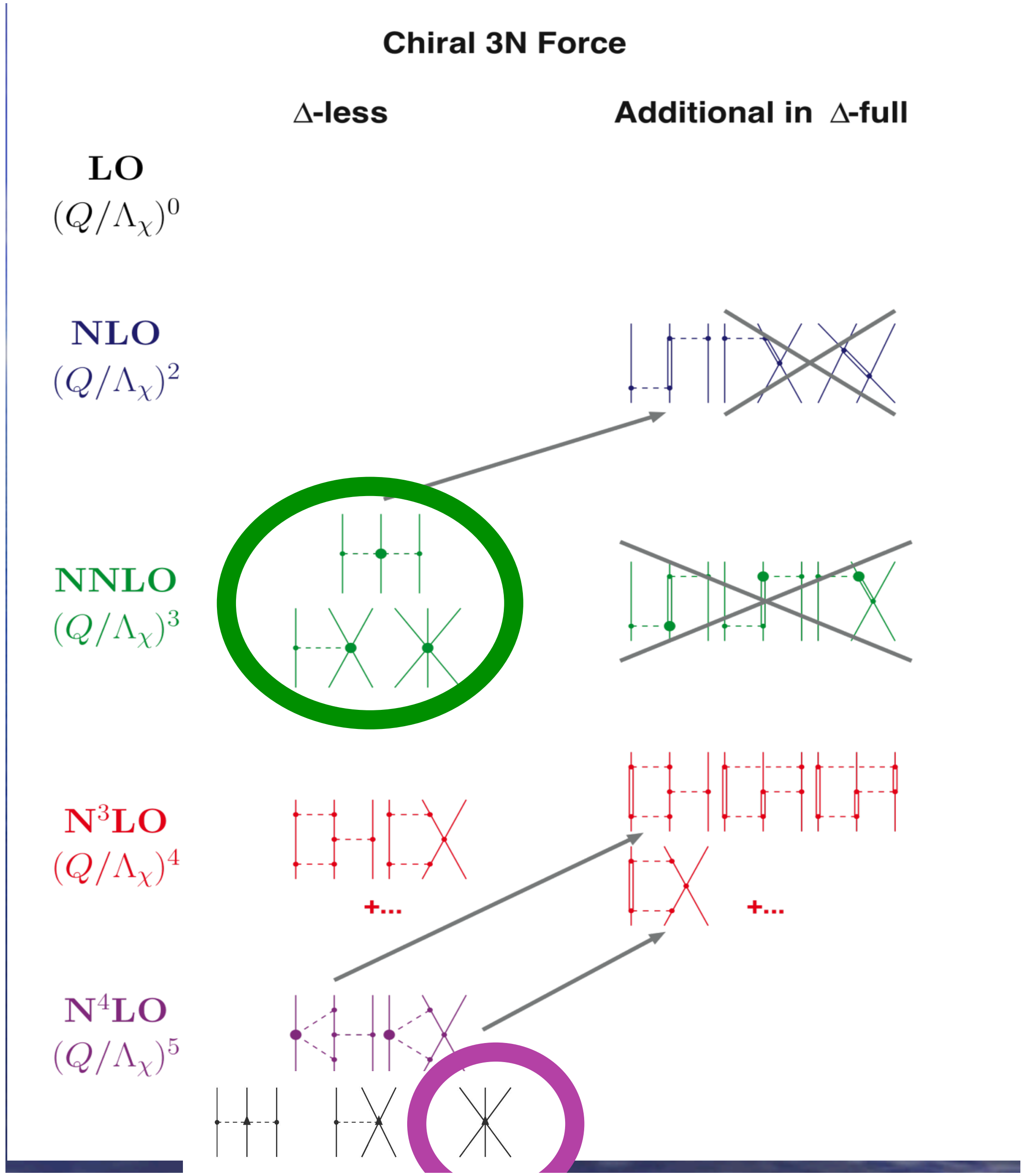
	$E_{g.s.}$	$\langle r_p \rangle^{1/2}$	$E_{g.s.}$	$\langle r_p \rangle^{1/2}$	$E_{g.s.}$	$\langle r_p \rangle^{1/2}$
NN	-8.25	1.60	-7.50		-27.59	1.43
NN+NNN	-8.48	1.58	-7.73	1.76	-28.46	1.42
Exp	-8.48	1.60	-7.72	1.77	-28.30	1.47

cD-cE fit of the $^3H/^3He$ binding energy and the ^3H half life (From P. Navratil and S. Quaglioni)

cD = -0.39 +/- 0.07,
cE = -0.398 +0.015/-0.016

$T_{\rm lab}$ (MeV)	0–35	35–125	125–183	183–290	0–290
pp χ^2/datum	1.11	1.56	23.95 4.35^a	29.26	17.10 14.03^a
np χ^2/datum	0.85	1.17	1.87	6.09	2.95

Gaute Hagen NTSE-2013



R. Machleidt, NTSE-2013

Questions?