Advances in nuclear structure calculations: extrapolations in finite model spaces and optimized chiral interactions at NNLO

Thomas Papenbrock

The University of Tennessee and Oak Ridge National Laboratory

R. J. Furnstahl, G. Hagen, TP, Phys. Rev. C 86, 031301(R) (2012); arXiv:1207.6100

Sushant N. More, A. Ekström, R. J. Furnstahl, G. Hagen, TP, arXiv:1302.3815

A. Ekström, G. Baardsen, C. Forssen, G. Hagen, M. Hjorth-Jensen, G. R. Jansen, R. Machleidt, W. Nazarewicz, TP, J. Sarich, S. M. Wild, arXiv:1303.4674

SciDAC Scientific Discovery through Advanced Computing

NUCLEI Nuclear Computational Low-Energy Initiative

Computational and Theoretical Advances for Exotic Isotopes in the Medium Mass Region

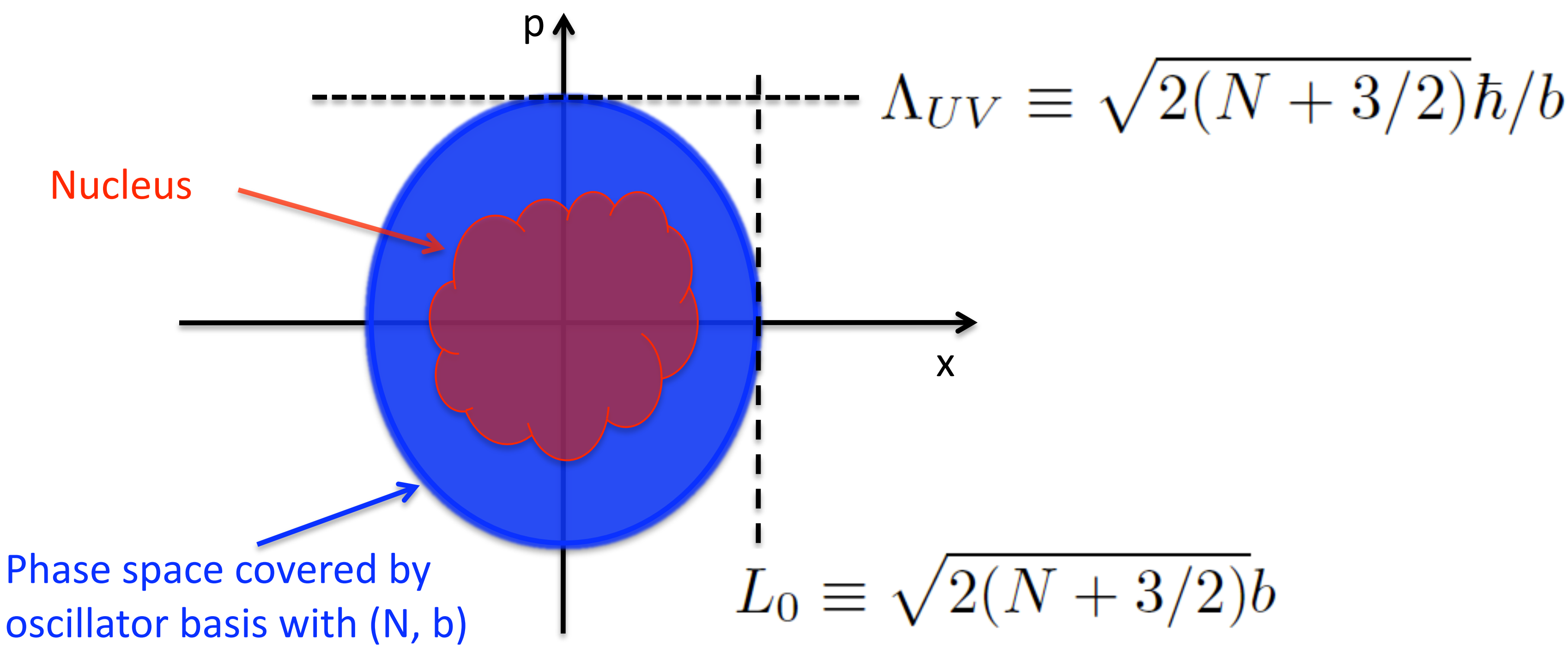
Institute for Nuclear Theory, Seattle — April 9, 2013

Research partly funded by the US Department of Energy

Convergence in finite oscillator spaces

Calculations are performed in finite oscillator spaces. How can one reliably extrapolate to infinity?

Convergence in momentum space (UV) and in position space (IR) needed



Nucleus needs to “fit” into basis:
- Nuclear radius R < L
- cutoff of interaction $\Lambda < \Lambda_{UV}$

What is the infrared cutoff in the HO basis?

(Question asked by Bira van Kolck at INT workshop in spring 2009. Bira's answer: 1/b [Stetcu, Barrett, van Kolck, Phys. Lett. B 653, 358 (2007); nucl-th0609023])

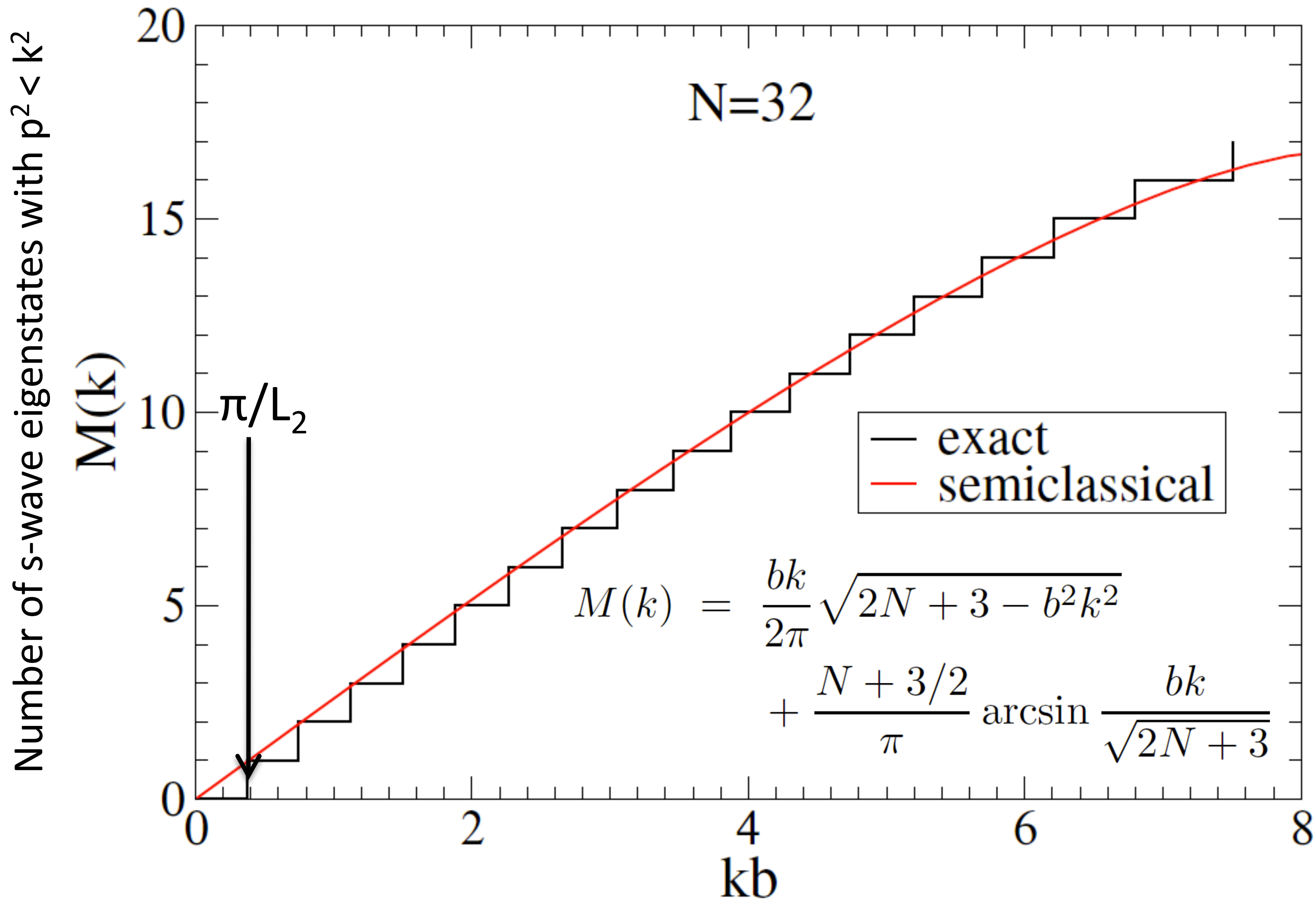
Very precise answer [More, Ekström, Furnstahl, Hagen, TP, 2013] based on length scale

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

1. At low energies, the HO basis looks like a "box" of radius L_2.
2. π/L_2 is the infrared cutoff.
3. Knowledge can be used for theoretically founded extrapolations in HO basis, computations of phase shifts in HO basis …

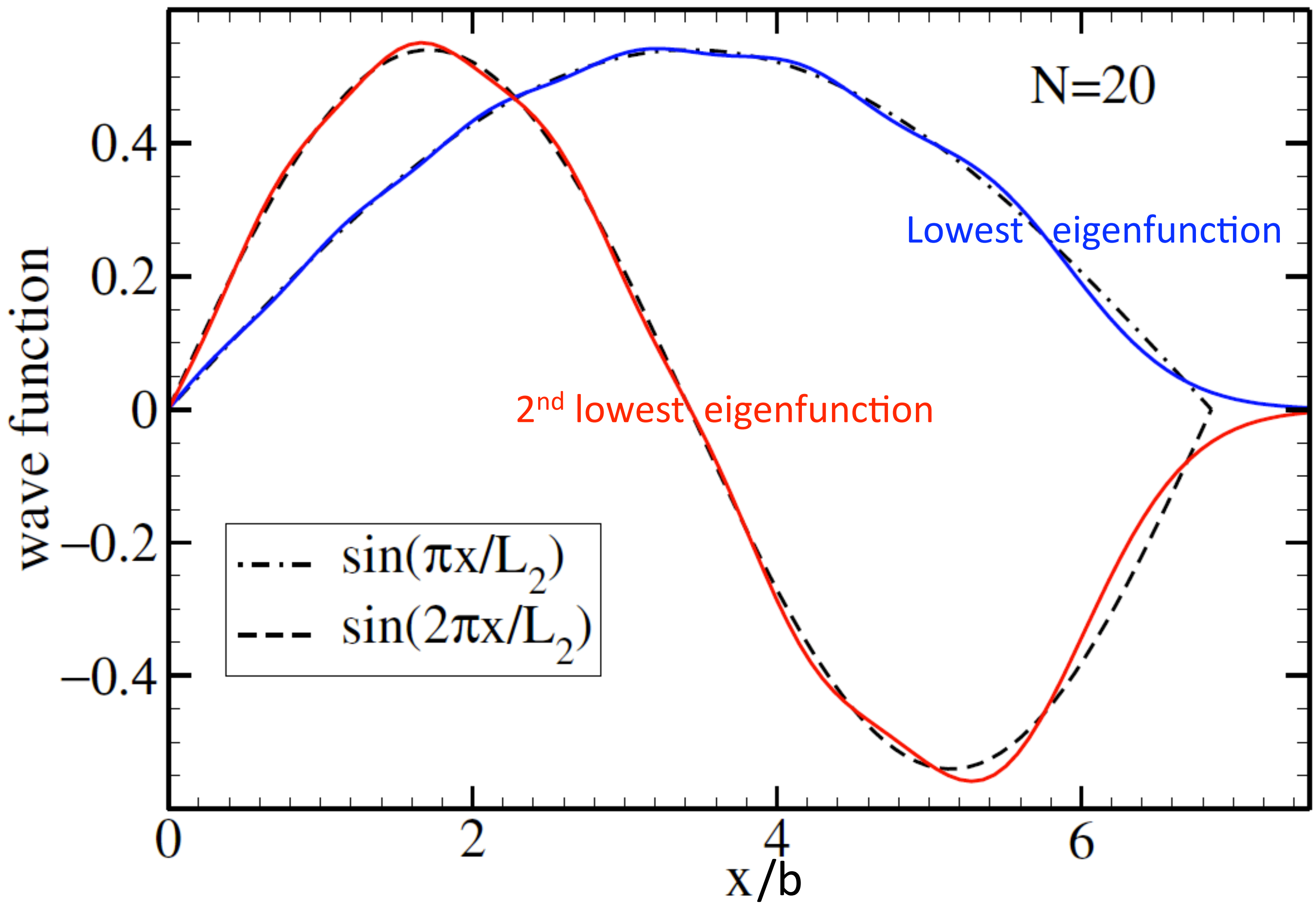
While 1/b can serve as an IR regulator [Stetcu, Barrett, van Kolck, Phys. Lett. B 653, 358 (2007); Stetcu, Rotureau, Barrett, van Kolck, J. of Phys. G 37, 064033 (2010); Coon, Avetian, Kruse, Kolck, Maris, Vary, Phys. Rev. C 86, 054002 (2012)], it is not the IR cutoff imposed by a finite HO basis.

Spectrum of the operator p^2 in the HO basis



- At low momentum, number of states increases linearly with increasing momentum
- Spectrum looks like that of the momentum operator in a box

Eigenfunctions of p^2 with lowest eigenvalues in oscillator basis



Eigenfunctions look like those from a box of size L_2.

Squared infrared cutoff is the lowest eigenvalue of p^2

The lowest eigenvalue κ_{min} can be computed analytically for N>>1. **Result: π/L_2**

Note: N>>1 does not imply impractically large model spaces

$$L_i \equiv \sqrt{2(N+3/2+i)}b$$

N	$\kappa_{\rm min}$	π/L_2	π/L_0
0	1.2247	1.1874	1.8138
2	0.9586	0.9472	1.1874
4	0.8163	0.8112	0.9472
6	0.7236	0.7207	0.8112
8	0.6568	0.6551	0.7207
10	0.6058	0.6046	0.6551
12	0.5651	0.5642	0.6046
14	0.5316	0.5310	0.5642
16	0.5035	0.5031	0.5310
18	0.4795	0.4791	0.5031
20	0.4585	0.4582	0.4791

1% deviation at N>2

0.1% deviation at N>14

π/L_2 is very precise value of the IR cutoff

IR corrections to bound-state energies

Simple view: A node in the wave function

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

at r=L_2 requires $\alpha_E = -\exp(-2k_E L_2)$. This yields a (kinetic) energy correction

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

Model-independent approach based on linear energy method [D. Djajaputra & B. R. Cooper, Eur. J. Phys. 21, 261 (2000)] yields energy correction

$$\Delta E_L \approx -u_\infty(L)\left(\left.\frac{du_E(L)}{dE}\right|_{E_\infty}\right)^{-1}$$

Final results [Furnstahl, Hagen, TP, Phys. Rev C 86, 031301 (2012); More, Ekström, Furnstahl, Hagen, TP, arXiv:1302.3815]

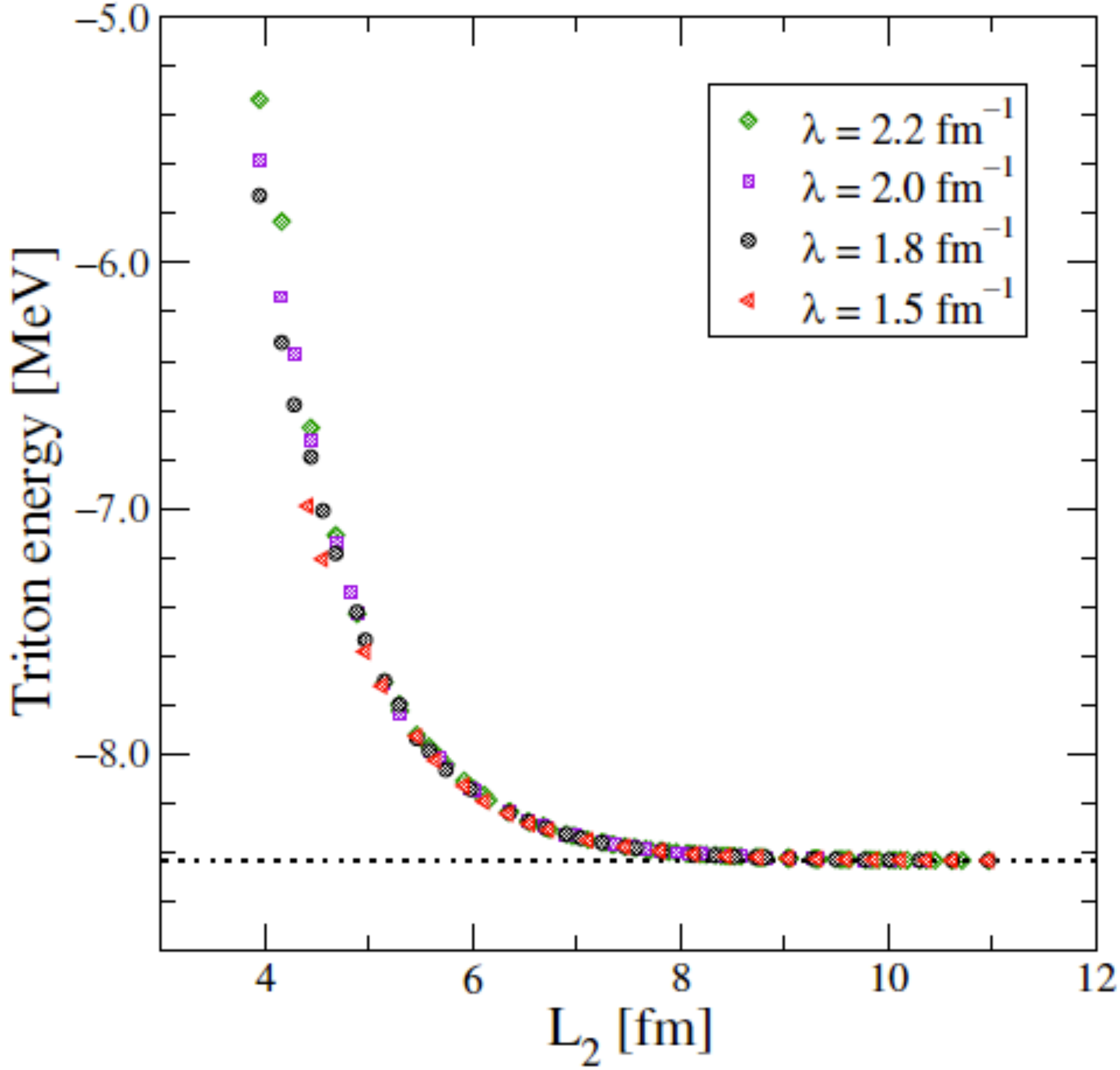
ANC^2 Binding momentum

$$\Delta E_L = \frac{\hbar^2 k_\infty \gamma_\infty^2}{\mu} e^{-2k_\infty L} + \mathcal{O}(e^{-4k_\infty L})$$ only observables enter

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

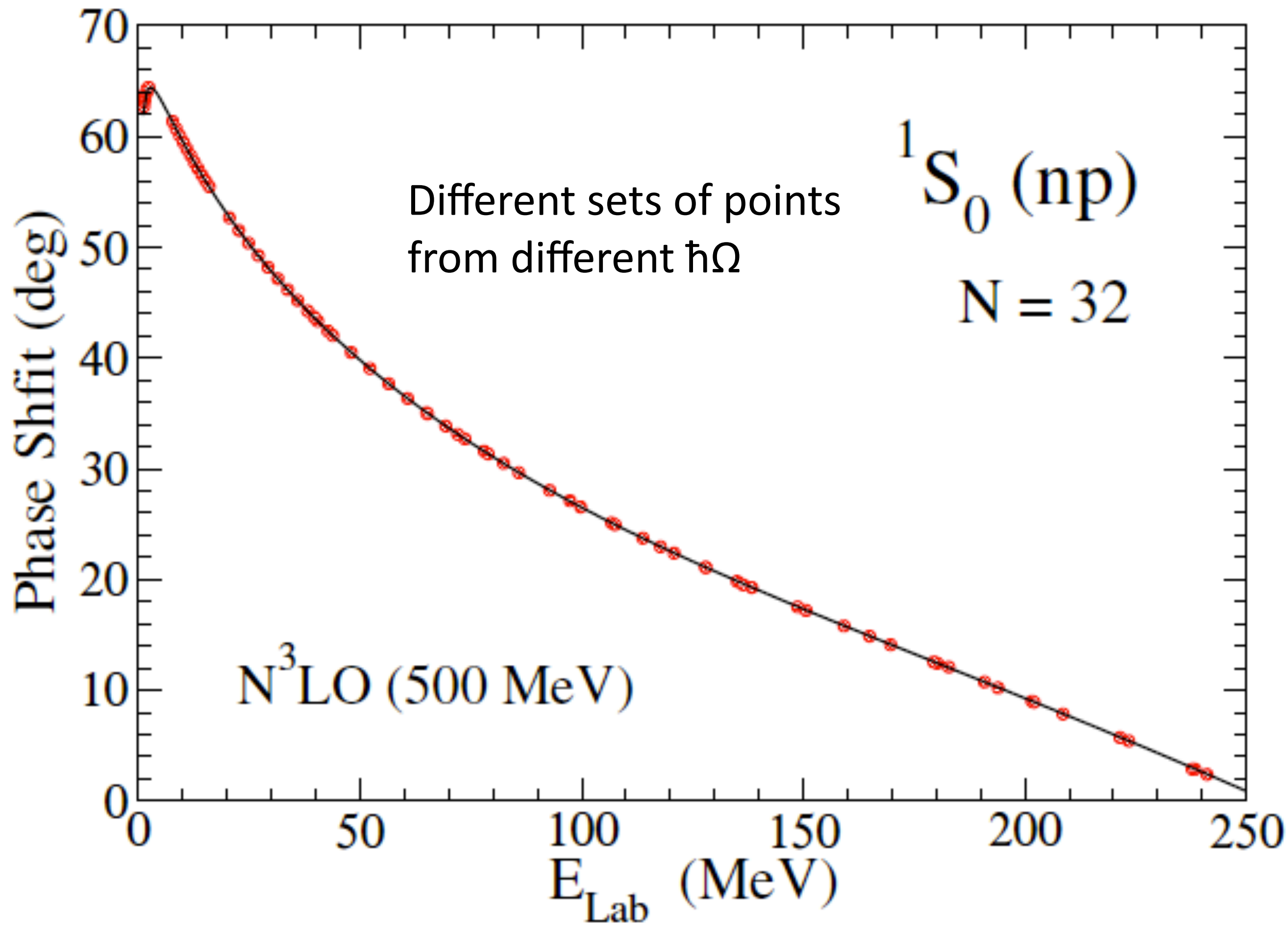
Energy extrapolation explains findings by Coon et al, Phys. Rev. C 86, 054002 (2012)

Triton binding energy from SRG interactions: only observables enter into the IR extrapolation

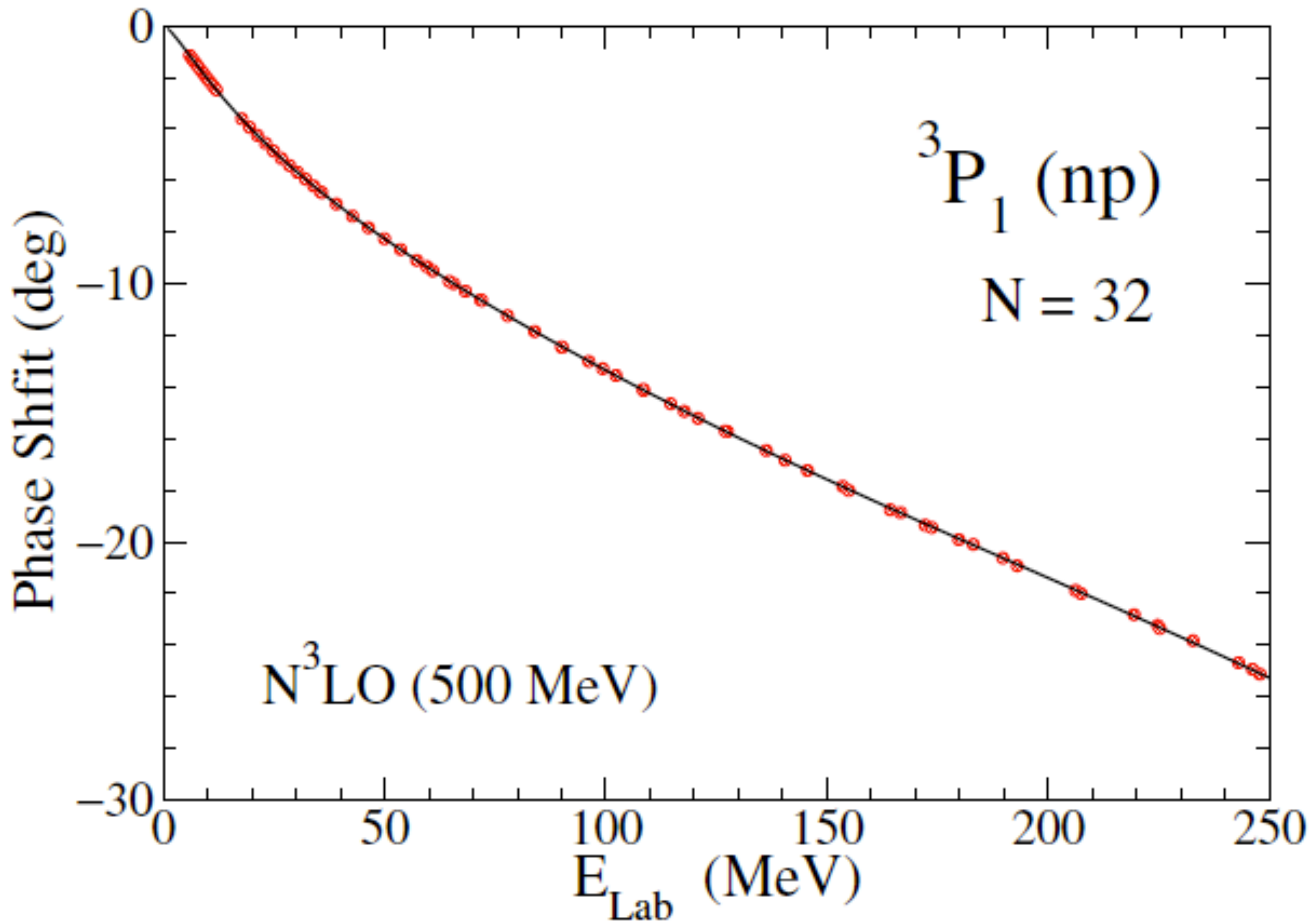


Phase shifts computed directly in the HO basis

1. Compute states in channel l with positive energies E_i and momentum p_i in HO basis at fixed N
2. In a box, the i^{th} state determines the box size $L_i = L(p_i)$ at that energy via $j_l(p_i L_i/\hbar) = 0$
3. Compute phase shift from usual formula: $\tan \delta_l(k_i) = \frac{j_l(k_i L(\hbar k_i))}{\eta_l(k_i L(\hbar k_i))}$
4. Repeat for several ħΩ



Phase shifts



Alternative approaches based on [Busch et al 1998] employ a harmonic potential and use ħΩ→0 for finite-range interactions.

T. Luu, M. J. Savage, A. Schwenk, and J. P. Vary, Phys. Rev. C 82, 034003 (2010).

I. Stetcu, J. Rotureau, B. R. Barrett, and U. van Kolck, J. Phys. G 37, 064033 (2010).

How well can one distinguish L_2 in practice?

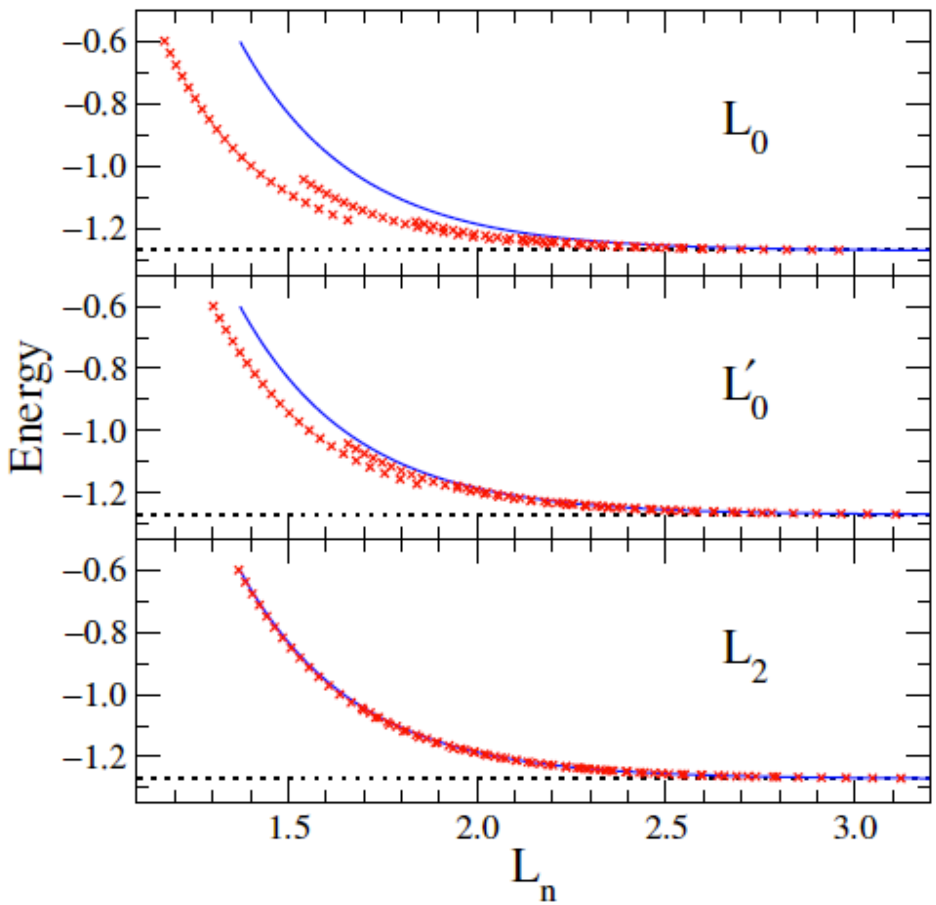
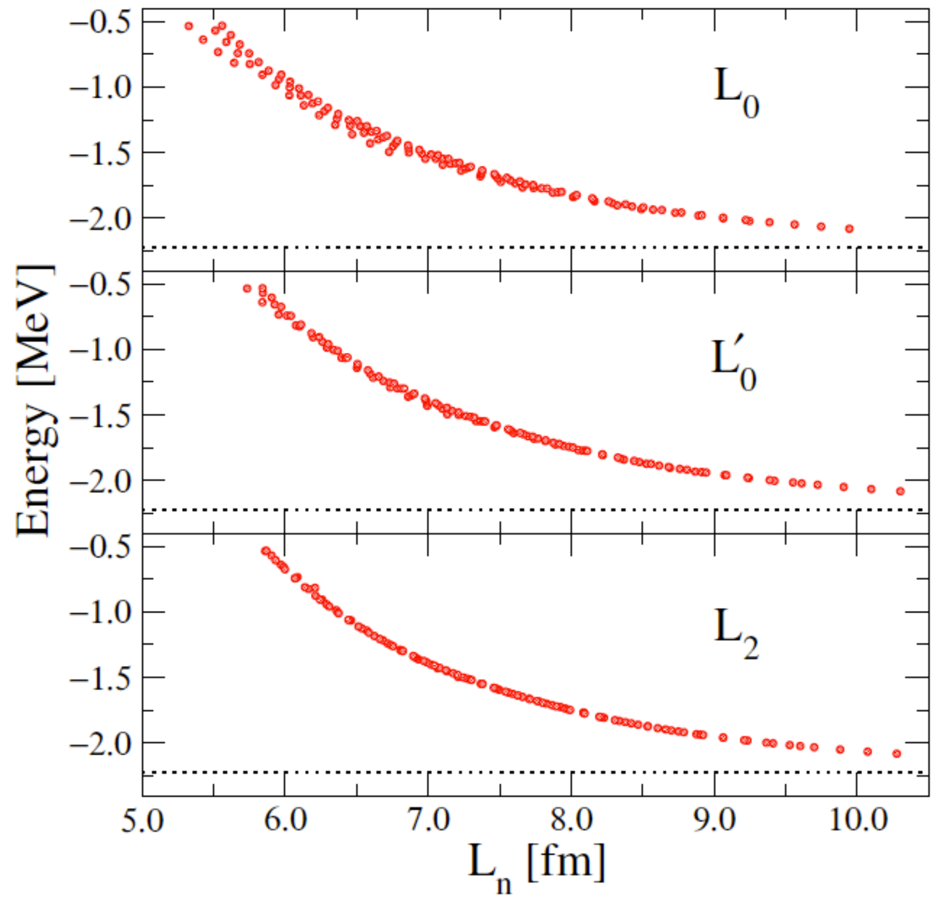
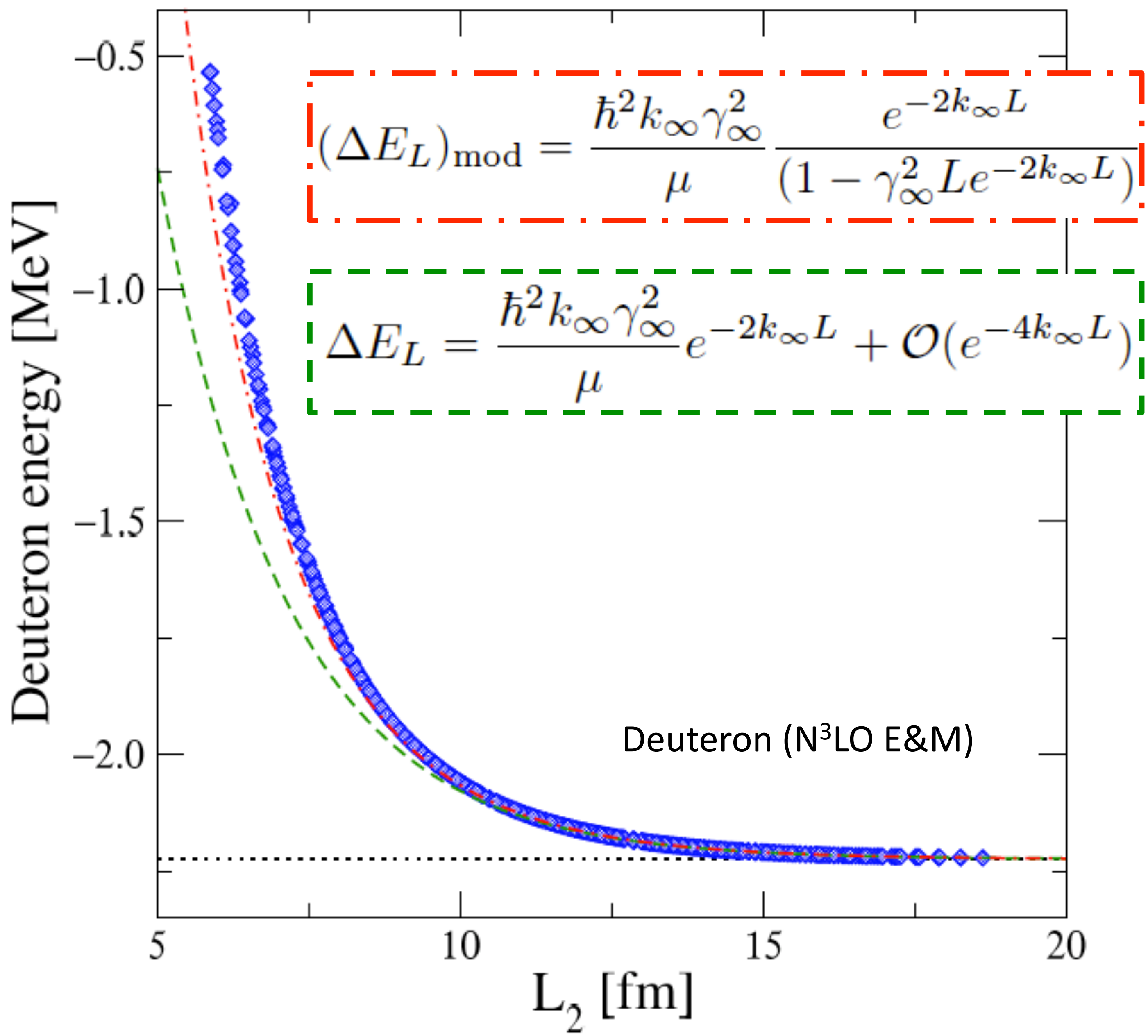


FIG. 2: (color online) Ground-state energies versus L_0 (top), L_0' (middle), and L_2 (bottom) for a Gaussian potential well Eq. (5) with $V_0 = 5$ and $R = 1$. The crosses are the energies from HO basis truncation. The energies obtained by numerically solving the Schrödinger equation with a Dirichlet boundary condition at L lie on the solid line. The horizontal dotted lines mark the exact energy $E_\infty = -1.27$.



Deuteron (N^3LO E&M)

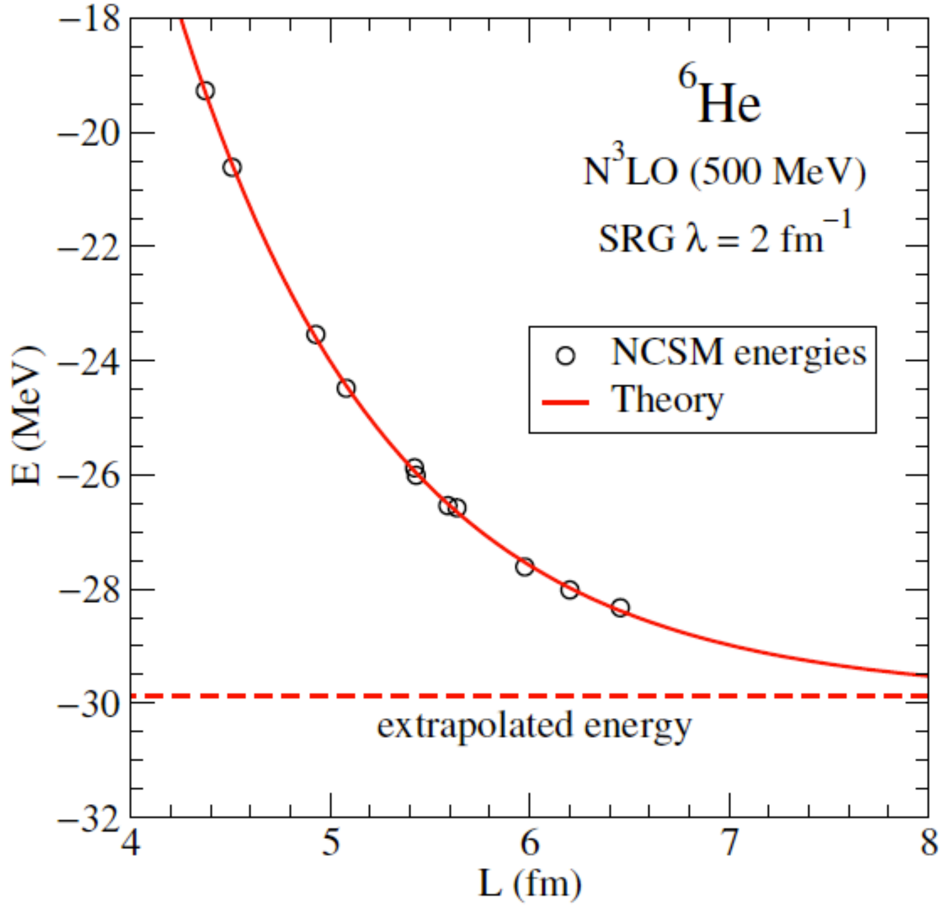
Corrections for shallow bound states



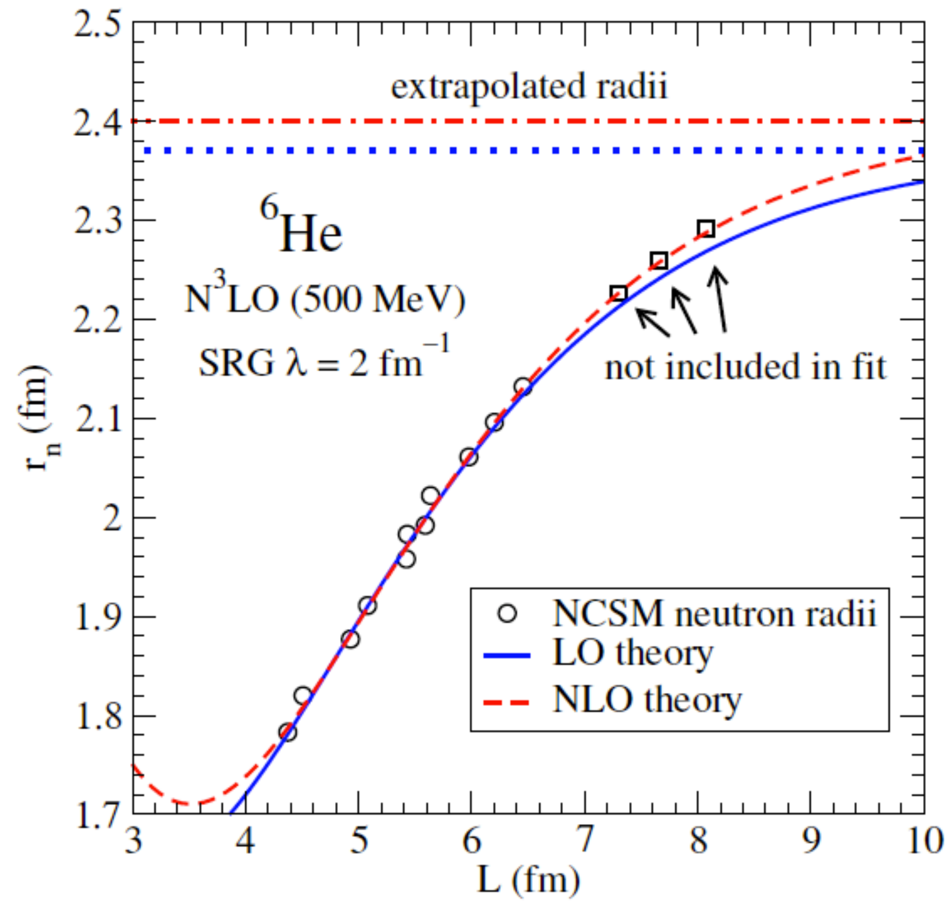
Corrections due to finite Hilbert spaces

- UV practically converged (because $\lambda < \Lambda_{UV}$)
- IR convergence is slower due to exponential decay of wave function
- Dirichlet boundary condition at x=L in position space

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



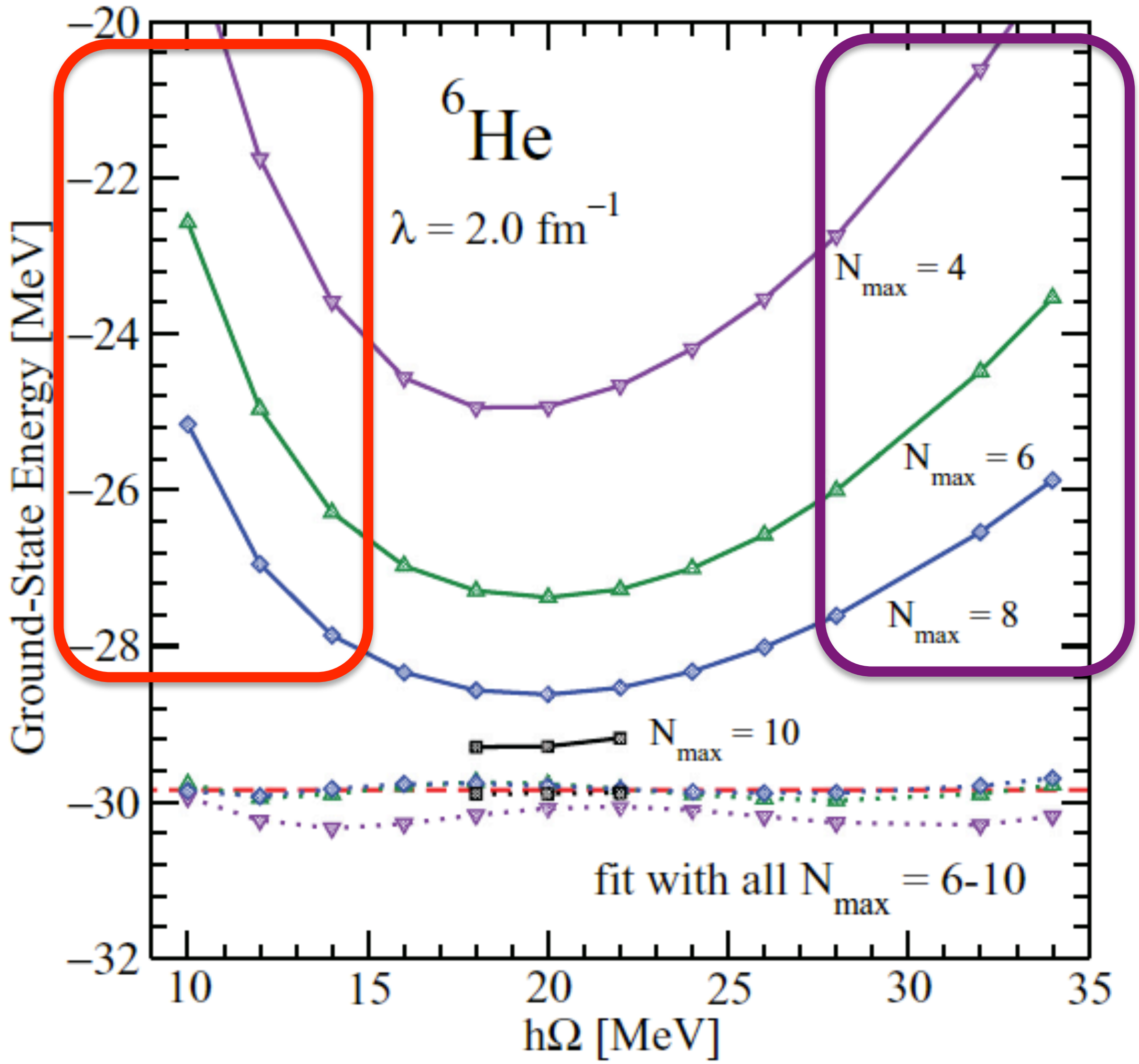
$$\langle r^2 \rangle_L \approx \langle r^2 \rangle_\infty [1 - (c_0 \beta^3 + c_1 \beta) e^{-\beta}]$$
$$\beta \equiv 2k_\infty L$$



Empirical approach: combined UV and IR fits for SRG interactions

$$E(\Lambda_{UV}, L) \approx E_\infty + A_0 e^{-2\Lambda_{UV}^2/A_1^2} + A_2 e^{-2k_\infty L}$$

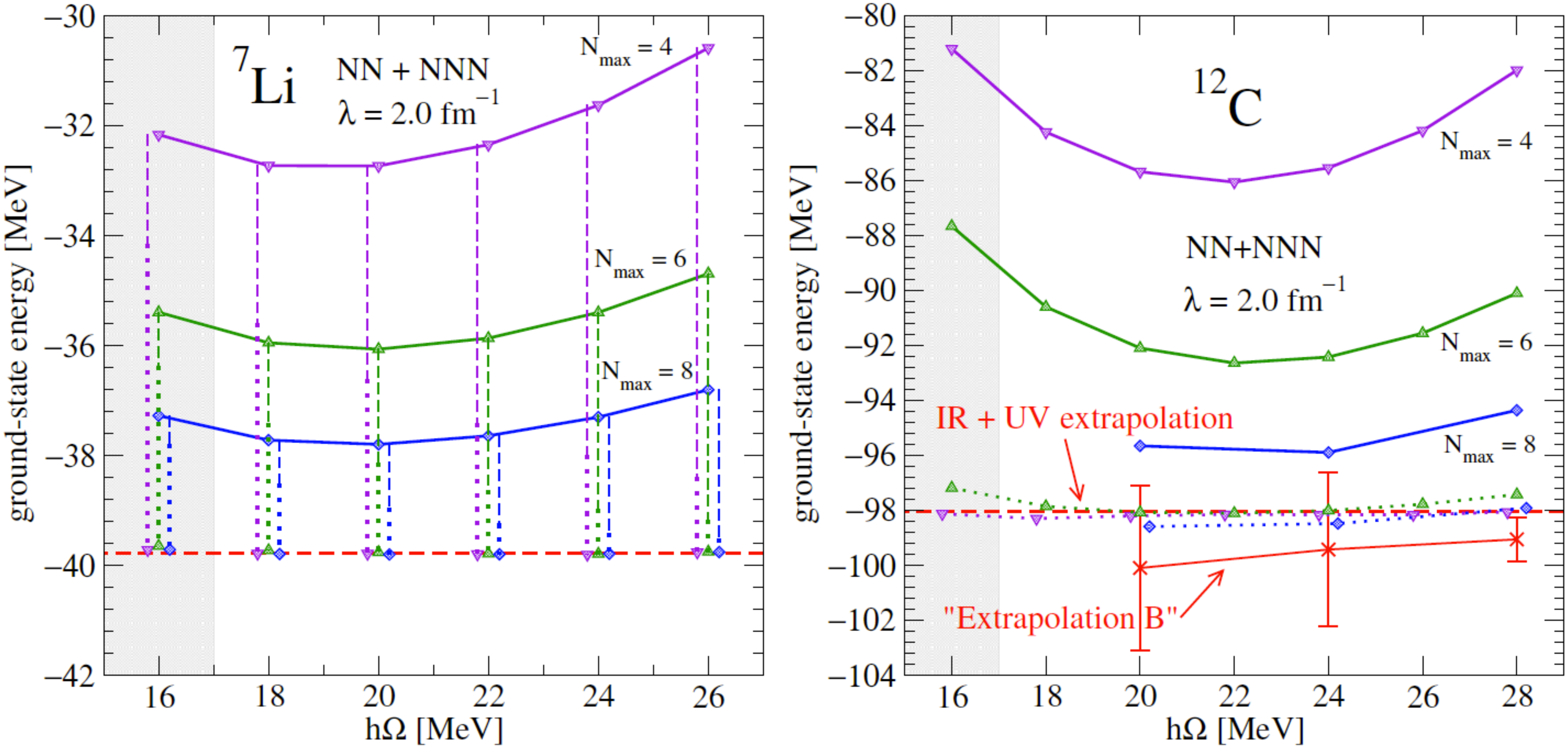
At lower ħΩ:
- IR converged
- extrapolate UV



At higher ħΩ:
- UV converged
- extrapolate IR

Empirical approach: combined UV and IR fits for SRG interactions

$$E(\Lambda_{UV}, L) \approx E_\infty + A_0 e^{-2\Lambda_{UV}^2/A_1^2} + A_2 e^{-2k_\infty L}$$



Error analysis of combined extrapolation lacking. Goodness-of-fit can be estimated.
"Extrapolation B" from [Maris, Vary, Shirokov, Phys. Rev. C 79, 014308 (2009)]

Figures from [Jurgenson, Maris, Furnstahl, Navratil, Ormand, Vary arXiv:1302.5473]

Recipe

1. Perform calculations at sufficiently large values of $\hbar\Omega$ (these have small or no UV corrections)
2. Plot results (energies, radii) vs. L_2 (UV converged results are expected to fall onto a single line)
3. Perform fit to extrapolation formulas and read off asymptotic value
4. General: Compute IR and UV cutoffs from diagonalization of p^2

Summary

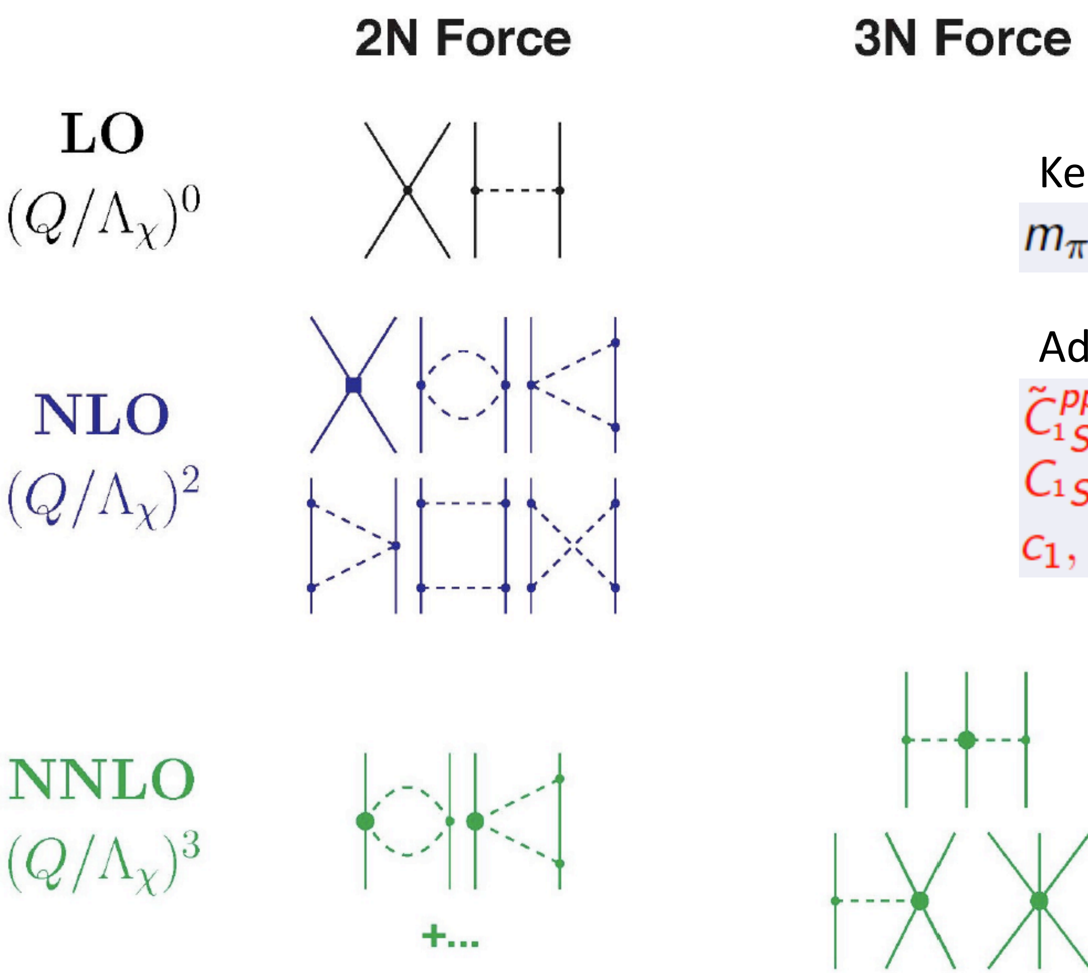
- Much improved understanding of IR properties of HO basis
- At low momenta, HO basis behaves as a box of size L_2
- π/L_2 is the IR cutoff
- Computation of phase shifts directly from the positive energy states in HO basis
- Energy extrapolation law expressed solely in terms of observables
- Corrections for shallow bound states worked out

Outlook: IR properties in *any localized* basis

- Diagonalize operator p^2 in a given model space → IR and UV cutoffs, and L for this model space.
- Be in the UV-converged regime.
- Plot energies and radii as a function of L, and extrapolate.

Optimization of chiral interaction an NNLO

Andreas Ekström, Baardsen, Forssen, Hagen, Hjorth-Jensen, Jansen, Machleidt, Nazarewicz, TP, Sarich, Wild, arXiv:1303.4674



Kept fixed

$m_{\pi^+}, m_{\pi^-}, m_{\pi^0}, m_n, m_p, g_A, f_\pi, \Lambda_{LS}, \Lambda_\chi$

Adjusted parameters

$\tilde{C}^{pp}_{^1S_0}, \tilde{C}^{nn}_{^1S_0}, \tilde{C}^{np}_{^1S_0}, \tilde{C}_{^3S_1}$
$C_{^1S_0}, C_{^3P_0}, C_{^1P_1}, C_{^3P_1}, C_{^3S_1}, C_{^3S_1-^3D_1}, C_{^3P_2}$
$c_1, c_3, c_4, (c_D, c_E)$

Weinberg; van Kolck; Epelbaum, Glöckle & Meißner; Entem & Machleidt; Krebs; …

Optimization to phase shifts; χ^2 from data

$$f(\vec{x}) = \sum_{q=1}^{N_q} \left(\frac{\delta_q^{\mathrm{NNLO}}(\vec{x}) - \delta_q^{\mathrm{Nijm93}}}{w_q} \right)^2$$

Weights for contacts scale as Q^3; for pion-nucleon couplings from Nijmegen analysis

Pion nucleon couplings determined from fits to peripheral D, F, G partial waves (NNLO contacts do not contribute for L≥2)

πN LEC	πN-scattering[1]	NN-PWA[2]	NNLO[3]	N3LO	POUNDerS
c_1 [GeV^{-1}]	-0.81±0.15	-0.76±0.07	-0.81	-0.81	-0.9186
c_3 [GeV^{-1}]	-4.69±1.34	-4.78±0.10	-3.40	-3.20	-3.8887
c_4 [GeV^{-1}]	+3.40±0.04	+3.96 ±0.22	+3.40	+5.40	+4.3103

[1] πN Fit 1, in P. Büttiker, U-G. Meißner Nucl. Phys. A **668**, 97 (2000)

[2] *NN* PWA, in M. C. M. Rentmeester *et al.* Phys. Rev C **67** 044001 (2003)

[3] E. Epelbaum et al., Eur. Phys. J. A19, 401 (2004)

χ^2/datum, *np* scattering data (1999 database)

The previous picture...

T_{lab} bin (MeV)	N3LO	NNLO[1]	NLO[1]	AV18
0-100	1.06	1.71	5.20	0.95
100-190	1.08	12.9	49.3	1.10
190-290	1.15	19.2	68.3	1.11
0-290	**1.10**	**10.1**	**36.2**	**1.04**

[1] E. Epelbaum et al., Eur. Phys. J. A19, 401 (2004)

... changes with POUNDerS

T_{lab} bin (MeV)	POUNDerS-NNLO(500)
0-35	0.85
35-125	1.17
125-183	1.87
183-290	6.09
0-290	**2.95**

χ^2/datum, *pp* scattering data (1999 database)

The previous picture...

T_{lab} bin (MeV)	N3LO	NNLO[1]	NLO[1]	AV18
0-100	1.05	6.66	57.8	0.96
100-190	1.50	28.3	62.0	1.31
190-290	1.93	66.8	111.6	1.82
0-290	**1.50**	**35.4**	**80.1**	**1.38**

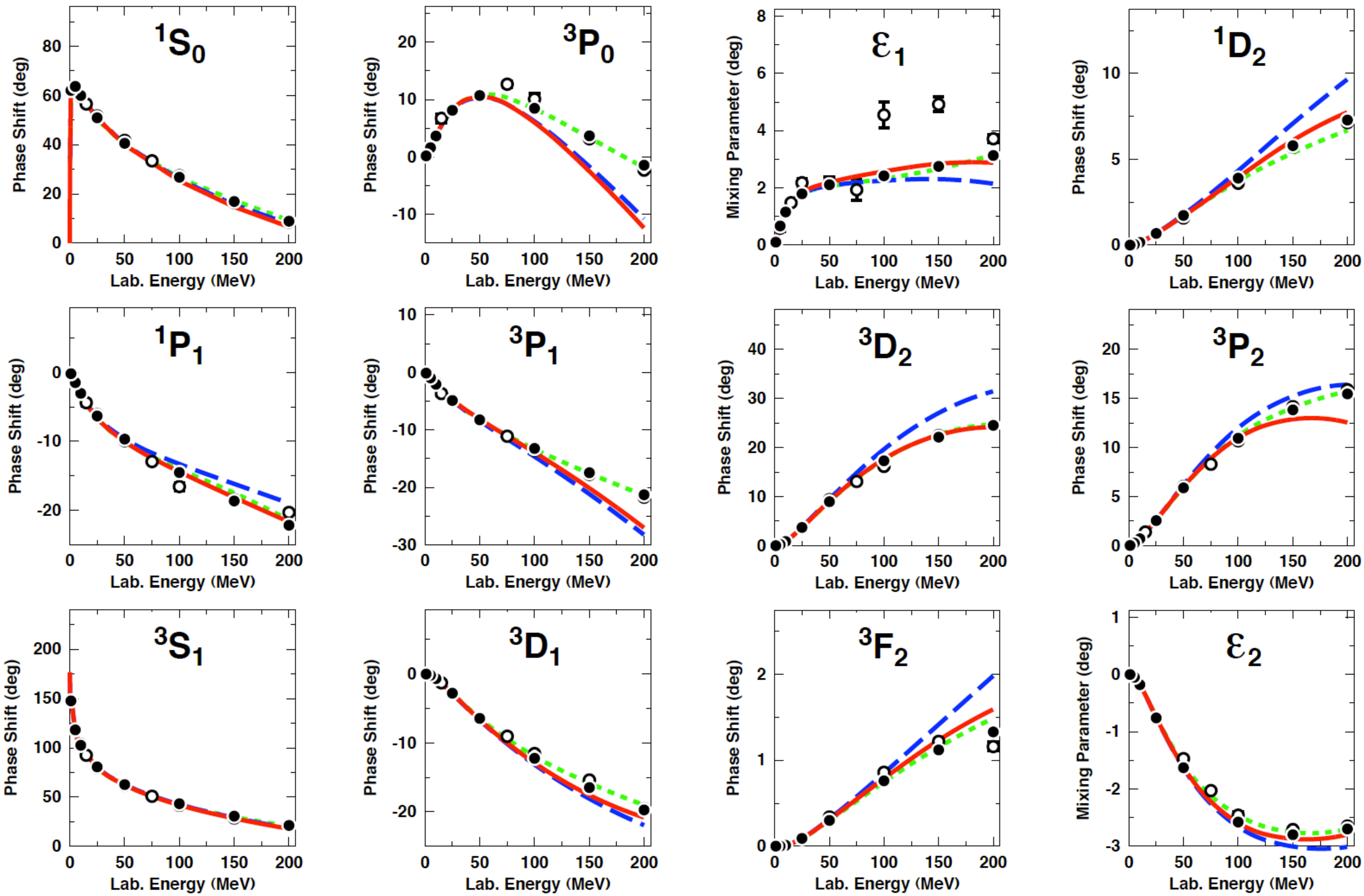
[1] E. Epelbaum et al., Eur. Phys. J. A19, 401 (2004)

... changes with POUNDerS

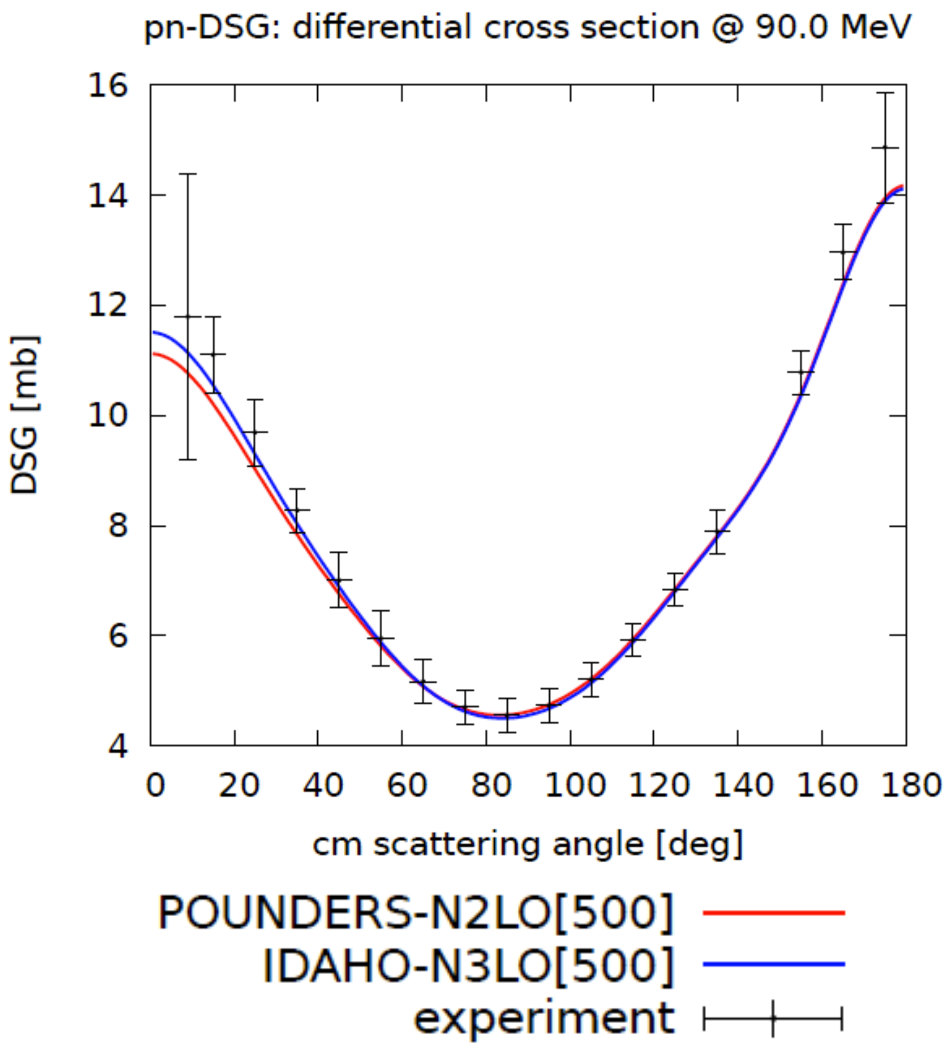
T_{lab} bin (MeV)	POUNDerS-NNLO(500)
0-35	1.11
35-125	1.56
125-183	23.95 (4.35[a])
183-290	29.26
0-290	**17.10 (14.03)**[2]

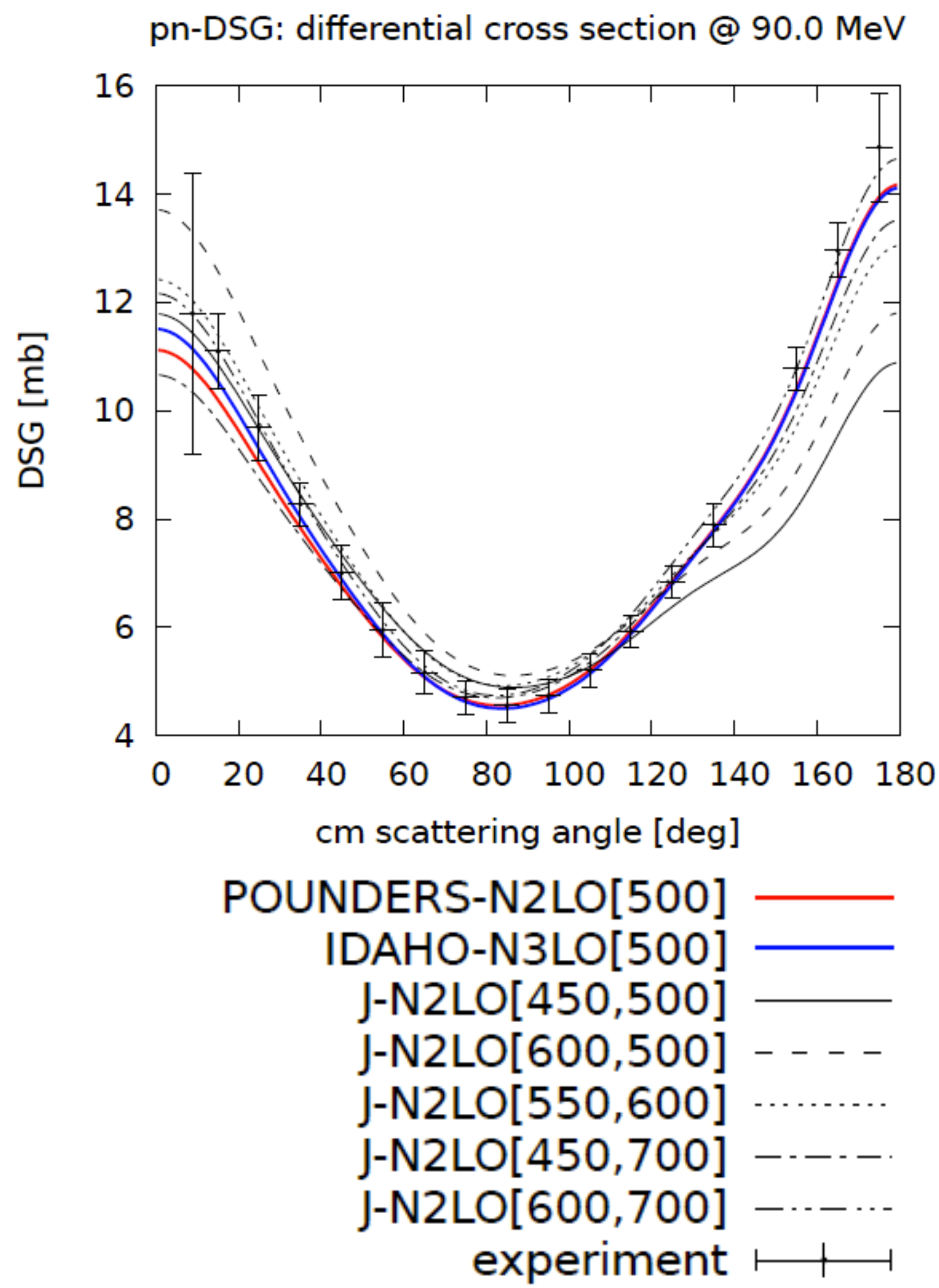
[2] Total (0-290) MeV *pp* χ^2/datum when excluding two low-uncertainty data sets.

Optimization with POUNDerS



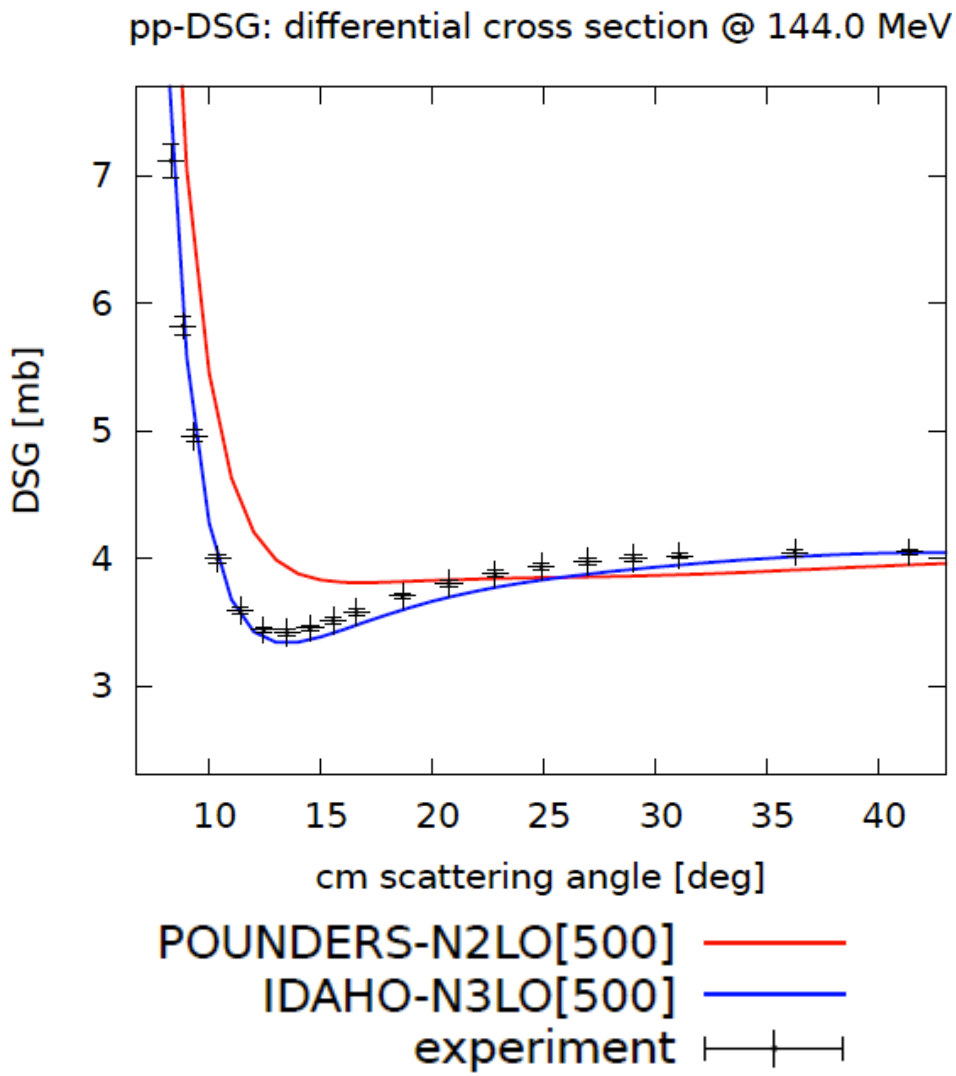
Differential cross sections at 90 MeV

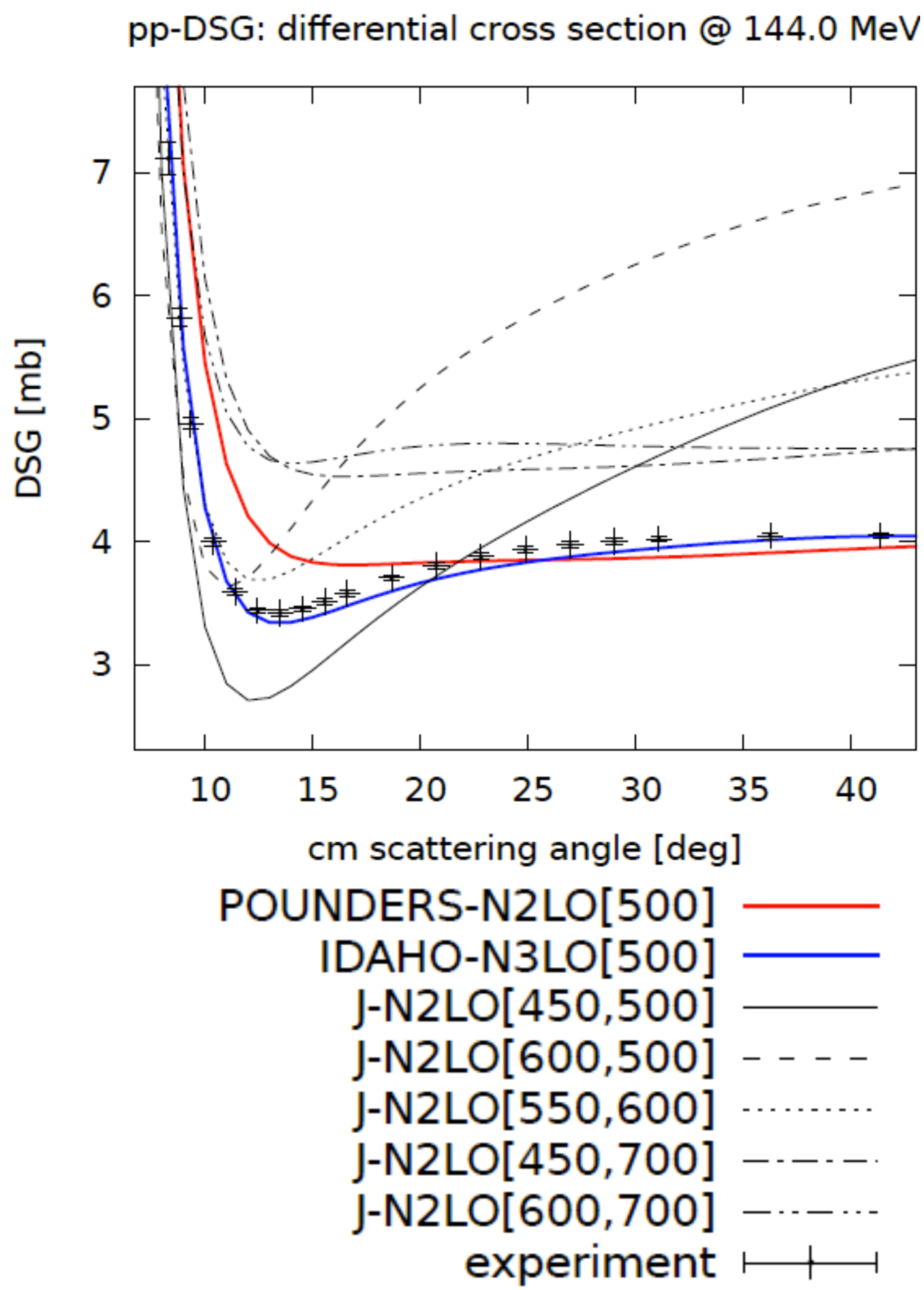




A. Ekström et al (2012), unpublished

Differential cross sections at 144 MeV

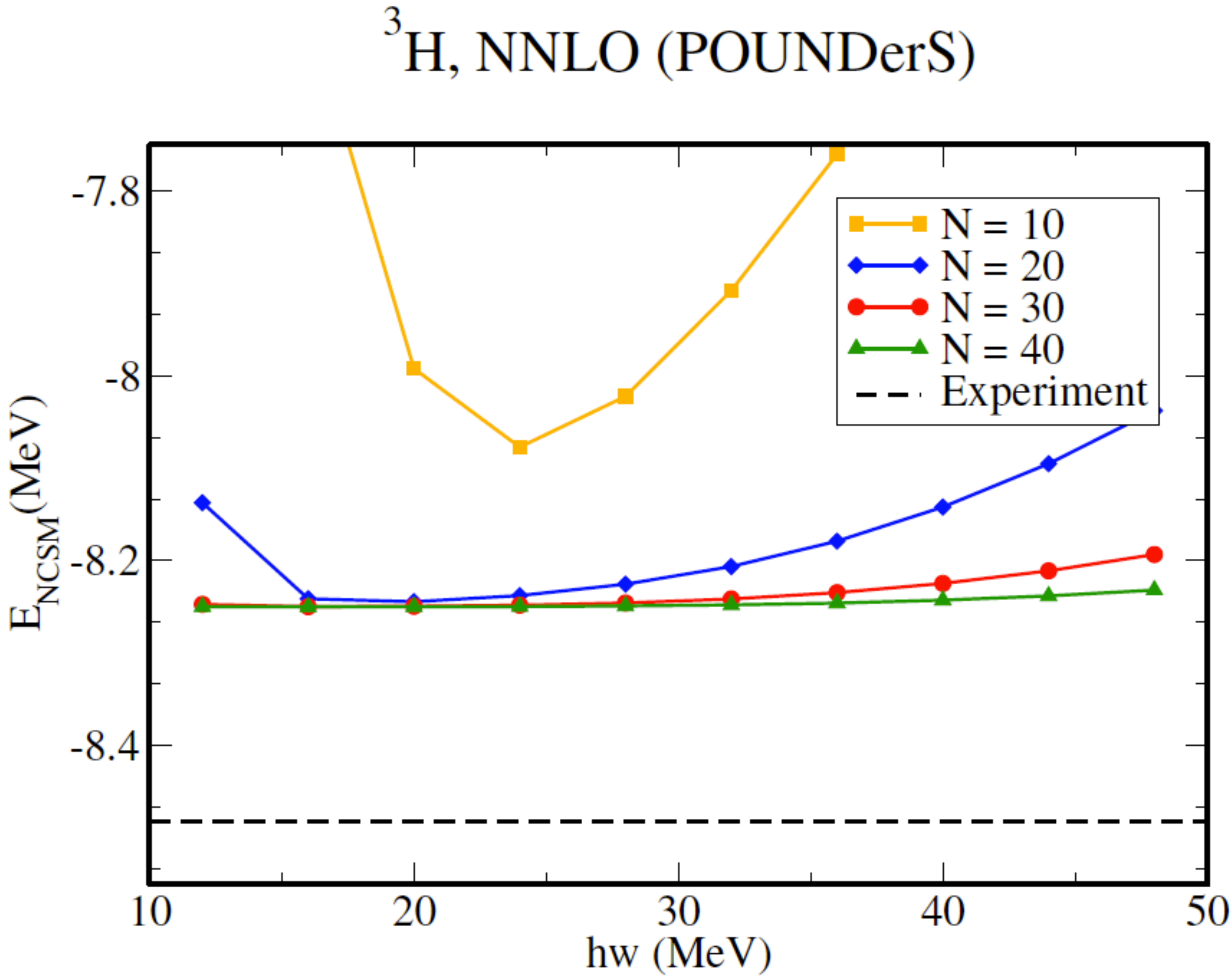




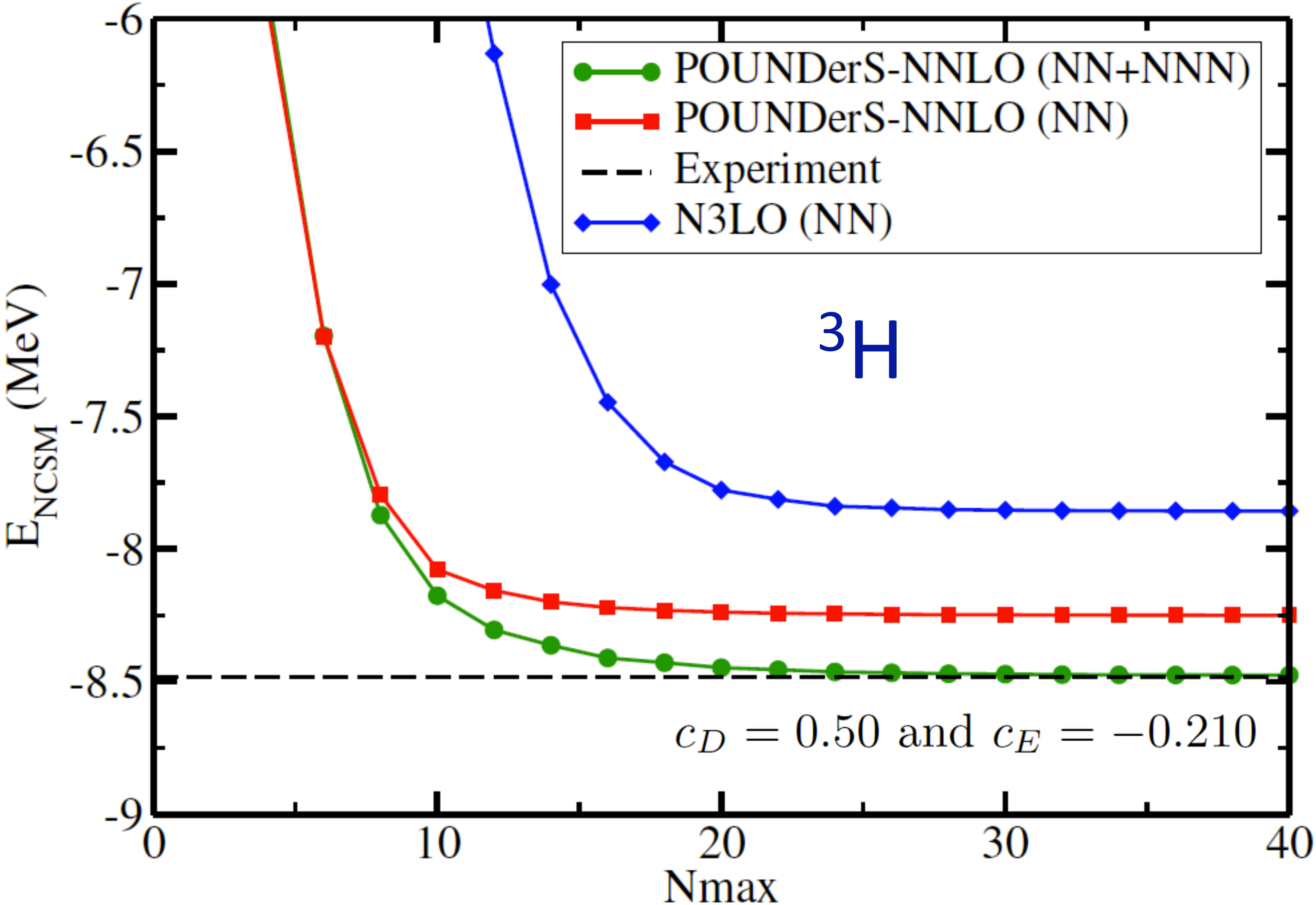
A. Ekström et al (2012), unpublished

Nucleon-nucleon properties

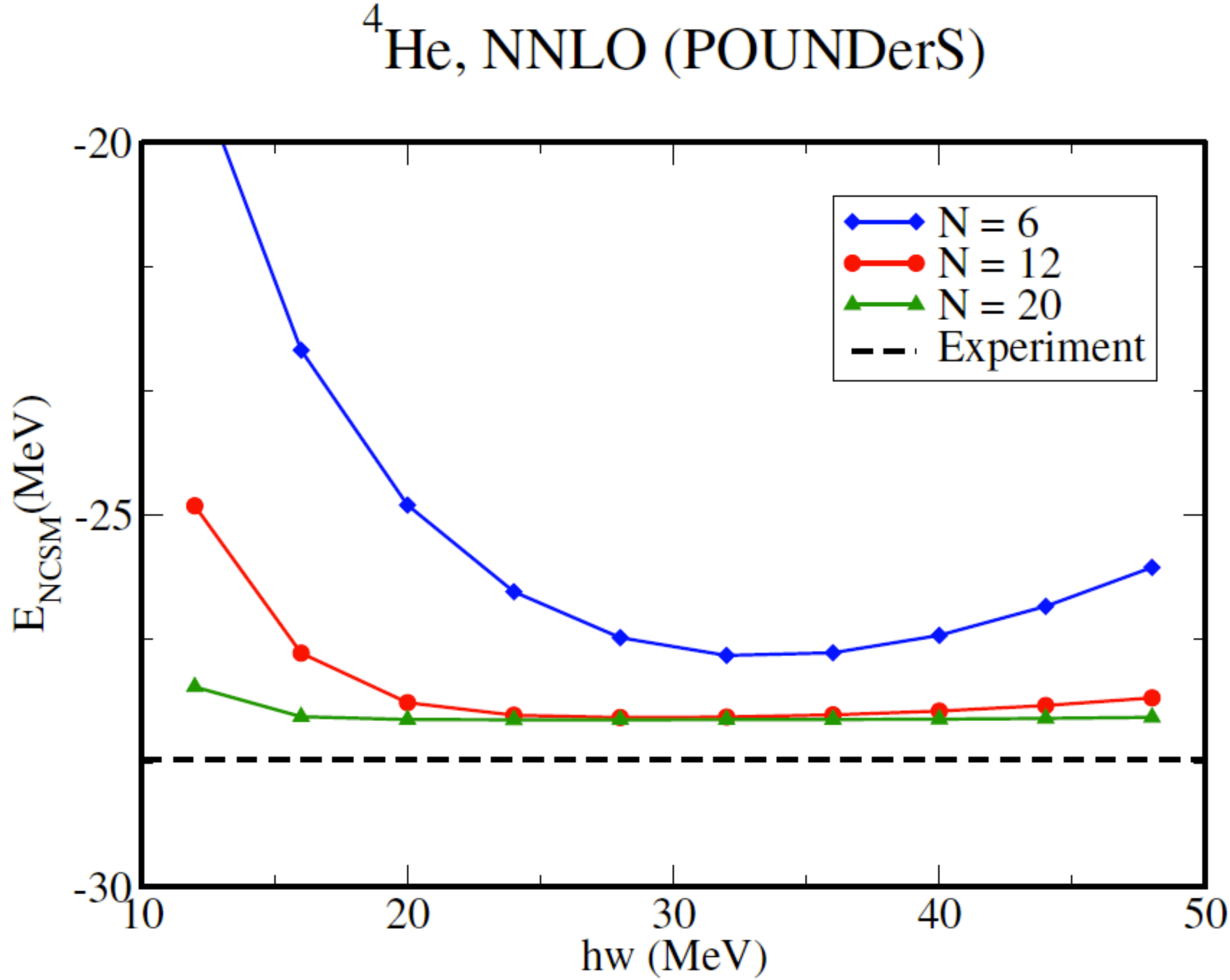
	N^3LO_{EM}	$NNLO_{opt}$	Exp.
a^C_{pp}	-7.8188	-7.8174	-7.8196(26) -7.8149(29)
r^C_{pp}	2.795	2.755	2.790(14) 2.769(14)
a^N_{pp}	-17.083	-17.825	
r^N_{pp}	2.876	2.817	
a_{nn}	-18.900	-18.889	-18.95(40)
r_{nn}	2.838	2.797	2.75(11)
a_{np}	-23.732	-23.749	-23.740(20)
r_{np}	2.725	2.684	2.77(5)
B_D (MeV)	2.224575	2.224582	2.224575(9)
r_D (fm)	1.975	1.967	1.97535(85)
Q_D (fm^2)	0.275	0.272	0.2859(3)
P_D (%)	4.51	4.05	



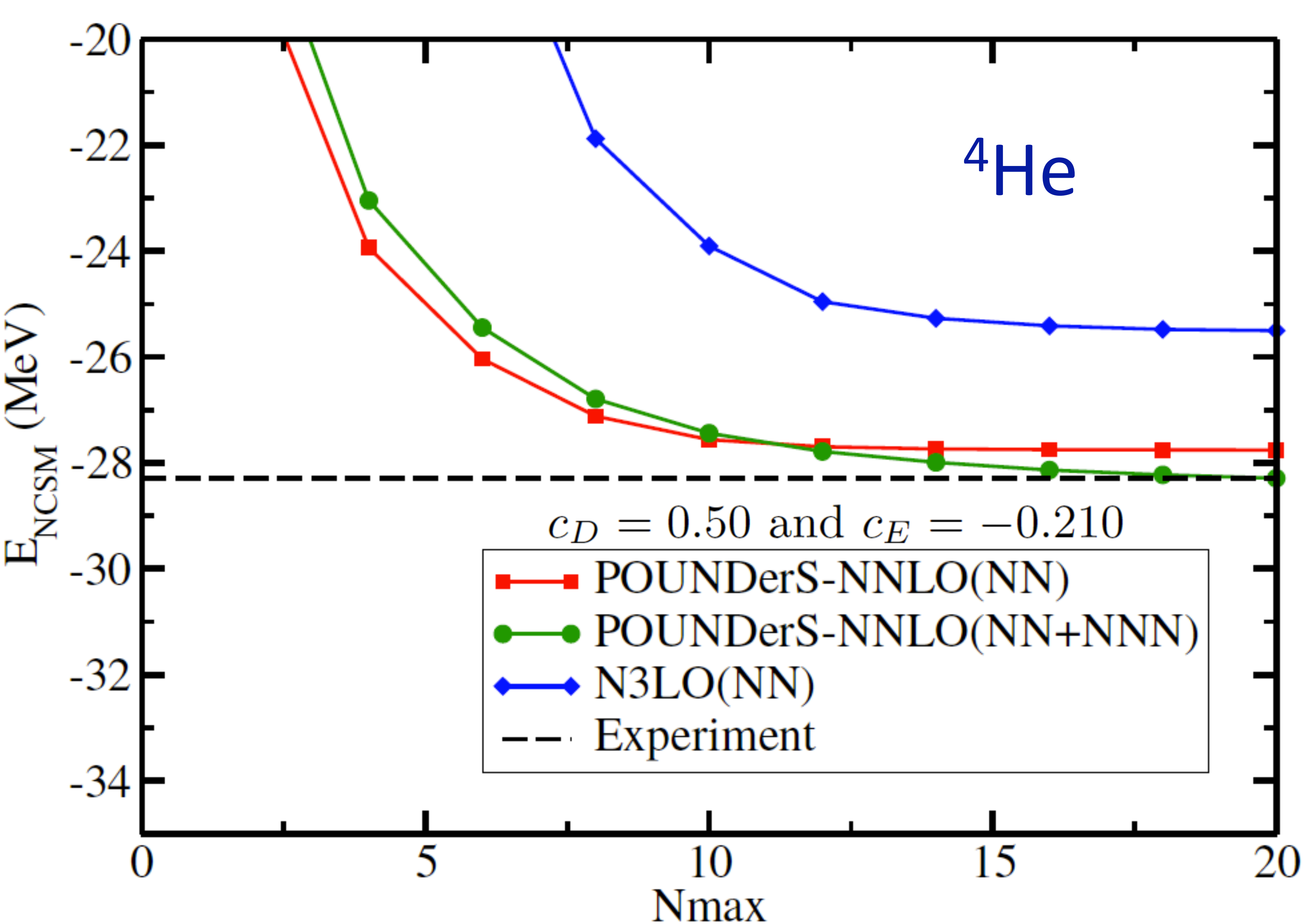
³H, NNLO (POUNDerS)
N = 10
N = 20
N = 30
N = 40
Experiment
-7.8
-8
-8.2
-8.4
E_NCSM(MeV)
10
20
30
40
50
hw (MeV)



POUNDerS-NNLO (NN+NNN)
POUNDerS-NNLO (NN)
Experiment
N3LO (NN)
^{3}H
$c_D = 0.50$ and $c_E = -0.210$
E_{NCSM} (MeV)
Nmax
-6
-6.5
-7
-7.5
-8
-8.5
-9
0
10
20
30
40



4He, NNLO (POUNDerS)
-20
-25
-30
10
20
30
40
50
E_NCSM (MeV)
hw (MeV)
N = 6
N = 12
N = 20
Experiment



^{4}He
E_{NCSM} (MeV)
-20
-22
-24
-26
-28
-30
-32
-34
0
5
10
15
20
Nmax
$c_D = 0.50$ and $c_E = -0.210$
POUNDerS-NNLO(NN)
POUNDerS-NNLO(NN+NNN)
N3LO(NN)
Experiment

Three nucleon force

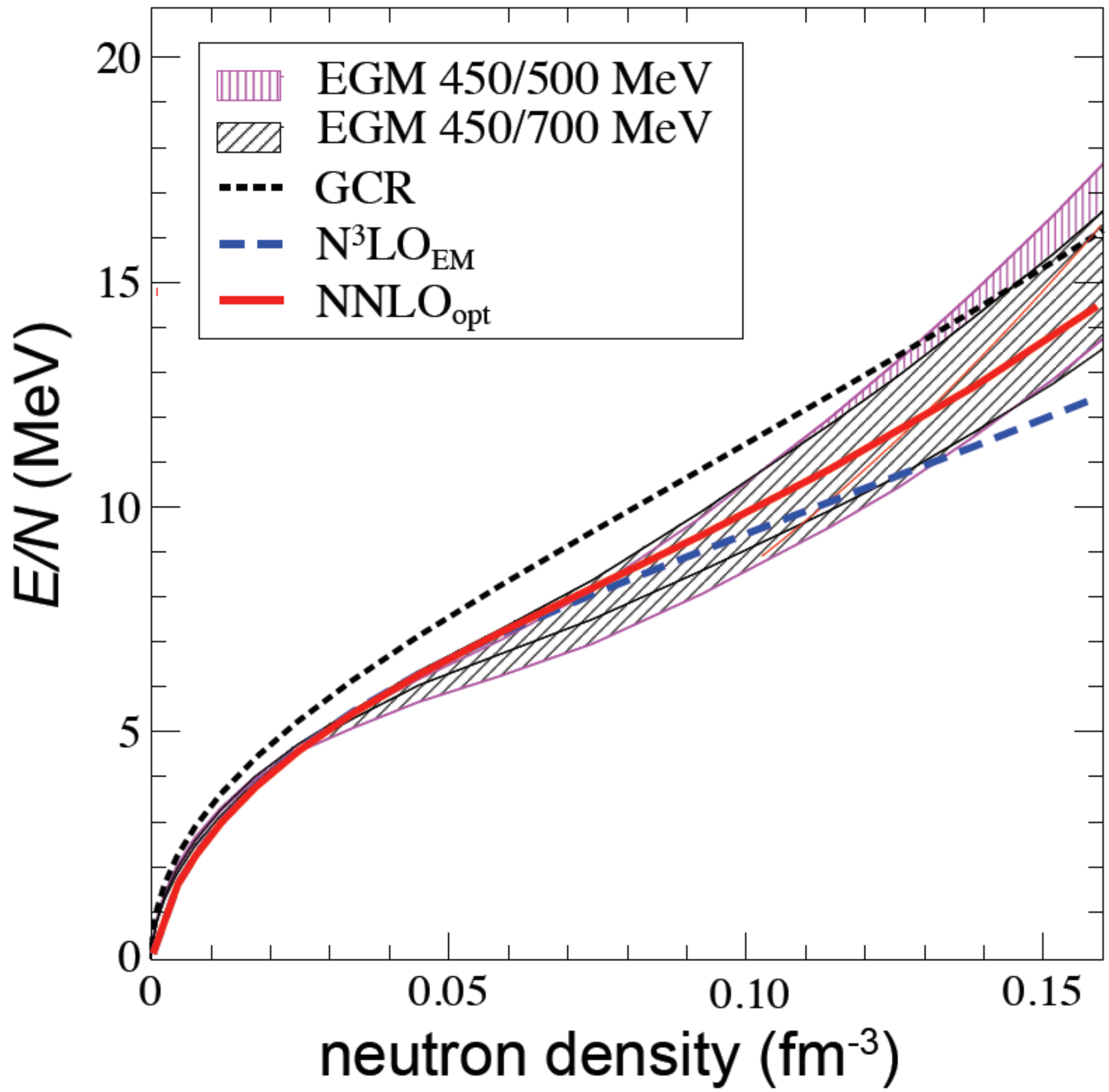
Local form of 3NF [Navratil, Few Body Syst. 41, 117 (2007)] based on [Epelbaum et al., Phys. Rev. C 66, 064001 (2002)].

TABLE IV. Ground-state energies (in MeV) and point proton radii (in fm) for ^{3}H, ^{3}He, and ^{4}He using the NNLO$_{\rm opt}$ with and without the NNLO 3NF interaction for $c_D = -0.20$ and $c_E = -0.36$.

	$E(^3\mathrm{H})$	$E(^3\mathrm{He})$	$E(^4\mathrm{He})$	$r_p(^4\mathrm{He})$
NNLO	-8.249	-7.501	-27.759	1.43(8)
NNLO+NNN	-8.469	-7.722	-28.417	1.43(8)
Experiment	-8.482	-7.717	-28.296	1.467(13)

→ See Gustav Jansen's talk this afternoon

Neutron matter with optimized chiral interactions at NNLO



GCR=Gandolfi, Carlson, Reddy, Phys. Rev. C 85, 032801 (2012)

EGM=I. Tews, T. Krüger, K. Hebeler, and A. Schwenk, Phys. Rev. Lett. 110, 032504 (2013)

Pauli-operator from [Suzuki et al. (2000)]; Coupled cluster (and Bruckner HF)

Summary

- Optimization of chiral interaction at NNLO
- acceptable $\chi^2 \approx 1$ per degree of freedom for lab energies $\lesssim$ 125 MeV
- NN interactions alone reproduce essential features in isotopes of oxygen and calcium → Gustav Jansen's talk this afternoon