Local chiral NN potentials and the structure of light nuclei

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Minimally nonlocal nucleon-nucleon potentials with chiral two-pion exchange including Δ resonances

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https://arxiv.org/abs/1606.06335

Local chiral potentials and the structure of light nuclei

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Nuclear χEFT Approach:

S. Weinberg, Phys. Lett. **B251**, 288 (1990); Nucl. Phys. **B363**, 3 (1991); Phys. Lett. **B295**, 114 (1992)

- χEFT uses the chiral-symmetry to constrain the interactions of π's among themselves or with baryons (N and Δ-isobar)

- π's couple by powers of its momentum Q, and the Lagrangian ($\mathcal{L}_{\rm eff}$) can be expanded systematically in powers of Q/Λ; ($Q \ll \Lambda \sim 1\,\mathrm{GeV}$ is the chiral-symmetry breaking scale and $Q \sim m_\pi$)

$$\mathcal{L}_{eff} = \mathcal{L}^{(0)} + \mathcal{L}^{(1)} + \mathcal{L}^{(2)} + ...$$

- χEFT allows for a perturbative treatment in terms of powers of Q

- The unknown coefficients of the perturbative expansion are called LEC's and are determined fitting the experimental data

- The χ-expansion gives rise to potentials and external currents can be naturally incorporated

The derivation of nuclear forces from χEFT has been a topic of active interest for the past 25 years

Previous work:

- S. Weinberg, Phys. Lett. B **251**, 288 (1990); Nucl. Phys. B **363**, 3 (1991)
- C. Ordóñez, L. Ray, and U. van Kolck, Phys. Rev. Lett. **72**, 1982 (1994); Phys. Rev. C **53**, 2086 (1996)
- N. Kaiser, R. Brockmann, and W. Weise, Nucl. Phys. A **625**, 758 (1997)
- N. Kaiser, S. Gerstendörfer, and W. Weise, Nucl. Phys. A **637**, 395 (1998)
- N. Kaiser, Phys. Rev. C **61**, 014003 (1999)
- N. Kaiser, Phys. Rev. C **62**, 024001 (2000)
- E. Epelbaum, W. Glöckle, and U.-G. Meißner, Nucl. Phys. A **637**, 107 (1998); **671**, 295 (2000)
- N. Kaiser, Phys. Rev. C **63**, 044010 (2001); **64**, 057001 (2001); **65**, 017001 (2001)
- D. R. Entem and R. Machleidt, Phys. Rev. C **66**, 014002 (2002); **68**, 041001 (2003)
- E. Epelbaum, W. Glöckle, and U.-G. Meißner, Eur. Phys. J. A **19**, 125 (2004)
- E. Epelbaum, W. Glöckle, and U.-G. Meißner, Nucl. Phys. A **747**, 362 (2005)
- H. Krebs, E. Epelbaum, and Ulf.-G. Meißner, Eur. Phys. J. A **32**, 127 (2007)

Recent work:

- A. Ekström, G. Baardsen, C. Forssen, G. Hagen, M. Hjorth-Jensen, G. R. Jansen, R. Machleidt, W. Nazarewicz, T. Papenbrock, J. Sarich, and S. M. Wild, Phys. Rev. Lett. **110**, 192502 (2013)
- A. Gezerlis, I. Tews, E. Epelbaum, S. Gandolfi, K. Hebeler, A. Nogga, and A. Schwenk, Phys. Rev. Lett. **111**, 032501 (2013)
- A. Gezerlis, I. Tews, E. Epelbaum, M. Freunek, S. Gandolfi, K. Hebeler, A. Nogga, and A. Schwenk, Phys. Rev. C **90**, 054323 (2014)
- D. R. Entem, N. Kaiser, R. Machleidt, and Y. Nosyk, Phys. Rev. C **91**, 014002 (2015); **92**, 064001 (2015)
- N. Kaiser, Phys. Rev. C **92**, 024002 (2015)
- E. Epelbaum, H. Krebs, and U.-G. Meißner Phys. Rev. Lett. **115**, 122301 (2015)

Motivations:

WHY?

Many of the available versions of chiral potentials are strongly non-local

- Non-localities due to contact interactions
- Non-localities due to regulator functions

$\Rightarrow \mathbf{p} \to -i\boldsymbol{\nabla}$ relative momentum operator

Non-local interactions hard (but not impossible; see A. Roggero *et al.* PRL **112**, 221103 (2014)) handle in for example Quantum Monte Carlo (QMC) methods

GOAL:

Construct a local χEFT NN potential with chiral TPE including Δ-isobar:

- Minimize the number of non-localities due to contact interactions and remove those due to the regulator functions

M. Piarulli *et al.* PRC **91**, 024003 (2015)
Minimally nonlocal nucleon-nucleon potentials with chiral two-pion exchange including Δ's

- The LECs multiplying these non-localities are now absent

M. Piarulli *et al.* arXiv/1606.06335
Local chiral NN potentials and the structure of light nuclei

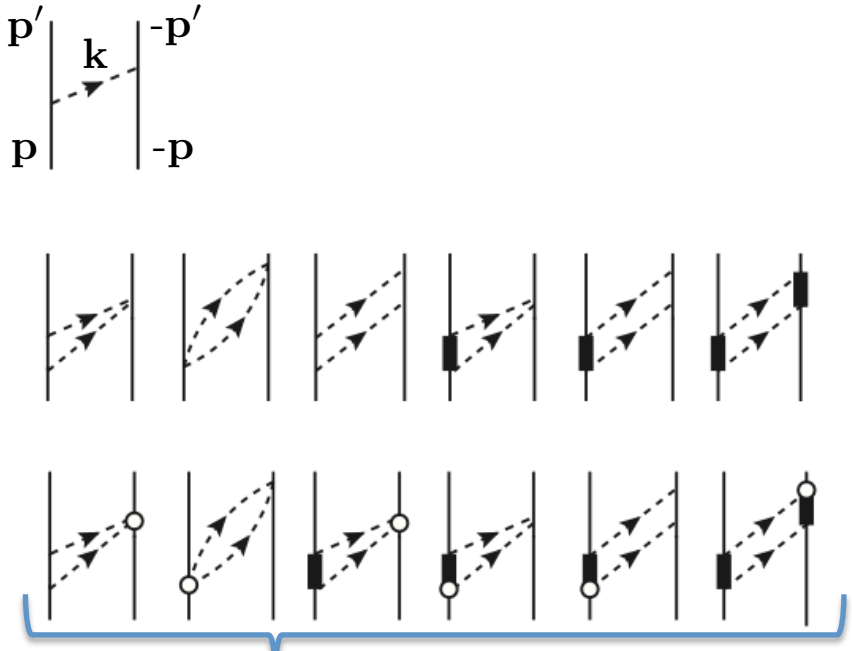
Local chiral NN Potentials:

$$v_{12} = v_{12}^{\rm EM} + v_{12}^{\rm L} + v_{12}^{\rm S}$$

$v_{12}^{\rm EM}$: EM interaction component

- Leading Coulomb interaction
- Second order Coulomb interaction
- Darwin-Foldy interaction
- Vacuum polarization interaction
- Magnetic moment interaction

$v_{12}^{\rm L}$: long-range component



- $\mathbf{k} = \mathbf{p}' - \mathbf{p}$
- Dependence on g_A, F_π and $h_A = 3\,g_A/\sqrt{2}$

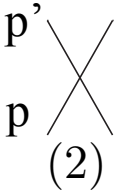
$c_1,\ c_2,\ c_3,\ c_4\ \ (\mathcal{L}_{\pi N}^{(2)})$

$b_3 + b_8\ \ (\mathcal{L}_{\pi N\Delta}^{(2)})$

taken from π-N scattering

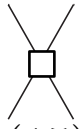
H. Krebs, E. Epelbaum, U.-G. Meissner (2007)

$v_{12}^{\rm S}$: short range component

LO : Q^0 

(2)

NLO : Q^2  (7)

N3LO : Q^4  (15)

- $\mathbf{K} = \frac{1}{2}(\mathbf{p} + \mathbf{p}')$
- $\mathbf{k} = \mathbf{p}' - \mathbf{p}$

- In the NLO and N3LO contact interactions terms proportional to K^2 and K^4 have been removed by Fierz rearrangements: $P^{\rm exc} \,|\, f\rangle = -\,|\, f\rangle$ $\langle f|O|i\rangle = -\langle f|P^{\rm exc}\, O|i\rangle$

$$P^{\rm exc} = \frac{1+\boldsymbol{\sigma}_1\cdot\boldsymbol{\sigma}_2}{2}\,\frac{1+\boldsymbol{\tau}_1\cdot\boldsymbol{\tau}_2}{2}\,P^{\rm space} \longrightarrow \mathbf{k}\to -2\,\mathbf{K} \text{ and } \mathbf{K}\to -1/2\,\mathbf{k}$$

$$K^m \longrightarrow -\frac{1+\boldsymbol{\tau}_1\cdot\boldsymbol{\tau}_2}{2}\,\frac{1+\boldsymbol{\sigma}_1\cdot\boldsymbol{\sigma}_2}{2}\,\frac{k^m}{2^m} \qquad \text{with m=2 or 4}$$

- Fierz rearrangement is effective in completely removing non-localities at NLO (see A. Gezerlis *et al.* PRC **90**, 054323 (2014), M. Piarulli *et al.* PRC **91**, 024003 (2015)), but it cannot do so at N3LO.

- Of course mixed terms as $k^2\,K^2$ or $\mathbf{K}\times\mathbf{k}$ can not Fierz-transformed away

$$k^2\,K^2 \quad\longrightarrow\quad -\frac{1+\boldsymbol{\tau}_1\cdot\boldsymbol{\tau}_2}{2}\,\frac{1+\boldsymbol{\sigma}_1\cdot\boldsymbol{\sigma}_2}{2}\,K^2\,k^2$$

Coordinate-space $v_{12}^{\rm L}$:

$$v_{12}^{\rm L} = \left[\sum_{l=1}^{6} v_{\rm L}^{l}(r)\, O_{12}^{l}\right] + v_{\rm L}^{\sigma T}(r)\, O_{12}^{\sigma T} + v_{\rm L}^{tT}(r)\, O_{12}^{tT}$$

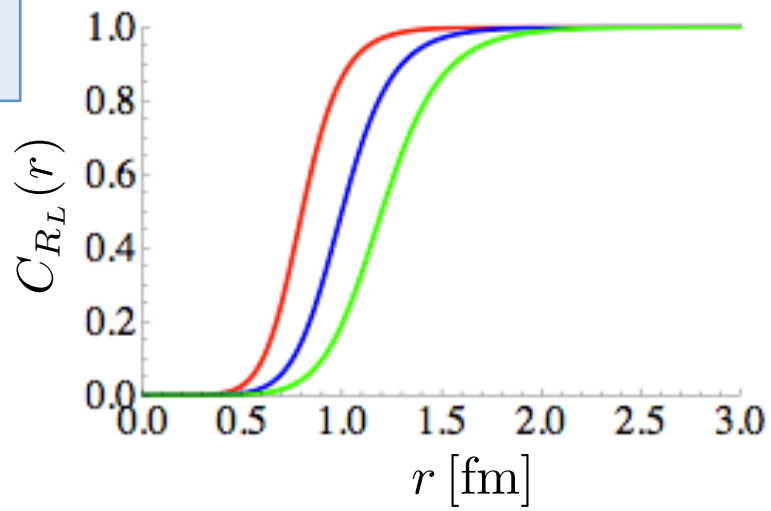
- $O_{12}^{l=1,\ldots,6} = [\mathbf{1}\,,\, \boldsymbol{\sigma}_1 \cdot \boldsymbol{\sigma}_2\,,\, S_{12}] \otimes [\mathbf{1}\,,\, \boldsymbol{\tau}_1 \cdot \boldsymbol{\tau}_2]$
- $O_{12}^{\sigma T} = \boldsymbol{\sigma}_1 \cdot \boldsymbol{\sigma}_2\, T_{12}$
- $O_{12}^{tT} = S_{12} T_{12}$

$T_{12} = 3\,\tau_{1z}\tau_{2z} - \boldsymbol{\tau}_1 \cdot \boldsymbol{\tau}_2$ } CIB terms

- $v_L^l(r)\;\; v_L^{\sigma T}(r)\;\; v_L^{tT}(r)$ ⇒ divergencies of type $1/r^n$, $1 \le n \le 6$

$$C_{R_{\rm L}}(r) = 1 - \frac{1}{(r/R_{\rm L})^6\, e^{(r-R_{\rm L})/a_L} + 1}$$

- $R_L = (0.8, 1.0, 1.2)$ fm
- $a_L = R_L/2$



Coordinate-space $v_{12}^{\rm S}$:

$$v_{12}^{\rm S} = \sum_{l=1}^{16} v_{\rm S}^{l}(r)\, O_{12}^{l}$$

- $O_{12}^{l=1,\ldots,6} = [\mathbf{1}\,,\, \boldsymbol{\sigma}_1\cdot\boldsymbol{\sigma}_2\,,\, S_{12}] \otimes [\mathbf{1}\,,\, \boldsymbol{\tau}_1\cdot\boldsymbol{\tau}_2]$
- $O_{12}^{l=7,\ldots,11} = \mathbf{L}\cdot\mathbf{S}\,,\, \mathbf{L}\cdot\mathbf{S}\,\boldsymbol{\tau}_1\cdot\boldsymbol{\tau}_2\,,\, (\mathbf{L}\cdot\mathbf{S})^2\,,\, \mathbf{L}^2\,,\, \mathbf{L}^2\,\boldsymbol{\sigma}_1\cdot\boldsymbol{\sigma}_2$
- $O_{12}^{l=12,\ldots,16} = T_{12}\,,\, (\tau_1^z+\tau_2^z)\,,\, \boldsymbol{\sigma}_1\cdot\boldsymbol{\sigma}_2\,T_{12}\,,\, S_{12}\,T_{12}\,,\, \mathbf{L}\cdot\mathbf{S}\,T_{12}$

- In this parametrization we removed

  $\{\, v_{\rm S}^{p}(r) + v_{\rm S}^{p\sigma}(r)\,\boldsymbol{\sigma}_1\cdot\boldsymbol{\sigma}_2 + v_{\rm S}^{pt}(r)\,S_{12} + v_{\rm S}^{pt\tau}(r)\,S_{12}\,\boldsymbol{\tau}_1\cdot\boldsymbol{\tau}_2\ ,\ \mathbf{p}^2\,\}$

  and also we considered CD terms

- For the short-range terms the regularization is achieved by employing a local regulator

$$\widetilde{C}_{R_{\rm S}}(k) = e^{-R_{\rm S}^2 k^2/4} \longrightarrow C_{R_{\rm S}}(r) = \frac{1}{\pi^{3/2} R_{\rm S}^3} e^{-(r/R_{\rm S})^2}$$

- In combination with $R_L = (0.8, 1.0, 1.2)$ fm ⇒ $R_S = (0.6, 0.7, 0.8)$ fm

  ⇒ $\Lambda_{\rm S} = 2/R_{\rm S}$ $(700, 600, 500)$ MeV

Fitting Procedure I:

In this work the LECs are fixed by fitting the pp and np Granada database up to laboratory frame energies $E_{\rm lab} = 125$ MeV and $E_{\rm lab} = 200$ MeV, the deuteron binding energy and the nn scattering length

- $3\,\sigma$-criterion to remove inconsistencies in the database [1]
- There are 2493 exp data up to 125MeV (3476 data up to 200 MeV)
- There are N sets each one corresponding to a different experiment
- Each data set contains measurements at fixed energy and different scattering angle (except total cross sections)

We fit first phase shifts and then refine the fit by minimizing the χ^2 obtained from a direct comparison with the database

[1] R. Navarro Pérez, J.E. Amaro, and E. Ruiz Arriola, Phys. Rev. C **88**, 064002 (2013)
http://www.ugr.es/ amaro/nndatabase/

Fitting Procedure II:

To minimize the total χ^2, we use the Practical Optimization Using No Derivatives (for Squares), POUNDerS (with the help of J. Sarich and S. Wild)

M. Kortelainen, PRC **82**, 024313 (2010)

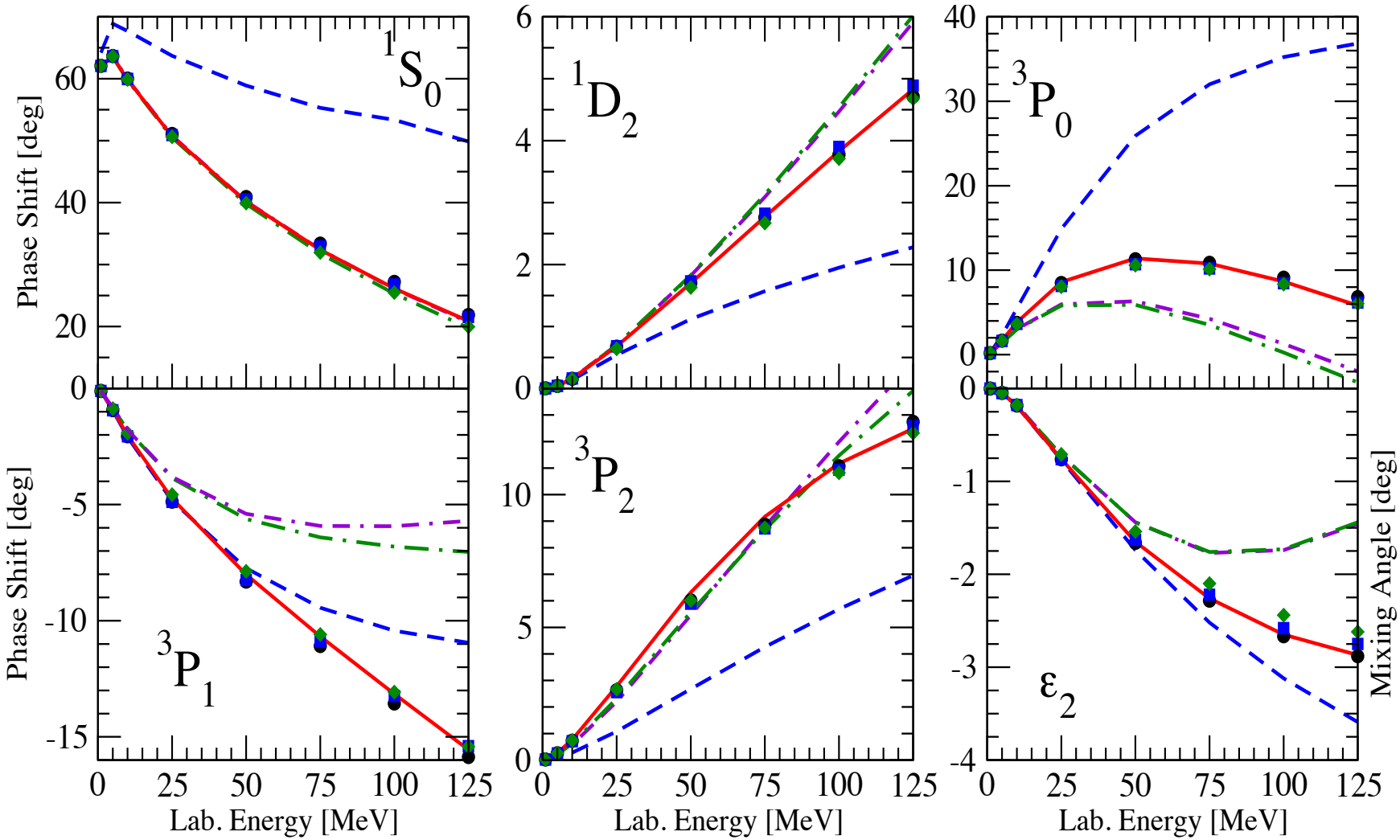
Model a : $(R_L, R_S) = (1.2, 0.8)$

Model b : $(R_L, R_S) = (1.0, 0.7)$

Model c : $(R_L, R_S) = (0.8, 0.6)$

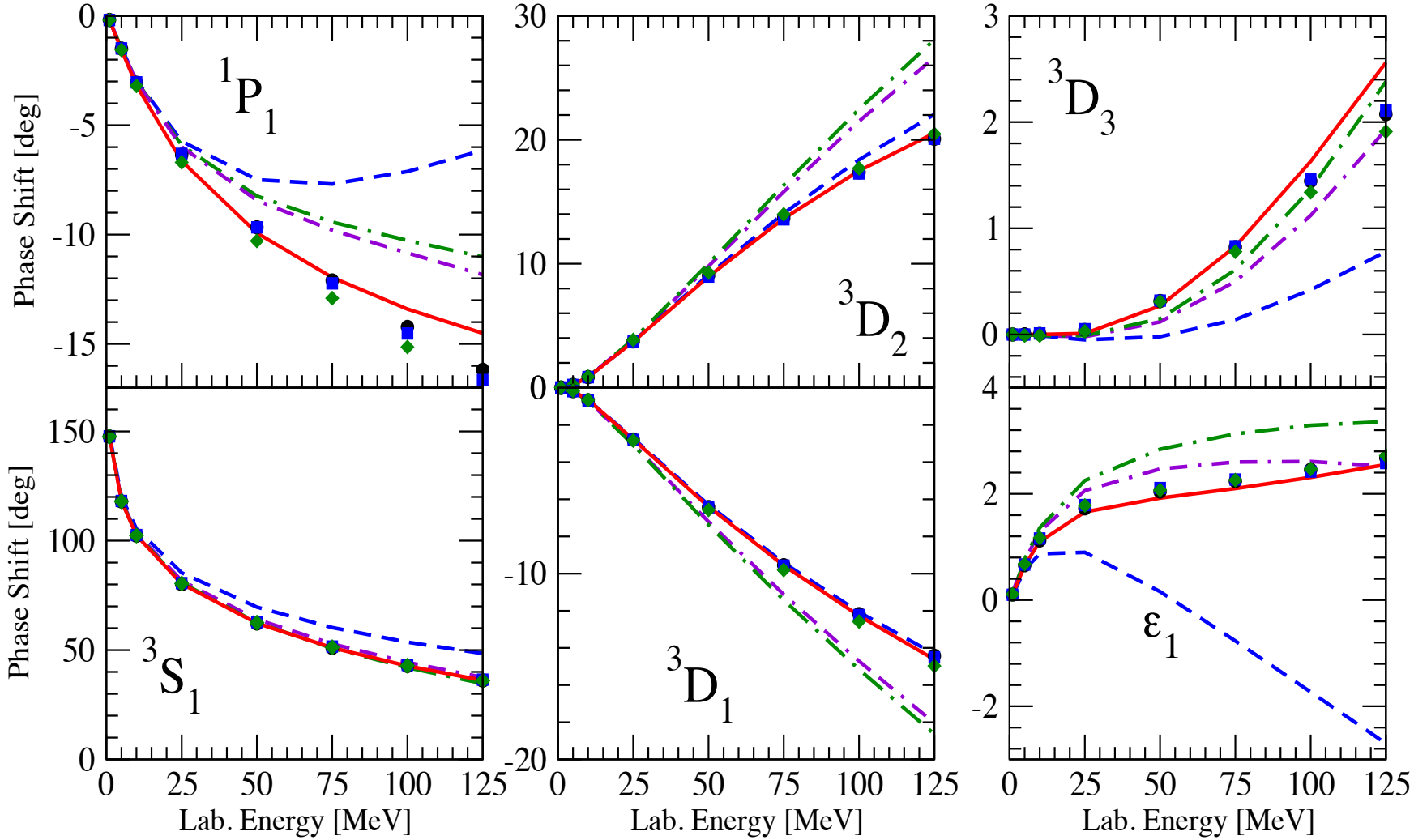
model	order	$R_{\rm L}$ (fm)	$R_{\rm S}$ (fm)	$E_{\rm LAB}$ (MeV)	χ^2/datum
Model b	LO	1.0	0.7	125	59.88
Model b	NLO	1.0	0.7	125	2.18
Model b	N2LO	1.0	0.7	125	2.32
Model b	N3LO	1.0	0.7	125	1.07
Model a	N3LO	1.2	0.8	125	1.05
Model c	N3LO	0.8	0.6	125	1.11
Model $\widetilde{a}$	N3LO	1.2	0.8	200	1.37
Model $\widetilde{b}$	N3LO	1.0	0.7	200	1.37
Model $\widetilde{c}$	N3LO	0.8	0.6	200	1.40

Phase shifts model b up to 125 MeV (order by order):



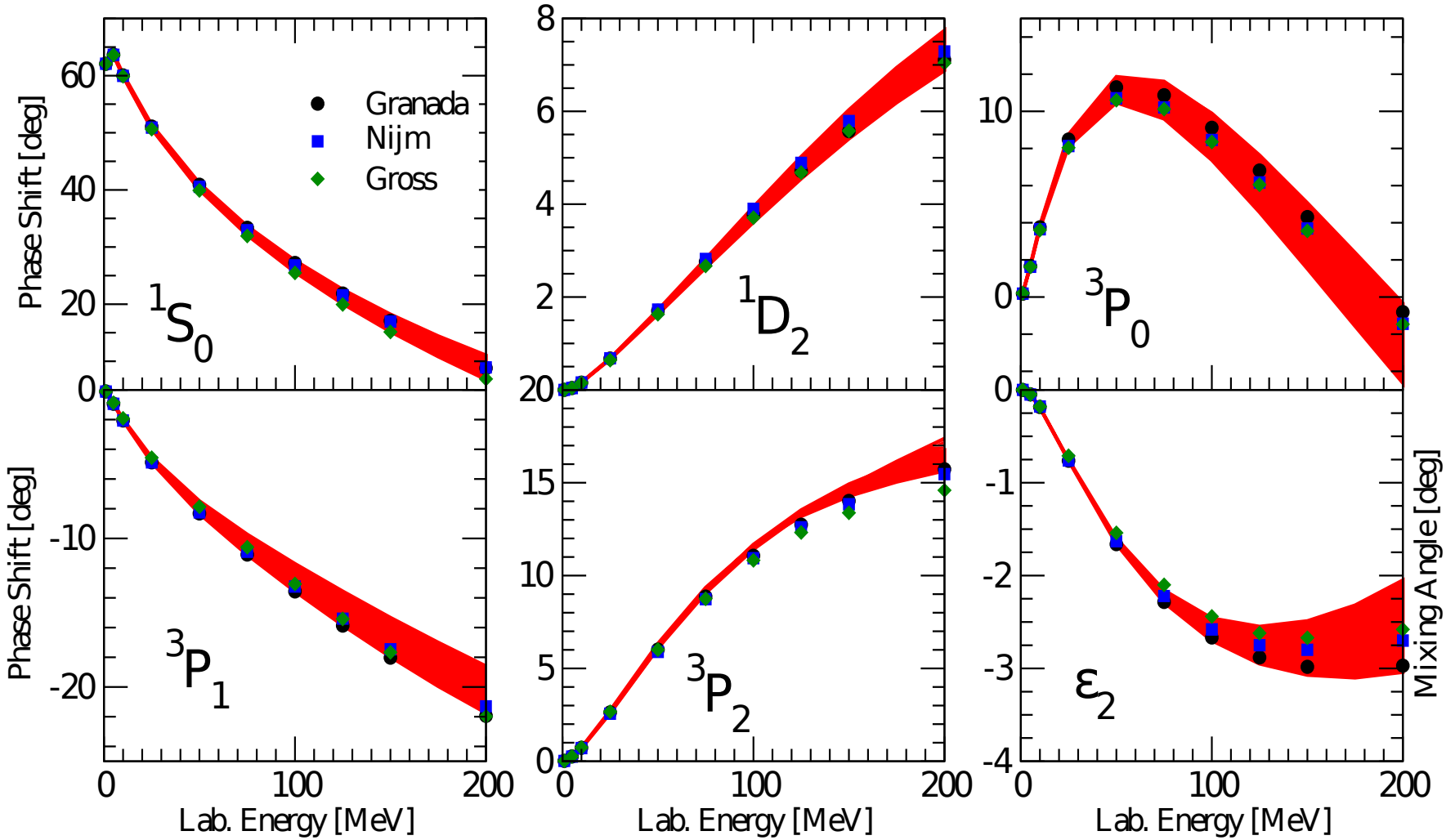
np T=1

Phase shifts model b up to 125 MeV (order by order):

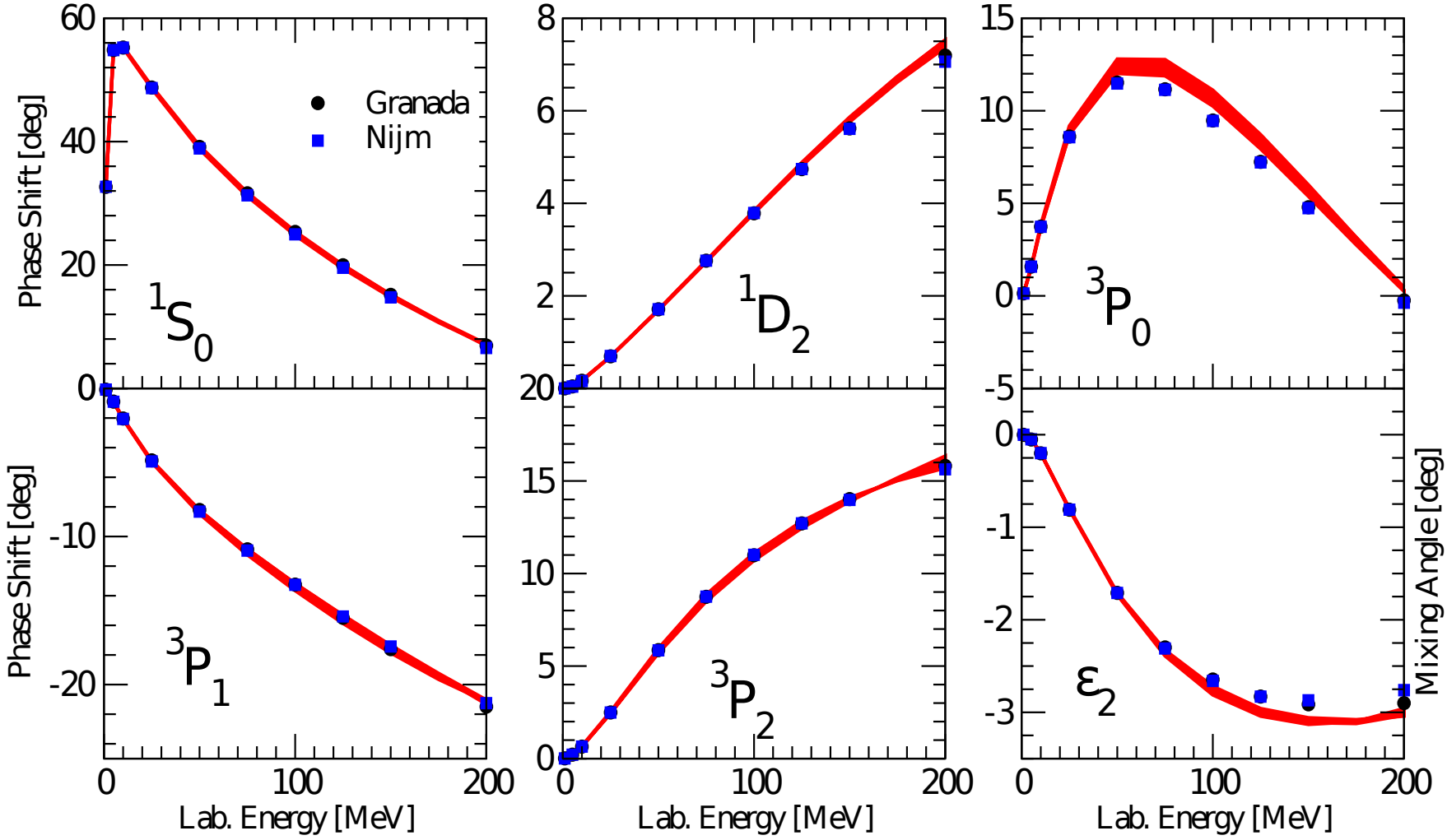


np T=0

Phase shifts: np T=1



Phase shifts: pp T=1



Nuclear Many-Body Problem:

- Few- and many-body systems provide a laboratory to study nuclear forces with a variety of numerical and computational techniques

$$H\,\Psi(\mathbf{R}; s_1, .., s_A; t_1, .., t_A) = E\,\Psi(\mathbf{R}; s_1, .., s_A; t_1, .., t_A)$$

$$H = -\frac{\hbar^2}{2\,m}\sum_i \nabla_i^2 + \sum_{i<j} v_{ij} + \sum_{i<j<k} V_{ijk}$$

$\mathbf{R} = (\mathbf{r}_1, \mathbf{r}_2, ..., \mathbf{r}_A)$ configuration space;
s_i are nucleon spins: $\pm\frac{1}{2}$;
t_i are nucleon isospins (proton or neutron): $\pm\frac{1}{2}$

- HH method (A. Kievsky *et al.*, NPA **577**, 511 (1994); A. Kievsky *et al.*, FBS **22**, 1 (1997); M. Viviani *et al.*, PRC **71**, 024006 (2005); A. Kievsky *et al.*, JPG: NPP **35**, 063101 (2008)) is used to calculate the ground-state energies of ^{3}H and ^{4}He: provide a benchmark for the corresponding QMC calculations
- QMC methods (J. Carlson *et al.*, RMP **87**, 1067 (2015)) are then applied to compute BE and rms radii of the ^{3}He ground state, of the ^{6}Li and ^{6}He ground and excited states

Variational Monte Carlo (VMC):

R.B. Wiringa, PRC **43**, 1585 (1991)

Minimize the expectation value of H:

$$E_T = \frac{\langle \Psi_T | H | \Psi_T \rangle}{\langle \Psi_T | \Psi_T \rangle} \geq E_0$$

Trial wave function (involves variational parameters):

$$|\Psi_T\rangle = \left[S \prod_{i<j}^{A} (1 + U_{ij}) \right] |\Psi_J\rangle$$

no three-body correlations induced by three-body force

- $|\Psi_J\rangle = \left[\prod_{i<j} f_c(r_{ij}) \right] |\Phi(JMTT_z)\rangle$ (s-shell nuclei): Jastrow wave function, fully antisymmetric
- $S \prod_{i<j}$ represents a symmetrized product
- pair correlation operators $U_{ij} = \sum_{p=2,6} u_p(r_{ij})\, O_{ij}^p$
- pair correlation obtained by solving the (two-body) Euler-Lagrange equations (in spin S and isospin T channels)

The search in parameter space is made using COBYLA (Constrained Optimization BY Linear Approximations) algorithm available in the NLopt library

http://ab-initio.mit.edu/wiki/index.php/NLopt

Green's Function Monte Carlo (GFMC):

J. Carlson, PRC **36**, 2026 (1987); J. Carlson, PRC, 1879 (1988)

Projects out lowest energy state from the best variational Ψ_T:

$$|\Psi_0\rangle \propto \lim_{\tau\to\infty} |\Psi(\tau)\rangle = \lim_{\tau\to\infty} e^{-(H-E_0)\,\tau}\,|\Psi_T\rangle \qquad |\Psi(\tau=0)\rangle = |\Psi_T\rangle$$

- the imaginary-time evolution operator is computed for small time steps $\Delta\tau$ ($\tau = n\,\Delta\tau$)

Propagator does not contain p^2, L^2, $(\mathbf{L}\cdot\mathbf{S})^2$:

- it is carried out with a simplified version H' of the full Hamiltonian H; H' contains a charge independent eight-operator projection:

$$[\mathbf{1}\,,\,\boldsymbol{\sigma}_1\cdot\boldsymbol{\sigma}_2\,,\,S_{12}\,,\mathbf{L}\cdot\mathbf{S}]\otimes[\mathbf{1}\,,\,\boldsymbol{\tau}_1\cdot\boldsymbol{\tau}_2]$$

Fermion sign problem limits maximum τ:

Constrained path approximation: R.B. Wiringa PRC **62**, 014001 (2000)

- limits the initial propagation to regions where the propagated $|\Psi(\tau)\rangle$ and trial $|\Psi_T\rangle$ wave functions have a positive overlap and discards those configurations that instead have a small or vanishing overlap
- small number of unconstrained time steps $n_{\rm uc} \sim 20$ are used when evaluating the expectation values

Results for binding energies: HH vs QMC

The ^{3}H ground-state energies E_0 (MeV) and rms proton radii r_p (fm)

	Model a		Model $\widetilde{a}$		Model b		Model $\widetilde{b}$	
Method	E_0	$\sqrt{\langle r_p^2 \rangle}$	E_0	$\sqrt{\langle r_p^2 \rangle}$	E_0	$\sqrt{\langle r_p^2 \rangle}$	E_0	$\sqrt{\langle r_p^2 \rangle}$
VMC	–7.592(6)	1.65	–7.691(6)	1.62	–7.317(7)	1.68	–7.643(5)	1.63
GFMC	–7.818(8)	1.62	–7.917(10)	1.60	–7.627(17)	1.65	–7.863(8)	1.57
HH	–7.818		–7.949		–7.599		–7.866	

The ^{4}He ground-state energies E_0 (MeV) and rms proton radii r_p (fm)

	Model a		Model $\widetilde{a}$		Model b		Model $\widetilde{b}$	
Method	E_0	$\sqrt{\langle r_p^2 \rangle}$	E_0	$\sqrt{\langle r_p^2 \rangle}$	E_0	$\sqrt{\langle r_p^2 \rangle}$	E_0	$\sqrt{\langle r_p^2 \rangle}$
VMC	–24.38(1)	1.51	–25.03(1)	1.49	–22.89(2)	1.54	–24.46(2)	1.49
GFMC	–25.13(5)	1.49	–25.71(3)	1.50	–23.88(5)	1.53	–25.21(4)	1.45
HH	–25.15		–25.80		–23.96		–25.28	

Results for binding energies:

The ^{3}H, ^{3}He, ^{4}He, ^{6}He, and ^{6}Li ground- and excited-state energies in MeV and proton rms radii r_p in fm with model $\widetilde{b}$ compared with the corresponding GFMC results obtained with the AV18.

	VMC		GFMC		GFMC(AV18)	
$^A Z(J^\pi;T)$	E_0	$\sqrt{\langle r_p^2\rangle}$	E_0	$\sqrt{\langle r_p^2\rangle}$	E_0	$\sqrt{\langle r_p^2\rangle}$
^{3}H$(\frac{1}{2}^+;\frac{1}{2})$	–7.643(5)	1.63	–7.863(8)	1.57	–7.610(5)	1.66
^{3}He$(\frac{1}{2}^+;\frac{1}{2})$	–6.907(5)	1.84	–7.115(9)	1.84	–6.880(5)	1.85
^{4}He$(0^+;0)$	–24.46(2)	1.49	–25.21(4)	1.45	–24.14(1)	1.49
^{6}He$(0^+;1)$	–22.58(3)	2.05	–24.53(6)	2.07(1)	–23.76(9)	2.06(1)
^{6}He$(2^+;1)$	–20.94(2)	2.06	–22.87(6)	2.18(2)	–21.85(9)	2.11(1)
^{6}Li$(1^+;0)$	–25.86(3)	2.58	–27.71(8)	2.62(1)	–26.87(9)	2.58(1)
^{6}Li$(3^+;0)$	–22.73(3)	2.59	–24.56(8)	2.59(1)	–24.11(7)	2.87(1)
^{6}Li$(2^+;0)$	–21.42(3)	2.61	–24.04(9)	2.79(2)	–22.75(11)	2.63(1)
^{6}Li$(1^+;0\,,{}^3$D[2])	–20.42(3)	2.58	–23.09(11)	2.89(2)	–21.99(12)	2.85(3)

Conclusions:

We constructed a family of local NN potential with chiral TPE including Δ-isobar up to N2LO (Q^3) and contact interactions up to N3LO (Q^4)

Three versions of this chiral potential for three different cutoffs have been developed with fits to np and pp data up to $E_{\rm lab} = 125$ MeV and 200 MeV, deuteron binding energy and nn scattering length

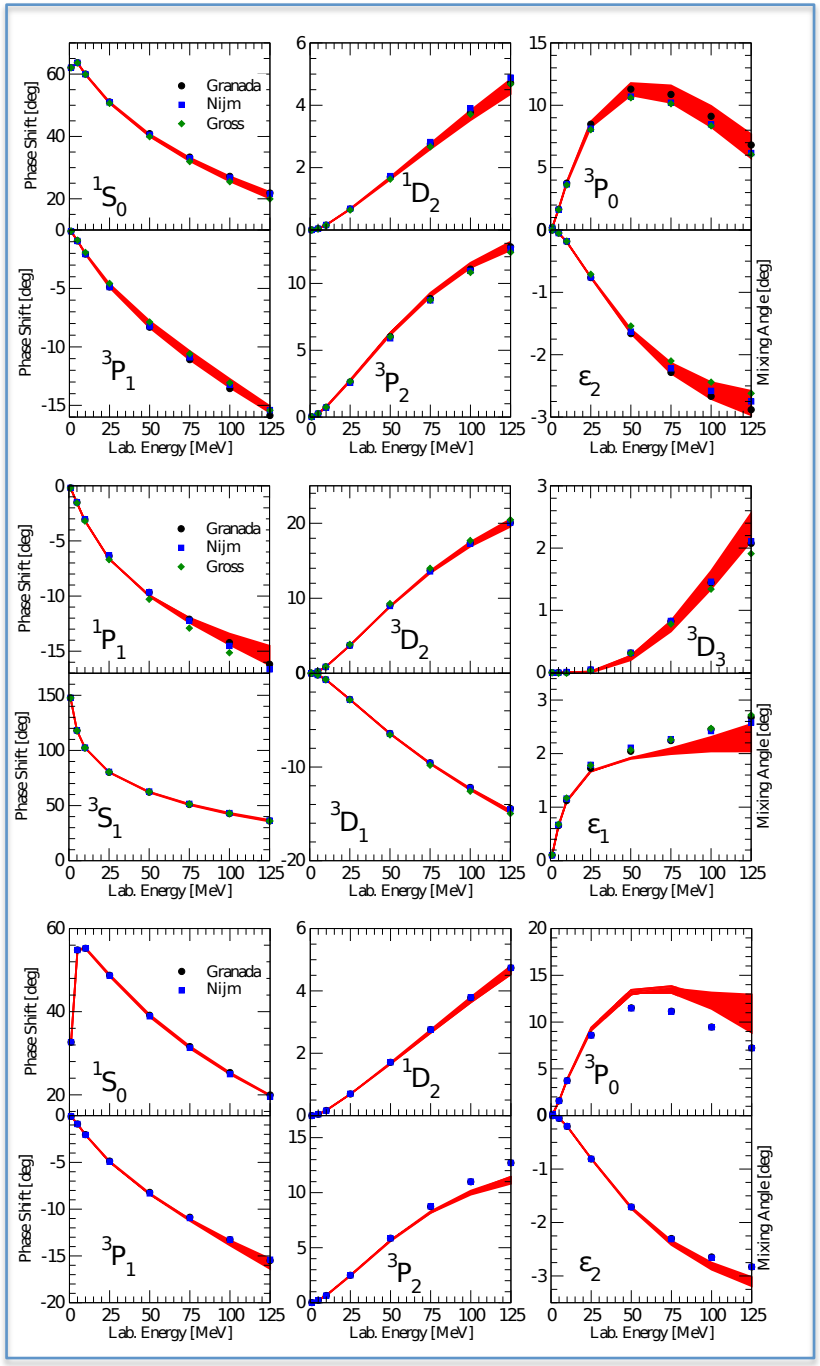
A subset of the potentials—a, $\widetilde{a}$, b, and $\widetilde{b}$—have been used in HH, VMC, and GFMC calculations of binding energies and proton rms radii of nuclei with $A = 2$–6

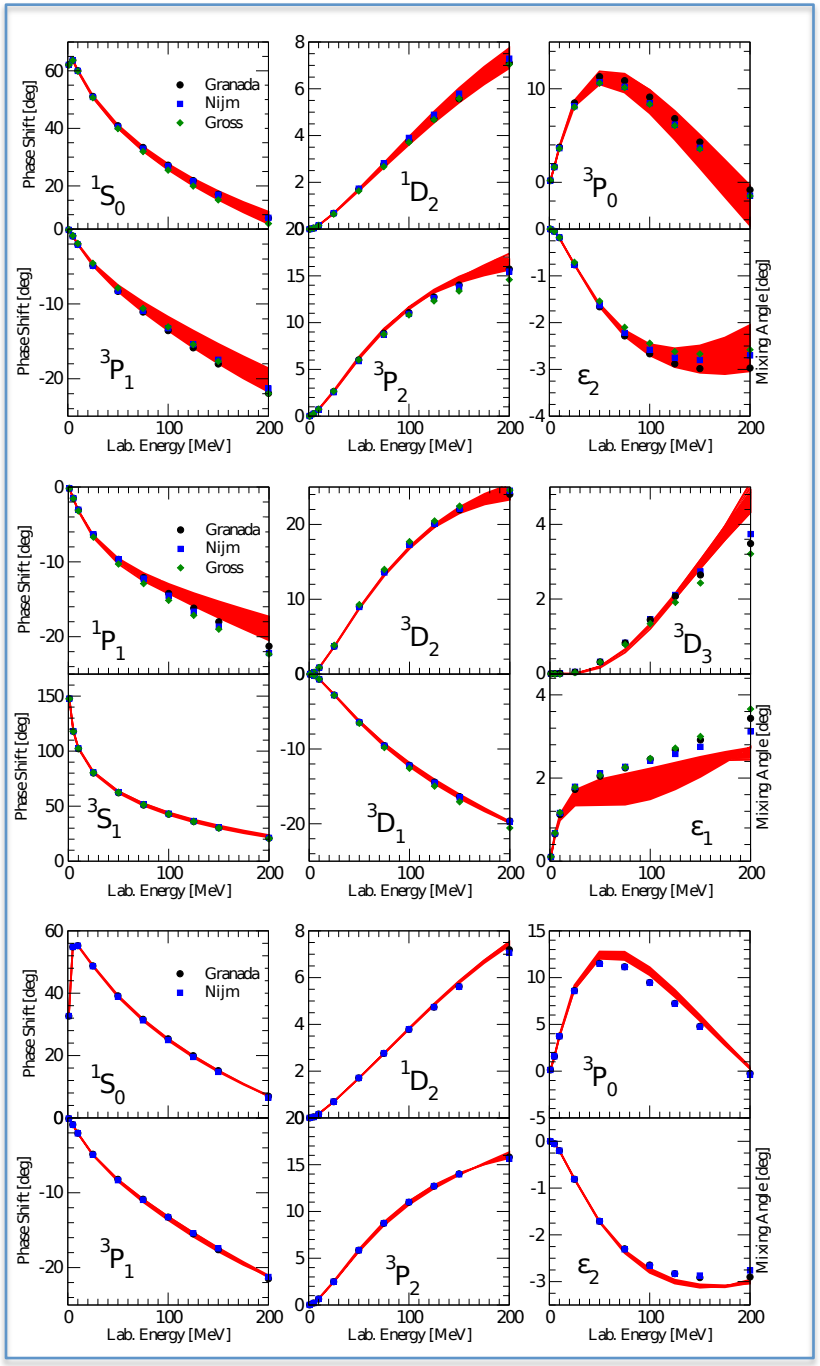
Plans:

The next stage in the program of studies of light nuclei structure with chiral interactions will be the inclusion of a 3N potential

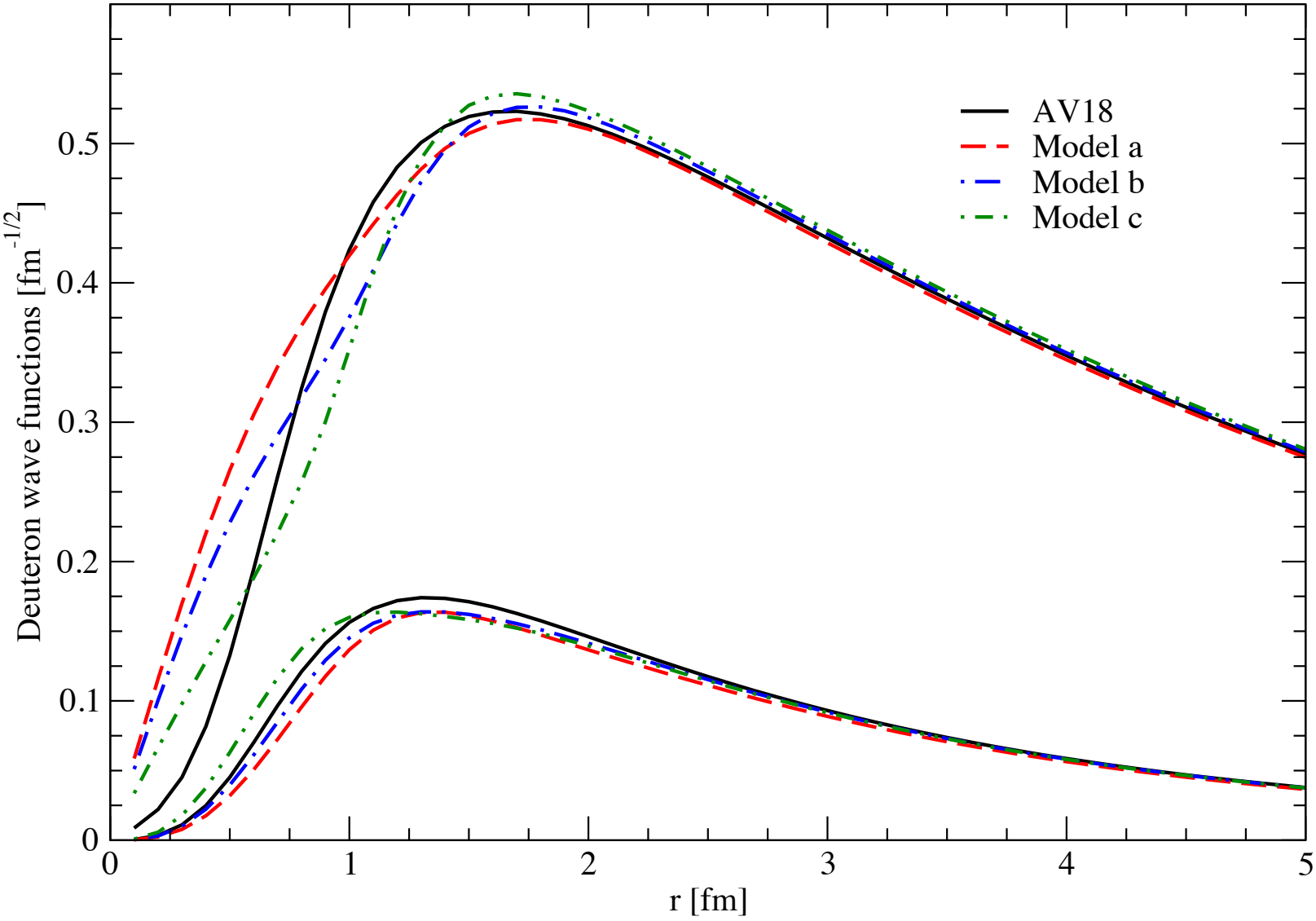
A chiral version of it at leading order, including Δ-isobar intermediate states, has been developed, and is currently being constrained by reproducing observables in the $A = 3$ systems.

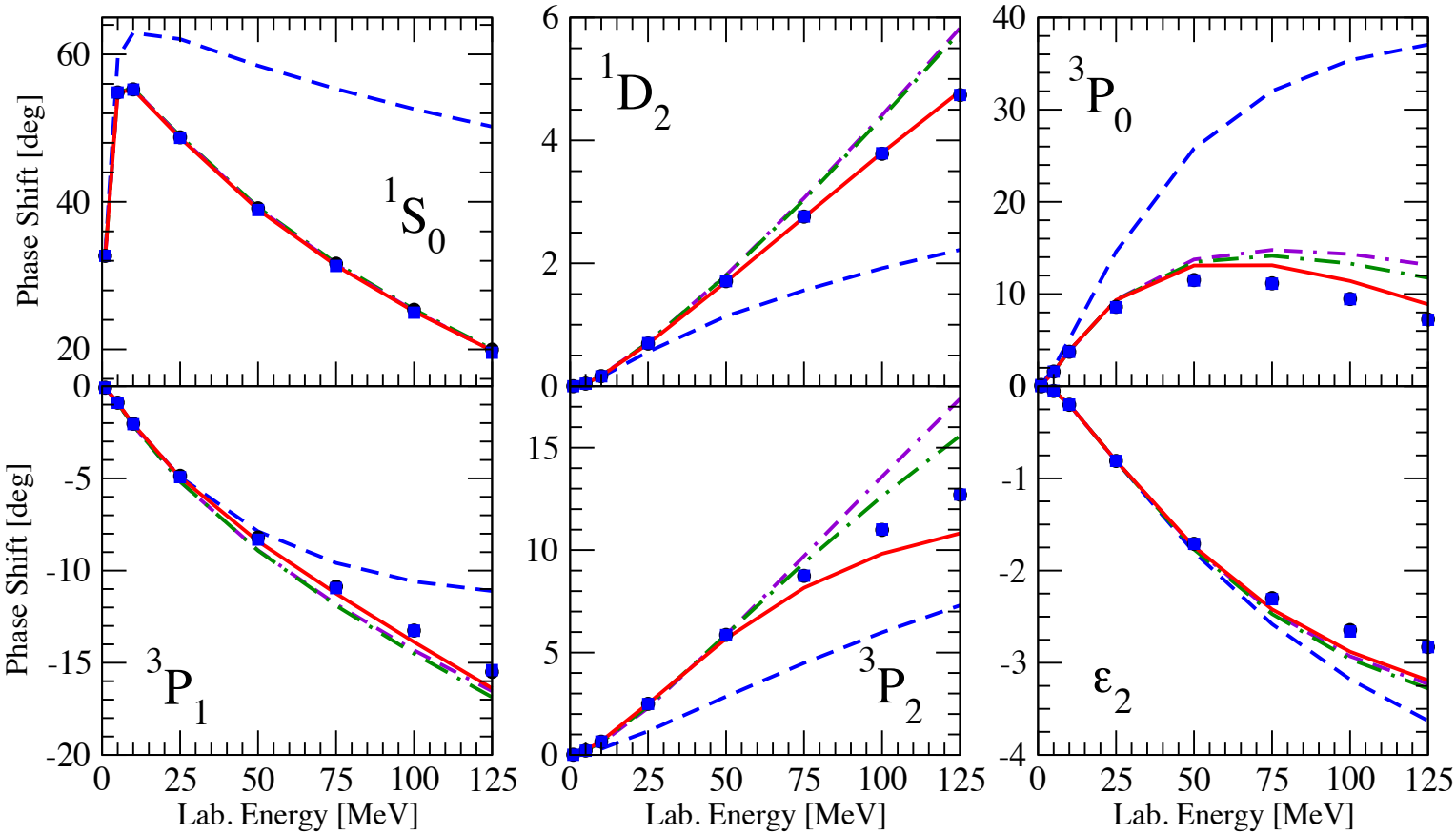
Phase Shifts: 125 and 200 MeV





The S-wave and D-wave components of the deuteron wave function corresponding to models a (dashed lines), b (dotted-dashed lines) and c (dotted-dashed-dotted lines) are compared with those corresponding to the AV18 (solid lines)




Phase Shift [deg]
$^1S_0$
$^1D_2$
$^3P_0$
$^3P_1$
$^3P_2$
ε_2
Lab. Energy [MeV]
Lab. Energy [MeV]
Lab. Energy [MeV]