

# **Nuclear interactions and quantum Monte Carlo methods**

Maria Piarulli—Washington University, St. Louis July 11-13, 2022

2022 National Nuclear Physics Summer School (NNPSS) – MIT





## Lecture 1: Nuclear Forces

- Introduction
- The microscopic model of nuclear theory
- The nucleon-nucleon scattering problem
- Phenomenological approach
- Empirical features of nuclear forces
- Chiral effective filed theory approach

## The big questions in NP

**1.** How did the universe come to be and how does it evolve?

**2.** How does subatomic matter organize itself and what phenomena emerge?

**3**. Are the fundamental interactions that are basic to the structure of matter fully understood?

**4**. How can the knowledge and technological progress provided by nuclear physics best be used to benefit society?

These are very broad and deep questions, and the challenges they pose provoke intriguing opportunities for the next decades to come!

VATIONAL RESEARCH EDUNCE.

- Hot QCD (relativistic heavy ions): examines the primordial form of matter existed in the universe shortly after the Big Bang
- Cold QCD (hadron structure): explores the characteristics of the strong force by which the quarks and gluons interact and resulting properties of the nucleons

#### Interface between Physics of Hadrons and Physics of Nuclei

- Nuclear structure and reactions: trying to build a coherent framework for explaining all properties of nuclei and nuclear matter and how they interact
- Nuclear astrophysics: explores those events and objects in the universe shaped by nuclei and nuclear reactions
- Fundamental symmetries: providing some understandings upon which a new, more comprehensive Standard Model will be built



## **NUclear Computational Low-Energy Initiative**



ATLAS (ANL): superconducting linear accelerator focusing on atomic nuclei near and far from stability, nuclear astrophysics, and fundamental symmetries

FRIB (MSU): scientific user facility for nuclear science access a wide range of nuclei far from stability

CEBAF (JLAB): Continuous Electron Beam Accelerator Facility focusing on electronnucleus scattering.



Nuclear astrophysics: JINA (Michigan State University, Notre Dame University, UChicago)

Nuclear Structure and astrophysics: ARUNA (Florida State U., Notre Dame U., Texas A&M, The Triangle Universities Nuclear Laboratory, Ohio U., Kentucky U., U. Washington)

#### **Domestic nuclear physics facilities**

and densities



DUNE (Fermilab): is an experiment under construction that will focus on neutrinos physics

double beta decay



## Physics of atomic nuclei



Question: where does the nuclear force which binds nucleons together gets its main characteristics, and how it is rooted in the fundamental theory of strong interactions?

• Atomic nuclei: complex quantum many-body systems of strongly interacting fermions (nucleons: p and n) displaying interesting properties. • Their structure and scattering by electron and neutrinos are the main focus of NP and HEP in domestic and worldwide research programs. • It is important for nuclear theory to guide and support such experimental activities, ultimately connecting low-energy nuclear properties with quantum chromodynamics (QCD). • QCD is the underlying theory of the strong interaction but nucleons are the relevant degree of freedom for the low-energy nuclear physics that

leads to the idea of effective potential.

# What Holds the Nucleus Together?

#### by Hans A. Bethe September 1953

Tn the preceding article Erwin Schrödinger deals with the basic nature L of matter (does it consist of particles or waves?) and touches on some of the questions about its construction. My assignment is to discuss what is by all odds the most mystifying of these questions: What holds the nucleus of the atom together? In the past quarter century physicists have devoted a huge amount of experimentation and mental labor to this problem-probably more man-hours than have been given to any other scientific question in the history of mankind. The problem is not only

tion. It is constructed of a heavy, positively charged nucleus surrounded by a "planetary system" of light, negatively charged electrons. The forces that govern the behavior of the electrons are thoroughly familiar: they are the forces of electric attraction and repulsion. To describe the motions of the electrons physicists had to invent a new mechanics known as quantum mechanics. Once this was worked out, it became possible to understand all the properties of atoms as a whole-their sizes, their chemical behavior, the light they emit, and so on-in terms of the motions of the elec-

humankind \_\_\_\_

person

Electrical forces bind the electron to the atom, but they cause nuclear particles to fly apart. The powerful cohesion of protons and neutrons must be explained by a wholly different phenomenon

> fact: whereas the density of the fluffy outer structure of atoms varies greatly from one kind of atom to another, all nuclei have a uniform density (about 100 trillion times that of water). Thus the total volume of an atom, insofar as its volume can be defined at all, is not necessarily proportional to its weight, a circumstance which makes some substances denser than others. But the volume of a nucleus is very nearly proportional to its weight, just as a piece of iron 10 times as heavy as another is also 10 times as large in volume.

This resemblance of nuclei to the mat-

#### Quantum Chromodynamcs







Nuclear forces: very complicated problem to derive in terms of quarks and gluons

- Cartoon of the exchange of a pion (OPE) between two nucleons in the quark picture
- OPE: describes the long range part of nuclear forces ( $r \ge 2$  fm) to describe the net attraction to form bound nuclei
- Meson exchange theory: introduced by Yukawa in 1935; in 1947 discovery of a massive particle called pion

### **Nevertheless Lattice QCD**

#### Lattice Quantum Chromodynamics



Scattering in the  ${}^{1}S_{0}$  channel  $m_{\pi} \sim 450 \,\mathrm{MeV}$ 



Orginos et Phys. Rev. D 92, 114512 (2015); NPLQCD

Despite the many advances, LQCD calculations are still limited to small nucleon numbers and/or large pion masses.

#### Atomic nuclei and nucleonic matter





LQCD predictions for magnetic moments A < 4,  $m_{\pi} \sim 800 \,\mathrm{MeV}$ 



Beane et al., PRL113, 252001 (2014); NPLQCD





## The microscopic model of nuclear theory

*Goal*: develop a predictive understanding of nuclei in terms of the interactions between individual nucleons and external probes

Nucleon-nucleon (NN) and 3N scattering data: "thousands" of experimental data available

Spectra, properties, and transition of nuclei: BE, radii, magnetic moments, beta decays rates, weak/radiative captures, electroweak form factors, etc,...

Nucleonic matter equation of state: for ex. EOS neutron matter

Disentangle new physics from nuclear effects: for ex.  $0\nu\beta\beta$ , BSM with  $\beta$ -decay, EDMs,  $\nu - A$  xsec, etc,..



## The microscopic model of nuclear theory

• What we need?

Electroweak current operators:



Ab-initio methods: solve the nuclear many-body problem



- Improved and novel many-body frameworks
- Increased computational resources
- Nuclear interactions and currents based on EFTs
- Theoretical uncertainty quantification

## What do we know about the nuclear force?

Our understanding of the nuclear force is based on three types of experimental information:

- conducted with spin-polarized projectiles/targets.
- Nuclear binding energies and masses, especially for light nuclei.
- especially for light nuclei.

Results of NN (particularly proton-proton and proton-neutron) scattering experiments which give us information about the two-body potential. Some of these experiments are

Nuclear structure information, such as spins, parities, magnetic and quadrupole moments,





### The nucleon-nucleon scattering



• The differential and total cross sections are given by:



• When V(r) = 0 (free scattering):  $R_l(k, r) = j_l(k, r) = -$ 

$$\frac{d\sigma}{d\Omega} = |f(\theta,\phi)|^2 \qquad \sigma = \int d\Omega \frac{d\sigma}{d\Omega}$$

$$\frac{1}{kr}\sin(kr-\frac{1}{2}l\pi)$$



• For elastic scattering from  $V(r > a) \rightarrow 0$  the asymptotic wave function can vary by an amount  $\delta_l$  – the phase shift:



• If  $\delta_l > 0$ , the node in sin(...) is reached at smaller r and the wave is "sucked in" indicating an attractive interaction. If  $\delta_l < 0$ , the wave is "pushed out" implying net repulsion.



$$-\frac{1}{2}l\pi + \delta_{\rm l}$$

• With a complete set of  $\delta_l$ , we can calculate cross sections:

$$f(\theta) = \frac{\sqrt{4\pi}}{k} \sum_{l=0}^{\infty} \sqrt{4\pi} \sum_{l=0}^{$$

$$\sigma = \int |f(\theta)|^2 d\Omega = \frac{4\pi}{k^2} \sum_{l=0}^{\infty} (2l+1) \sin^2 \delta_l$$

- in terms of  $\delta_l$ .

$$k \cot \delta_0(k) = -\frac{1}{a} + \frac{1}{2}rk^2$$
$$\lim_{k \to 0} \sigma = 4\pi a^2 = 4\pi \frac{\sin^2 \delta_0}{k^2}$$

• Things are somewhat more complicated when long-range Coulomb potentials are included.

 $\sqrt{2l+1}e^{i\delta_l}\sin\delta_l Y_{l0}(\theta)$ 

• Other observables include polarizations, analyzing powers, spin correlation parameters, all of which have specific expressions

• At low energy (< 1 MeV, l = 0) the cross section is expressed in terms of the scattering length a and effective range r:

#### **Allowed NN scattering states**

- Wave function for two nucleons must be antisymmetric in space  $\otimes$  spin  $\otimes$  isospin
- The allowed partial waves in spectroscopic notation  ${}^{2S+1}L_i$

L = even (+) S = 1 (+) T =S=0(-)T=L = odd(-) S = 1 (+) TS=0(-)T

$$S = \begin{pmatrix} e^{2i\delta_{L}=J-1}\cos(2\varepsilon_{J}) \\ ie^{\delta_{L}=J-1+\delta_{L}=J+1}\sin(2\varepsilon_{J}) \end{pmatrix}$$

characterized by two phases  $\delta_{L=J-1}$  and  $\delta_{L=J+1}$  and mixing angle parameter  $\epsilon_i$ 

$$=0 (-): {}^{3}S_{1} - {}^{3}D_{1}, {}^{3}D_{2}, {}^{3}D_{3} - {}^{3}G_{3}, ...$$
  
$$=1 (+): {}^{1}S_{0}, {}^{1}D_{2}, {}^{1}G_{4}, ...$$
  
$$=1 (+): {}^{3}P_{0}, {}^{3}P_{1}, {}^{3}P_{2} - {}^{3}F_{2}, {}^{3}F_{3}, ...$$
  
$$=0 (-): {}^{1}P_{1}, {}^{1}F_{3}, ...$$

• Note that J is a conserved quantum number but L is not – different partial waves can be mixed by the tensor force in S = 1 states, i.e., L = J - 1 L = J + 1. For coupled-channels, the scattering matrix encodes this information as:

$$ie^{\delta_{L}=J-1+\delta_{L}=J+1}sin(2\varepsilon_{J})$$
$$e^{2i\delta_{L}=J+1}cos(2\varepsilon_{J})$$

## Partial wave analysis: Nijmegen database

Data selection in the 1993 Nijmegen PWA from all pp [Bergervoet, et al., PRC 41, 1435 (1990)] and np [Stoks, *et al.*, PRC 48, 792 (1993)] elastic scattering data with  $E_{lab} < 350$  MeV published between 1955 and 1992:

> observables rejected in  $3\sigma$  test remainder (groups) normalizations (floated) total data to fit

Post 1992 data have increased the "accepted" database to 2932 pp [Machleidt, PRC 63, 024001 (2000)] and 3788 *np* [Gross & Stadler, PRC 78, 014005 (2008)] data.

Useful up-to-date resources include: the SAID program from http://gwdac.phys.gwu.edu/ and NN-OnLine from http://nn-online.org/

pp		np	
1947		3298	
-291		-932	
1656	(215)	2366	(211)
+131	(22)	+148	(16)
1787		2514	

### Partial wave analysis: Granada database

The analysis includes data within the years 1950 to 2013.

More than 7800 elastic scattering data



http://www.ugr.es/~amaro/nndatabase/

## **Empirical features of the nuclear force**

#### What do binding energies and phase shifts tell us about the nuclear force?

1. Nuclear force has a finite range:

"Saturation": Nuclei A > 4 show saturation. Binding energy of light nuclei increase rapidly as the number of pairs increase, but stabilize in larger nuclei at  $\sim$  8 MeV/nucleon (force range is about the size of the  $\alpha$  or 2 fm)



#### 2. NN force has an attractive long-range component ( $r \ge 2$ fm ):

► Net attraction necessary to form bound nuclei. Yukawa (1935) suggested that it could be modeled by the exchange of a massive particle (one-pion exchange OPEP)

$$\begin{split} \mathbf{N} & \| \mathbf{N} \\ \mathbf{$$

▶ S-wave phase shifts are positive ( $\delta_{l=0} > 0$ ) for  $E_{lab} < 250$  MeV.



$$S_{12} = 3\,\boldsymbol{\sigma}_1 \cdot \hat{\mathbf{r}}\,\boldsymbol{\sigma}_2 \cdot \hat{\mathbf{r}} - \boldsymbol{\sigma}_1 \cdot \boldsymbol{\sigma}_2$$

#### 3. Nuclear force has a repulsive core

S-wave phase shifts are negative ( $\delta_{l=0} < 0$ ) for  $E_{lab}$  > 250 MeV, while D-wave phase shift remains positive to momentum barrier in D-wave. Simple classical argument gives the core radius  $\sim$ 0.6 fm.

4. NN force depends on spins and isospins of the nucleons: Only the combination S=1 and T=0 has a weakly bound state of np, deuteron.



much larger energy. Can be understood as repulsive core of short range seen by S-wave, but masked by angular

S=0,1 and T=0,1 possibilities. Phase shifts vary greatly among the four possible S=0,1 and T=0,1 combinations.

Notation:  $2S + 1L_{J}$ 

5. NN force has a tensor component: the tensor operator

can can mix states of different orbital angular momentum, L = J - 1 and L = J + 1. The deuteron is predominantly an S-state, but it has magnetic and quadrupole moments that indicate it is not spherical, but has a D-state admixture. B = -2.2224575(9) MeV

Deuteron:

![](_page_22_Picture_3.jpeg)

 $J^{+} = 1^{+}$ L = 0, 2

 $Q = 0.2859(3) \text{ fm}^2$ 6. NN force has a spin-orbit component: Nuclear spectra show evidence for an effective spin-orbit component  ${f L} \cdot {f S}$ which is very important in determining which nuclei are most stable.  ${}^{3}P_{0,1,2}$  phase shifts cannot be explained by

central and tensor forces alone. 20

![](_page_22_Figure_7.jpeg)

$$S_{12} = 3\boldsymbol{\sigma}_1 \cdot \hat{\mathbf{r}} \boldsymbol{\sigma}_2 \cdot \hat{\mathbf{r}} - \boldsymbol{\sigma}_1 \cdot \boldsymbol{\sigma}_2$$

- quadratic in momentum such as  $(\mathbf{L} \cdot \mathbf{S})^2$  and  $L^2$
- or np) in the same state are almost the same.
  - "Almost the same": isospin is slightly broken.
    - Equality between the pp and nn forces: Charge symmetry.
    - Equality between pp/nn force and np force: Charge independence.

**Charge-symmetry breaking (CSB):**  $a_{pp}^{N} = -17.3 \pm 0.4 \,\text{fm}$   $a_{nn}^{N} = -18.8 \pm 0.5 \,\text{fm}$ 

**Charge-independence breaking (CIB):**  $a_{np}^N = -23.74 \pm 0.02 \,\text{fm}$ 

9. There are many-nucleon forces: the NN potential does not give adequate description of nuclei A  $\geq$  3. Since nucleons are composite objects with low-lying excitation spectra we expect many-nucleon forces such as:

$$\begin{array}{c} \pi \\ \Delta \\ \pi \end{array}$$

![](_page_23_Picture_9.jpeg)

7. NN force has quadratic dependence in momentum: higher partial wave phase shifts for given S, T are not fit well by the same potential for the corresponding lowest phase shifts (S-P- and D-waves). This indicates the needs for terms

8. Isospin symmetry breaking: After correcting for the electromagnetic interaction, the forces between nucleons (pp, nn,

![](_page_23_Figure_15.jpeg)

## Phenomenological approach

• Use the general form of a potential allowed by the symmetries:

- Translation invariance
- Galilean invariance
- Rotation invariance
- Space reflection invariance
- Time reversal invariance
- Invariance under the interchange of particle 1 and 2
- Isospin symmetry
- Hermiticity

 Most general two-body potential under those symmetries: (Okubo and Marshak, Ann. Phys. 4, 166 (1958))  $V_{NN} = V_0(r) + V_{\sigma} \sigma_1 \cdot \sigma_2 + V_{\tau} \tau_1 \cdot \tau_2 + V_{\sigma\tau} \sigma_1 \cdot \sigma_2 \tau_1 \cdot \tau_2$  central

 $+V_T(r)S_{12} + V_{T_T}(r)S_{12}\tau_1 \cdot \tau_2$  tensor

+ $V_{LS}(\mathbf{L} \cdot \mathbf{S})$  +  $V_{LS\tau}(\mathbf{L} \cdot \mathbf{S})\boldsymbol{\tau}_1 \cdot \boldsymbol{\tau}_2$  spin-orbit

+ $V_Q Q_{12}$  +  $V_{Q\tau} Q_{12} \tau_1 \cdot \tau_2$  quadratic spin-orbit

+ $V_{PP}(r)(\boldsymbol{\sigma}_1 \cdot \mathbf{p})(\boldsymbol{\sigma}_2 \cdot \mathbf{p}) + V_{PP\tau}(r)(\boldsymbol{\sigma}_1 \cdot \boldsymbol{p})(\boldsymbol{\sigma}_2 \cdot \mathbf{p})\boldsymbol{\tau}_1 \cdot \boldsymbol{\tau}_2$  p-dependent

 $S_{12} = 3 \sigma_2 \cdot \mathbf{r} \sigma_2 \cdot \mathbf{r} - r^2 \sigma_1 \cdot \sigma_2 \quad Q_{12} = 1/2\{(\sigma_1 \cdot \mathbf{L})(\sigma_2 \cdot \mathbf{L}) + (\sigma_2 \cdot \mathbf{L})(\sigma_1 \cdot \mathbf{L})\}$ 

# Examples:

- Gammel-Thaler potential (Phys. Rev. 107, 291, 1339 (1957)), hard-core.
- Hamada-Johnston potential (Nucl. Phys. 34, 382 (1962)), hard core.
- Reid potential (Ann. Phys. (N.Y.) 50, 411 (1968)), soft core.
- Argonne V14 potential (Wiringa et al., Phys. Rev. C 29, 1207 (1984)), uses 14 operators.
- Argonne **V18** potential (Wiringa et al., Phys. Rev. C **51**, 38 (1995)), uses 18 operators.

#### Phenomenological nucleon-nucleon AV18

range parts:

Argonne  $v_{18}$  $v_{ij} = v_{ij}^{\gamma} + v_{ij}^{\pi} + v_{ij}^{I} + v_{ij}^{S} = \sum v_p(r_{ij})O_{ij}^{p}$ 

plus two tensor and two spin-orbit terms in S = 1 states for different T.

$$O_{ij}^{p=1,8} = [1, \sigma_i \cdot \sigma_j, S_{ij}, \mathbf{L} \cdot \mathbf{S}] \otimes [1, \tau_i \cdot \tau_j]$$

• To fit higher partial waves, momentum-dependent terms are needed, e.g.,

$$O_{ij}^{p=9,14} = [L^2, \ L^2 \sigma_i \cdot \sigma_j, \ (\mathbf{L} \cdot \mathbf{S})^2] \otimes [1, \ \tau_i \cdot \mathbf{S})^2$$

• Add electromagnetic and small isospin-breaking terms:

$$O_{ij}^{p=15,22} = [1, \ \sigma_i \cdot \sigma_j, \ S_{ij}, \ \mathbf{L} \cdot \mathbf{S}] \otimes [T_{ij}, \ \tau_{\mathbf{z}i} + \tau_{\mathbf{z}j}] \qquad T_{ij} = 3 \ \tau_{iz} \tau_{jz} - \tau_i \cdot \tau_j$$

• It is a r-space potential expressed as a sum of EM and OPE terms and phenomenological intermediate- and short-

$$v_{ij}^{\gamma}: pp, pn \& nn \text{ electromagnetic terms}$$
$$v_{ij}^{\pi} \sim [Y_{\pi}(r_{ij})\sigma_i \cdot \sigma_j + T_{\pi}(r_{ij})S_{ij}] \otimes \tau_i \cdot \tau_j$$
$$v_{ij}^I = \sum_p I^p T_{\pi}^2(r_{ij})O_{ij}^p$$
$$v_{ij}^S = \sum_p [P^p + Q^p r + R^p r^2] W(r)O_{ij}^p$$

• Minimum of eight different potential terms needed to fit S- and P- wave data: four for different S, T combinations,

$$S_{ij} = 3 \,\boldsymbol{\sigma}_i \cdot \mathbf{r} \,\boldsymbol{\sigma}_j \cdot \mathbf{r} - r^2 \,\boldsymbol{\sigma}_i \cdot \boldsymbol{\sigma}_j$$

 $\tau_i$ 

![](_page_25_Picture_14.jpeg)

Wiringa, Stoks, Schiavilla, PRC 51, 38 (1995)

![](_page_25_Picture_16.jpeg)

## **Argonne nucleon-nucleon V18**

![](_page_26_Figure_1.jpeg)

- The AV18 model uses 42  $I^p, P^p, Q^p, R^p$  parameters, one cutoff parameter in  $Y_{\pi}(r), T_{\pi}(r)$ . • These parameters have been fix by fitting the Nijmegen database of ~4300 np and pp scattering data for  $E_{lab} \leq 350$  MeV with a total  $\chi^2 \approx 1$  plus nn scattering length and deuteron binding
- energy.

![](_page_26_Figure_4.jpeg)

## Phenomenological three-nucleon potentials: Urbana-Illinois

• 3N Urbana-Illinois (UIX-IL7): an Hamiltonian which only includes AV18 does not provide enough binding in the light nuclei. In light nuclei we find [thanks to large cancellations between  $\langle T \rangle$  and  $\langle v_{ij} \rangle$ ]:  $\langle V_{ijk} \rangle \sim (0.02 - 0.07) \langle v_{ij} \rangle \sim (0.2 - 0.5) \langle H \rangle$ 

Urbana: J. Carlson et al. NP A401, 59 (1983) contains the attractive Fujita and Miyazawa two-pion exchange interaction and a phenomenological repulsive term

![](_page_27_Figure_3.jpeg)

2 independent parameters controlled by <sup>3</sup>H binding energy & saturation density of symmetric nuclear matter. Good description for s-shell nuclei (A=3,4) and neutron stars; *inadequate description of the* absolute p-shell and spin-orbit splitting of heavier nuclei

![](_page_27_Figure_6.jpeg)

![](_page_27_Figure_7.jpeg)

Illinois: S. Pieper et al. PRC 64, 014001 (2001) also includes terms originating from three-pion rings containing one or two  $\Delta s$  and the two-pion S-wave contribution. This interaction is attractive in *nnn* triplets with T = 3/2 and provides extra attraction observed in neutron rich nuclei.

![](_page_28_Figure_1.jpeg)

5 independent parameters controlled by ground-state energies of A  $\leq$  10. Good description for light nuclei up to A=12; inadequate description of the neutron star matter equation of state.

![](_page_28_Picture_3.jpeg)

## Phenomenological potentials & QMC

GFMC calculations of the spectra of light-nuclei using **AV18** without and with **UIX** or **IL7** 

![](_page_29_Figure_2.jpeg)

electroweak currents

The EoS of pure neutron matter (PNM): useful tool

![](_page_29_Figure_5.jpeg)

- They do not provide rigorous schemes to consistently derive NN and 3N forces and compatible

# Chiral effective field theory: the framework in a nutshell S. Weinberg, Phys. Lett. B251, 288 (1990); Nucl. Phys. B363, 3 (1991); Phys. Lett B295, 114 (1992)

![](_page_30_Picture_1.jpeg)

Symmetries in particular the approximate chiral symmetry between hadronic d.o.f ( $\pi$ , N,  $\Delta$ )

Effective chiral Lagrangian  $\mathcal{L}_{eff}(\pi, N, \Delta)$ 

Calculate amplitudes+prescription to obtain potentials + regularization (of high momentum components)

> Few- and many-body methods: QMC, NCSM, CC, etc

Approximate chiral symmetry requires the pion to couple to other pions and to baryons by powers of its momentum

![](_page_30_Figure_7.jpeg)

- The  $\mathscr{L}_{\mathrm{eff}}$  can be constructed in a straightforward way using covariantly transforming building blocks defined in terms of the pion fields.
- A non-relativistic treatment of the nucleon fields is used: heavy-baryon formalism to eliminate the nucleon mass *m* from the leading-order Lagrangian.
- ullet The individual terms in the  $\mathscr{L}_{
  m eff}$  are multiplied by the corresponding coupling constants (lowenergy constants, LECs): not fixed by the symmetry and typically need to be determined from experimental data.
- For instance the nuclear potentials at fifth order in the chiral expansion, i.e., at N4LO, require input from the following effective Lagrangians:

$$\begin{aligned} \mathscr{L}_{\text{eff}} &= \mathscr{L}_{\pi}^{(2)}(m_{\pi}, F_{\pi}) + \mathscr{L}_{\pi}^{(4)}(l_{1,...,7}) \\ &+ \mathscr{L}_{\pi N}^{(1)}(g_{A}) + \mathscr{L}_{\pi N}^{(2)}(m, c_{1,...,7}) + \mathscr{L}_{\pi N}^{(3)}(d_{1,...,23}) + L_{\pi N}^{(4)}(e_{1,...,118}) \\ &+ \mathscr{L}_{NN}^{(0)}(C_{S}, C_{T}) + \mathscr{L}_{NN}^{(2)}(C_{1,...,7}) + \mathscr{L}_{NN}^{(4)}(D_{1,...,12}) + \mathscr{L}_{\pi NN}^{(1)}(D) + \dots \\ &+ \mathscr{L}_{NNN}^{(0)}(E) + \mathscr{L}_{NNN}^{(2)}(E_{1,...,10}) \end{aligned}$$

Epelbaum, Krebs, Patrick, Frontiers in Physics, 8 (2020)

## **Chiral perturbation theory for nuclear potentials**

Different ways to derive nuclear potentials using chiral perturbation theory— for example:

- Epelbaum, Krebs, Patrick, Frontiers in Physics, 8 (2020) and references therein].
- (2016)].

• The method, referred to as the unitary transformation (UT) method, is based on TOPT and exploits the Okubo (unitary) transformation, one containing only pure nucleonic states and the other involving states that retain at least one pion (Bochum-Bonn group) [see Epelbaum at al. Nucl. Phys. A 671, 295 (2000); Nucl. Phys. A 714,535 (2003); Nucl. Phys. A 747, 362 (2005);

• The JLab-Pisa group utilizes a different approach by starting with the on-shell transfer matrix T and "inverting" it to obtain the effective potential. This is carried out in perturbation theory by counting the nucleon mass via  $m \sim \Lambda_h$  [see Pastore *et al.* Phys. Rev. C 80, 034004 (2009), Phys. Rev. C 84, 024001 (2011); Piarulli et al. Phys. Rev. C 87, 014006 (2013), Baroni at al. Phys. Rev. C 93, 015501

![](_page_32_Figure_6.jpeg)

## **JLab-Pisa formalism: transition Amplitude in TOPT**

#### 1. Nucleon-nucleon potential: $(NN \rightarrow NN)$

- Degrees of freedom: non-relativistic N's and  $\Delta$ 's, relativistic  $\pi$ 's
- Time-ordered perturbation theory (TOPT)

$$\langle N'N'|T|NN\rangle = \langle N'$$

 $H_1$  = interaction Hamiltonians among  $\pi$ , N, and  $\Delta$  implied by  $\mathscr{L}_{eff}$ 

• The evaluation of this amplitude is carried out in practice by inserting complete sets of  $H_0$  eigenstates,  $\sum |I_i\rangle\langle I_i|$ , between successive terms of  $H_1$ 

$$\langle f|T|i\rangle = \langle f|H_1|i\rangle + \sum_{I_1} \langle f|H_1|I_1\rangle \frac{1}{E_i - E_1 + i\eta} \langle I_1|H_1|i\rangle + \sum_{I_1,I_2} \langle f|H_1|I_2\rangle \frac{1}{E_i - E_2 + i\eta} \langle I_2|H_1|I_1\rangle \frac{1}{E_i - E_1 + i\eta} \langle I_1|H_1|i\rangle + \dots$$

$$\begin{split} \langle f|H_{1}|i\rangle &+ \sum_{I_{1}} \langle f|H_{1}|I_{1}\rangle \frac{1}{E_{i} - E_{1} + i\eta} \langle I_{1}|H_{1}|i\rangle \\ &+ \sum_{I_{1},I_{2}} \langle f|H_{1}|I_{2}\rangle \frac{1}{E_{i} - E_{2} + i\eta} \langle I_{2}|H_{1}|I_{1}\rangle \frac{1}{E_{i} - E_{1} + i\eta} \langle I_{1}|H_{1}|i\rangle + \dots \end{split}$$

1

 $\frac{N'|H_1}{N} \sum_{n=1}^{\infty} \left( \frac{1}{E_i - H_0 + i\eta} H_1 \right)^{n-1} |NN\rangle$  $H_0$  = free  $\pi$ , N, and  $\Delta$  Hamiltonians

### **JLab-Pisa formalism: transition Amplitude in TOPT**

- Two kinds of diagrams: reducible and irreducible
- N vertices represented by  $\langle I_i | H_1 | I_k \rangle$
- N-1 energy denominators  $(E_i E_k + i\eta)^{-1}, k = 1, ..., (N-1)$ 
  - N<sub>K</sub> denominators involving only nucleonic energies scales as  $Q^{-2}$
  - $\sim N-N_{\rm K}-1$  denominators involving nucleons,  $\pi$ 's, and  $\Delta$ 's energies
- A contribution with N interaction vertices and L loops scales as

$$m = \prod_{i=1}^{N} Q^{\alpha_i - \beta_i/2} \times Q^{\alpha_i - \beta_i/2}$$

$$H_1 \text{ scaling}$$

![](_page_34_Figure_8.jpeg)

Irreducible

Reducible

![](_page_34_Figure_11.jpeg)

![](_page_34_Picture_12.jpeg)

### **JLab-Pisa formalism: transition Amplitude in TOPT**

• A N-N<sub> $\kappa$ </sub>-1 denominators can be further expanded:

$$\frac{1}{E_i - E_j + i\eta} \equiv \frac{1}{E_i - E_{I_j} - \Omega + i\eta}$$

•  $E_{I_i}$ : kinetic energies of intermediate states (2N or 1N+1 $\Delta$  or 2 $\Delta$ ) •  $\Omega \equiv \omega_{\pi}$  (if one or more pion are involved) •  $\Omega \equiv \omega_{\pi} + \Delta$  (if one or more pion are involved and a  $\Delta$  ), etc...  $\Delta = m_{\Delta} - m_N \sim 300 \,\mathrm{MeV} \sim 2m_{\pi}$ 

• The expansion in power of Q is:  $-\frac{1}{Q}\left[1+Q+Q^2+\ldots\right]$ 

static limit  $m_N, m_\Lambda \to \infty$ 

• In chiral-expansion T-matrix can be expanded as:

 $T = T^{(0)} + T^{(1)} + T^{(2)} + \dots$ with

$$-\frac{1}{\Omega} \left[ 1 + \frac{E_i - E_{I_j}}{\Omega} + \frac{(E_i - E_{I_j})^2}{\Omega^2} + \dots \right]$$

![](_page_35_Figure_13.jpeg)

non-static corrections

 $T^{(m)} \sim Q^{(m)}$ 

![](_page_35_Picture_16.jpeg)

## Few remarks about this prescription!

- 1. Reducible diagrams are enhanced compared to the irreducible ones by a factor Q for each purely nucleonic intermediate states.
- 2. In the static limit, these contributions are infrared-divergent (since reducible diagrams involve nucleonic kinetic energy denominators which lead to infinities for  $m_N \to \infty$ ).
- the irreducible contributions only.
- 4. Reducible contributions, instead, are generated by solving the Lippmann-Schwinger (or Schrodinger) equation iteratively with the nuclear potential (and currents) arising from the irreducible amplitudes.
- the nuclear operators.

3. According to the prescription proposed by Weinberg the nuclear potentials (and current operators) are given by

5. The reducible part of the amplitude which is not generated by iteration (i.e. the one that is obtained going beyond the static limit) needs to be incorporated order by order—along with the irreducible amplitude— in the definition of

![](_page_36_Figure_11.jpeg)

### From amplitudes to potentials

• Construct potential v such that when inserted in Lippmann-Schwinger (LS) equation

$$v + vG_0v + vG_0vG_0v + \dots$$

leads to T-matrix order by order in the power counting

• Assume: 
$$v = v^{(0)} + v^{(1)} + v^{(2)} + \dots$$
 (with  $v^{(m)} \sim$ 

• Matching expansion for *T* with the LS equation order by order:

$$\begin{aligned} v^{(0)} &= T^{(0)} \\ v^{(1)} &= T^{(1)} - \left[ v^{(0)} G_0 v^{(0)} \right] \\ v^{(2)} &= T^{(2)} - \left[ v^{(0)} G_0 v^{(0)} G_0 v^{(0)} \right] - \left[ v^{(1)} G_0 v^{(0)} + v^{(0)} G_0 v^{(1)} \right] \\ v^{(3)} &= T^{(3)} - \left[ v^{(0)} G_0 v^{(0)} G_0 v^{(0)} G_0 v^{(0)} \right] - \left[ v^{(1)} G_0 v^{(0)} G_0 v^{(0)} + \text{permutations} \right] \\ &- \left[ v^{(1)} G_0 v^{(1)} \right] - \left[ v^{(2)} G_0 v^{(1)} + v^{(0)} G_0 v^{(2)} \right] \end{aligned}$$

• A term like  $v^{(m)}G_0v^{(n)} \sim Q^{m+n+1}$ 

 $G_0 =$  two-nucleon propagator ( $Q^{-2}$ )  $G_0 = 1/(E_i + E_I + i\eta)$ 

 $\sim Q^m$  )

 $v^{(m)}$  up to order m=1

• Time-ordered diagrams contributing to the  $\chi$ EFT T-matrix up to order  $Q^1$ 

![](_page_38_Figure_2.jpeg)

•  $v^{(0)} = T^{(0)}$  consists of (static) OPE and contact terms (LO)

•  $v^{(1)} = T^{(1)} - \left[ v^{(0)} G_0 v^{(0)} \right]$  vanishes

2. EM Charge/Current operators  $(NN\gamma \rightarrow NN)$ 

- Similar prescription for potential  $v_{\gamma} = A^{\mu}J_{\mu} = A^{0}\rho$  -
- Power counting of the EM interaction (treated in firs
- In the context of LS:  $v_{\gamma} = v_{\gamma}^{(-3)} + v_{\gamma}^{(-2)} + v_{\gamma}^{(-1)} + \dots$

• Matching expansion for T with the LS equation order by order:

![](_page_39_Figure_5.jpeg)

• Charge and current operators up to one loop (eQ) consistent with v at  $Q^2$ 

. . . . . .

$$-\mathbf{A} \cdot \mathbf{J}$$

st order) 
$$T_{\gamma} = T_{\gamma}^{(-3)} + T_{\gamma}^{(-2)} + T_{\gamma}^{(-1)} \dots$$

$$\begin{array}{l} & 3^{3} G_{0} \upsilon^{(0)} + \upsilon^{(0)} G_{0} \upsilon^{(-3)} \\ & 3^{3} G_{0} \upsilon^{(0)} G_{0} \upsilon^{(0)} + \text{permutations} \\ \end{array}$$

$$\begin{array}{l} & 2^{3} G_{0} \upsilon^{(0)} + \upsilon^{(0)} G_{0} \upsilon^{(-2)} \\ & & & & \\ \end{array} \end{array}$$

LS terms

## **Some technical issues:**

absorbed in the redefinition of the relevant LECs

to arbitrarily high values but should be kept of the order of the breakdown scale  $\Lambda \sim \Lambda_b$ .

• Ultraviolet divergencies (UV) associated with nuclear and electromagnetic loop diagrams: one way is to remove them via dimensional regularization (DR) and the divergent part of these loops are

• Resulting renormalized operators have power-law behavior for large momenta: one way is to further regularization needs to be employed before these operators can be for solving Schrödinger equation and for calculation of current matrix elements, cutoff functions  $C_{\Lambda}$  where the cutoff  $\Lambda$  must not be set

![](_page_40_Picture_5.jpeg)

## State-of-the art of Chiral EFT interactions

![](_page_41_Figure_1.jpeg)

#### Advantages:

- Consistent description of two- and manybody interactions and currents
- Different processes described on the same footing: piN, NN, electroweak
- UQ due to the truncation in the chiral expansion
- Scheme can be systematically improved

#### **Disadvantages:**

- Increase in number of diagrams at higher orders; When do we stop in the chiral expansion? Convergence, power counting, etc....
- Consistency between strong- and electrowea sector very hard to achieve
- More LECs appearing at higher orders; challenging optimization problem

![](_page_41_Figure_11.jpeg)

## How to fix the LECs?

**First Challenge:** What experimental data should we use to find the LECs?

LECs appear in different low energy processes

![](_page_42_Figure_3.jpeg)

piN scattering NN interaction 3N interaction

![](_page_42_Picture_5.jpeg)

Scattering observables: piN, NN, NNN..

#### <u>Second Challenge:</u> What is the best fitting procedure?

#### "Traditional" approach: separate fits

![](_page_42_Picture_9.jpeg)

![](_page_42_Picture_10.jpeg)

![](_page_42_Picture_11.jpeg)

#### Light nuclei, A=2,3,4

![](_page_42_Picture_13.jpeg)

- A. Gezerlis et al., Phys.Rev. C 90, 054323 2014
- M. Piarulli et al., Phys. Rev. C, 024003 2015
- E. Epelbaum et al., Eur. Phys. J. A 51, 53 2015
- P. Reinert et al., Eur.Phys.J. A54 no.5, 86 2018
- Ekström et al. Phys. Rev. Lett. 110, 192502 2013 (NNLOopt)
- Ekström et al. Phys. Rev. C **97**, 024332 2018
- B. Carlsson et al., Phys. Rev. X, 011019 2015 (NNLOsep)

![](_page_42_Figure_24.jpeg)

![](_page_42_Picture_25.jpeg)

Static and dynamic properties of bound states

#### A "more modern" approach: simultaneous fits

![](_page_42_Figure_28.jpeg)

#### Computationally a very challenging problem!

## **Optimization procedure for the LECs**

Third Challenge: Minimize a objective function to find a\* (LECs) in the parameter space

Least-square objective function for a set of observables

$$\mathbf{a}^* = \min_{\mathbf{a}} \chi^2(\mathbf{a})$$
 with  $\chi^2(\mathbf{a}) = \sum_{i=1}^{N} \chi^2(\mathbf{a})$ 

#### "Conventional" least-square minimization:

- Take  $\delta o_i$  to be the experimental error (or same modification to take into account theoretical errors)
- Many optimization techniques suitable for this problem such as POUNDers, Newtons Methods,....
- UQ addressed as: Covariance methods, Bootstrapping, standard protocols for chiral truncation errors, cutoff dependence
- over/under-fitting, parameter ,...

![](_page_43_Figure_9.jpeg)

- $O_i$  : measured values
- $t_i$  : calculated values
- $\delta o_i$ : uncertainty observables

![](_page_43_Figure_13.jpeg)

- Assumptions are made explicit (e.g. naturalness of LECs, truncation errors)
- Parameter estimation: conventional
   optimization recovered as special case
- Clear prescriptions for combining errors

<u>BUQEYE</u> collaboration <u>BAND</u> collaboration

## **Chiral NN potentials: some recent developments**

- JPG **42**, 034003 2015)
- N2LO potential: a simultaneous fit of NN and 3N forces to low NN data (Elab=35 MeV), deuteron BE, BE and CR of hydrogen, helium, carbon and oxygen isotopes; Carlsson et al. (PRC 91, 051301(R) 2015)
- New generation of chiral NN potentials up to N4LO: improved choice of the regulator, no SFR; Epelbaum et al. (PRL. **112**, 102501, 2014; EPJ A **51**, 53 2015; PRL. **115**, 122301, 2015)
- Chiral  $2\pi$  and  $3\pi$  exchange up to N4LO and up to N5LO in NN peripheral scattering; Entem et al. (PRC 91, 014002) 2015; PRC **92**, 064001 2015, PRC 96, 024004 (2017)
- 497-501 (2020)

•

- Many of the available versions of chiral potentials are formulated in p-space and are strongly nonlocal: NOTE: Nonlocalities due to contact interactions  $\rightarrow p \rightarrow -i \nabla$ Nonlocalities due to regulator functions
  - Nonlocal interactions hard to handle in for example Quantum Monte Carlo (QMC) methods
  - 192501, 2014)
  - Minimally nonlocal NN potentials up to N3LO (including N2LO  $\Delta$  contributions); Piarulli et al. (PRC 91, 024003 2015) Local chiral potential with Δ-intermediate states up to N3LO; Piarulli et al. (PRC 94, 054007 2016)

• Optimized N2LO NN potential ( $\pi$ N LECs are tuned to NN peripheral scattering): Ekström et al. (PRL **110**, 192502 2013;

• High-Precision Nucleon-Nucleon Potentials from Chiral EFT; Reinert, Krebs, Epelbaum (Springer Proc. Phys. 238

• Local NN potentials up to N2LO: Gezerlis et al. (PRL 111, 032501 2013, PRC 90, 054323 2014); Lynn et al. (PRL 113

![](_page_44_Picture_14.jpeg)

![](_page_44_Picture_15.jpeg)

![](_page_44_Picture_16.jpeg)

![](_page_44_Picture_17.jpeg)

## **Example: Local chiral NN Hamiltonian with \Delta's**

16 spin-isospin operators (NV2s – Norfolk interactions)

![](_page_45_Figure_2.jpeg)

- Contact component parametrized by 26 LECs:
  - the functional form taken as  $C_{R_s}(r) \propto e^{-(r/R_s)}$  with  $R_s = 0.8 (0.7)$  fm a (b) models
  - models a (b) cutoff~500 MeV (600 MeV) in p-space

model	order	$E_{\rm Lab} ({\rm MeV})$	$N_{pp+np}$	$\chi^2/\text{datum}$
NV2-Ia	N3LO	$0\!-\!125$	2668	1.05
NV2-Ib	N3LO	$0\!-\!125$	2665	1.07
NV2-IIa	N3LO	0-200	3698	1.37
NV2-IIb	N3LO	0-200	3695	1.37

Local NN potentials including N2LO Δ-contributions and N3LO contacts have ben also devised and expressed as a sum of

![](_page_45_Figure_10.jpeg)

![](_page_45_Figure_11.jpeg)

MP et al. PRC **91**, 024003 (2015); PRC **94**, 054007 (2016)

## Fitting procedure for the $\Delta$ -full local chiral interactions

• We first fit the partial wave phase shifts then we refine the fit with a direct comparison with the database: good starting point for Practical Optimization Using No Derivatives (for Squares), POUNDers.

Given N data sets associated with a specific experiment

An experiment may have a specific systematic error (normalized data), no systematic error (absolute data), or a arbitrary systematic error (floated data)

In all cases  $\chi_t^2$  is given by

$$\chi_t^2 = \sum_{i=1}^n \frac{\left(o_i/Z_t - t_i\right)^2}{\left(\delta o_i/Z_t\right)^2} + \frac{(1 - 1/Z_t)^2}{\left(\delta_{\text{sys}}/Z_t\right)^2}$$

 $o_i$  and  $t_i$  are the measured and calculated values of the observable at point i  $\delta o_i$  and  $\delta_{sys}$  are the statistical and systematic errors  $Z_t$  is a scaling factor chosen to minimize the  $\chi_t^2$ 

$$Z_t = \left(\sum_{i=1}^{n} \frac{o_i t_i}{\delta o_i^2} + \frac{1}{\delta_{\text{sys}}^2}\right) \left/ \left(\sum_{i=1}^{n} \frac{t_i^2}{\delta o_i^2} + \frac{1}{\delta_{\text{sys}}^2}\right)$$

nt: 
$$\chi^2 = \sum_{t=1}^N \chi_t^2$$

![](_page_46_Picture_11.jpeg)

#### **Example: Local chiral NNN Hamiltonian with** \Delta's

• Inclusion of 3N forces at N2LO:  $V_{ijk} = V_{ijk}^{2\pi} + V_{ijk}^{CT}$ 

#### 1) Fit to: $E_0({}^{3}\text{H}) = -8.482 \text{ MeV}$ ${}^{2}a_{nd} = (0.645 \pm 0.010) \text{ fm}$

	Model	$c_D$	$c_E$
	Ia	3.666	-1.638
VV2+3s	Ib	-2.061	-0.982
	IIa	1.278	-1.029
	IIb	-4.480	-0.412

![](_page_47_Figure_4.jpeg)

![](_page_47_Figure_5.jpeg)

#### 2) Fit to: $E_0(^{3}\text{H}) = -8.482 \text{ MeV}$

GT m.e. in <sup>3</sup> H $\beta$ -decay			
Model	$c_D$	$c_E$	
Ia*	-0.635(255)	-0.09(8)	
Ib*	-4.705(285)	0.550(150)	
IIa*	-0.610(280)	-0.350(100)	
$\mathrm{IIb}^*$	-5.250(310)	0.05(180)	

NV2+3s\*

![](_page_47_Figure_9.jpeg)

![](_page_48_Figure_0.jpeg)

## **Example: EM Observables at N3LO fixing LECs**

 $C'_{15}, C'_{16}$   $d'_8, d'_9, d'_{21}$  • Five LECs: it is convenient to introduce the dimensionless set  $d_i^{S,V}$ :

 $C_{15}' = d_1^S / \Lambda^4 ,$  $C_{16}' = d_1^V / \Lambda^4 ,$ 

Fixed in A=2-3 nucleons' sector

 $d_1^S$  and  $d_2^V$  from expt  $\mu_d$  and

 $d_1^V$  from expt  $\mu_V({}^{3}\text{He}/{}^{3}\text{H})$  m.m. and  $d_2^V/d_3^V = 1/4$  from  $\Delta$  resonance-saturation

Λ	$d_1^S$	$d_2^S \times 10$	$d_1^V$	$d_2^V$	
500	4.072	2.190	-7.981	3.458	
600	11.38	3.231	-11.69	4.980	

$$d_2^V = \frac{4\,\mu_{\gamma N\Delta}\,h_A\,\Lambda^2}{9\,m_N\,(m_\Delta - m_N)}$$

 $(k) \qquad (j)$ 

Pastore et al. PRC 78, 064002 (2008), PRC 80, 034004 (2009)

$$d'_{9} = d_{2}^{S} / \Lambda^{2},$$
  
$$d'_{8} = d_{2}^{V} / \Lambda^{2}, \qquad d'_{21} = d_{3}^{V} / \Lambda^{2}$$

d 
$$\mu_{S}({}^{3}\text{He}/{}^{3}\text{H})$$
 m.m.