

Maria Piarulli-Washington University, St. Louis May 10, 2019

## Ab initio calculations of nuclear systems

Atomic nuclei are complex quantum many-body systems of strongly correlated nucleons

Their structure and scattering by electrons and neutrinos are at the forefront of the nuclear physics and high-energy physics

## ab-initio $=$ in medias res

- Baryons and mesons degrees of freedom
- Understand nuclei at the level of interactions between individual nucleons (nuclear structure) as well as their interactions with external probes (nuclear dynamics)


## Ex. ab-initio method: Quantum Monte Carlo (QMC)

- work with bare interactions
- good for strongly correlated systems
- statistical errors quantifiable and improvable
- limitations in the systems we can study
- limitation in the type of interactions to be used



## The basic model of nuclear theory

The basic model of nuclear theory: description of the static and dynamic properties of nuclear systems.

Nucleon-nucleon (NN) scattering data: "thousands" of experimental data available The spectra, properties, and transition of nuclei: BE, radii, magnetic moments, beta decays rates, weak/radiative captures, electroweak form factors, etc.
The nucleonic matter equation of state: for ex. EOS neutron matter

Inputs for the basic model:
Many-body interactions between the constituents

Electroweak current operators:

$$
\begin{aligned}
& H=\sum_{i=1}^{A} \frac{\mathbf{p}_{i}^{2}}{2 m_{i}}+\sum_{i<j=1}^{A} \overbrace{v_{i j}}^{\text {th+exp }}+\sum_{i<j<k=1}^{A} \overbrace{V_{i j k}}^{\text {th+exp }}+\ldots . \\
& \text { One-body Two-body (NN) Three-body (3N) } \\
& \left.\right|_{N} ^{N}+\left.\left.\left.\right|_{N} ^{N}\right|_{N} ^{N}\right|_{N} ^{N}+\ldots \\
& j^{\mathrm{EW}}=\sum_{\substack{i=1 \\
\text { One-body }}}^{A} j_{i}+\sum_{\substack{i<j=1 \\
\text { Two-body }}}^{A} j_{i j}+\sum_{\substack{i<j<k=1 \\
\text { Many-body }}}^{A} j_{i j k}+\ldots
\end{aligned}
$$

## Chiral EFT: from QCD to nuclear systems

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

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

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

$$
\mathcal{L}_{e f f}=\mathcal{L}^{(0)}+\mathcal{L}^{(1)}+\mathcal{L}^{(2)}+\ldots
$$

Given a power counting scheme
Calculate amplitudes+prescription to obtain potentials + regularization

$$
\mathcal{L}^{(n)} \sim\left(\frac{Q}{\Lambda_{\chi}}\right)^{n} \sim 100 \mathrm{MeV} \text { soft scale }
$$ (of high momentum components)

$\mathcal{L}^{(n)} \sim\left(\frac{Q}{\Lambda_{\chi}}\right)^{n} \sim 100 \mathrm{MeV}$ soft scale
Nuclear forces and currents

Few- and many-body methods: QMC, NCSM,


CC, etc

## Nuclear interactions in chiral EFT

## $\Delta$-less

## Chiral 2N




Kaiser et al.'97

## NNLO

$\left(Q / \Lambda_{\chi}\right)^{3}$
$\mathrm{N}^{5} \mathrm{LO}$
$\left(Q / \Lambda_{\chi}\right)^{6}$
$\mathrm{N}^{3} \mathrm{LO}$
$\left(Q / \Lambda_{\chi}\right)^{4}$
$\mathrm{N}^{4} \mathrm{LO}$
$\left(Q / \Lambda_{\chi}\right)^{5}$


$$
\left(Q / \Lambda_{\chi}\right)^{5}
$$

$$
(\infty)=x)
$$

Entem \& Machleidt ‘02




Ordonezet al.'96;Kaiser et al.'98; Krebs et al. ‘07
$\Delta$-less

## Chiral 3N

Additional in $\Delta$-full

U. van Kolck '94; Epelbaum et al.'02; Epelbaum et al. '08


Krebs at al. '12-'13; Girlanda et.al '11

## Chiral potentials and QMC

Many of the available versions of chiral potentials are formulated in momentumspace and are strongly nonlocal: $\Rightarrow \mathbf{p} \rightarrow-i \boldsymbol{\nabla}$ hard to use in QMC methods (limitation of the method)

Nonlocalities due to contact interactions and to regulator functions


Nonlocal regulator

Local regulator

$$
V_{\mathrm{NN}}\left(\mathbf{p}, \mathbf{p}^{\prime}\right) \rightarrow \exp \left[-\left[\left(\mathbf{p}^{2}+\mathbf{p}^{\prime 2}\right) / \Lambda^{2}\right]^{n}\right] V_{\mathrm{NN}}\left(\mathbf{p}, \mathbf{p}^{\prime}\right)
$$

$$
V_{\mathrm{NN}}\left(\mathbf{p}, \mathbf{p}^{\prime}\right) \rightarrow \exp \left[-\left[\left(\mathbf{p}^{\prime}-\mathbf{p}\right)^{2} / \Lambda^{2}\right]^{n}\right] V_{\mathrm{NN}}\left(\mathbf{p}, \mathbf{p}^{\prime}\right)
$$

- Local NN potential up to N2LO:

Gezerlis et al. PRL 111, 032501 2013; PRC 90, 054323 2014; Lynn et al. PRL 113, 192501 2014

- Minimally nonlocal/local NN potentials including N2LO $\Delta$-contributions and N3LO contacts: Piarulli et al. PRC 91, 024003 2015; PRC 94, 0540072016

We use QMC (VMC, GFMC, AFDMC) and HH methods to solve the many-body Schrödinger equation

$$
H \Psi\left(\mathbf{R} ; s_{1}, . ., s_{A} ; t_{1}, . ., t_{A}\right)=E \Psi\left(\mathbf{R} ; s_{1}, . ., s_{A} ; t_{1}, . ., t_{A}\right)
$$

## Local chiral NN potential with $\Delta$ 's

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

$v_{12}^{\mathrm{EM}}$ : EM component including corrections up to $\alpha^{2}$

$$
\mathrm{LO}:\left.Q_{\mathrm{p}}^{0}\right|^{\mathbf{p}^{\prime}}\left|-\frac{\mathbf{-}}{}-\right|_{-\mathbf{p}}^{-\mathbf{p}^{\prime}}
$$

$v_{12}^{\mathrm{L}}$ : chiral OPE and TPE component with $\Delta$ 's

- dependence only on the momentum transfer $\mathbf{k}=\mathbf{p}^{\prime} \mathbf{- p}$

$v_{12}^{\mathrm{S}}$ : short-range contact component up to order N3LO $\left(\mathrm{Q}^{4}\right)$ parametrized by $(2+7+11) \mathrm{Cl}$ and (2+4) IB LECs
- the functional form taken as $C_{R_{S}}(r) \propto e^{-\left(r / R_{S}\right)^{2}}$ with $R_{S}=0.8(0.7) \mathrm{fm}$ a (b) models

In coordinate-space it reads as:

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

$$
\begin{aligned}
& O_{12}^{l=1, \ldots, 6}=\left[\mathbf{1}, \boldsymbol{\sigma}_{1} \cdot \boldsymbol{\sigma}_{2}, S_{12}\right] \otimes\left[\mathbf{1}, \boldsymbol{\tau}_{1} \cdot \boldsymbol{\tau}_{2}\right] \\
& O_{12}^{l=7, \ldots, 11}=\mathbf{L} \cdot \mathbf{S}, \mathbf{L} \cdot \mathbf{S} \boldsymbol{\tau}_{1} \cdot \boldsymbol{\tau}_{2},(\mathbf{L} \cdot \mathbf{S})^{2}, \mathbf{L}^{2}, \mathbf{L}^{2} \boldsymbol{\sigma}_{1} \cdot \boldsymbol{\sigma}_{2} \\
& O_{12}^{l=12, \ldots, 16}=T_{12},\left(\tau_{1}^{z}+\tau_{2}^{z}\right), \boldsymbol{\sigma}_{1} \cdot \boldsymbol{\sigma}_{2} T_{12}, S_{12} T_{12}, \mathbf{L} \cdot \mathbf{S} T_{12}
\end{aligned}
$$

## Fitting procedure: NN PWA and database

The 26 LECs are fixed by fitting the pp and np Granada database up to two ranges of $E_{\text {lab }}=125 \mathrm{MeV}$ and 200 MeV , the deuteron BE and the nn scattering length

To minimizing the $\chi^{2}$ we have used the Practical Optimization Using No Derivatives (for Squares), POUNDers (M. Kortelainen, PRC 82, 024313 2010)

| model | order | $E_{\text {Lab }}(\mathrm{MeV})$ | $N_{p p+n p}$ | $\chi^{2} /$ datum |
| :---: | :---: | :---: | :---: | :---: |
|  |  |  |  |  |
| Ia | N3LO | $0-125$ | 2668 | 1.05 |
| Ib | N3LO | $0-125$ | 2665 | 1.07 |
| IIa | N3LO | $0-200$ | 3698 | 1.37 |
| IIb |  |  |  |  |
| IIb | N3LO | $0-200$ | 3695 | 1.37 |








## Local chiral 3N potential with $\Delta$ 's

## Inclusion of 3 N forces at N2LO:



1) Fit to:

- $E_{0}\left({ }^{3} \mathrm{H}\right)=-8.482 \mathrm{MeV}$
${ }^{2} a_{n d}=(0.645 \pm 0.010) \mathrm{fm}$

| Model | $c_{D}$ | $c_{E}$ |
| :---: | ---: | ---: |
| Ia | 3.666 | -1.638 |
| Ib | -2.061 | -0.982 |
| IIa | 1.278 | -1.029 |
| IIb | -4.480 | -0.412 |



(CD
\&
(CE) $\sim \tau_{i} \cdot \tau_{j}$
2) Fit to:

- $E_{0}\left({ }^{3} \mathrm{H}\right)=-8.482 \mathrm{MeV}$
- GT m.e. in ${ }^{3} \mathrm{H} \beta$-decay

| Model | $c_{D}$ | $c_{E}$ |
| :---: | ---: | ---: |
| $\mathrm{Ia}^{*}$ | $-0.635(255)$ | $-0.09(8)$ |
| $\mathrm{Ib}^{*}$ | $-4.705(285)$ | $0.550(150)$ |
| $\mathrm{IIa}^{*}$ | $-0.610(280)$ | $-0.350(100)$ |
| $\mathrm{IIb}^{*}$ | $-5.250(310)$ | $0.05(180)$ |



## The Nuclear Many-Body Problem

We need to solve the many-body Schrödinger equation of the system under consideration

$$
H \Psi\left(\mathbf{R} ; s_{1}, . ., s_{A} ; t_{1}, . ., t_{A}\right)=E \Psi\left(\mathbf{R} ; s_{1}, . ., s_{A} ; t_{1}, . ., t_{A}\right)
$$

input:
$H=\sum_{i} \frac{\mathbf{p}_{i}^{2}}{2 m}+\sum_{i<j} v_{i j}+\sum_{i<j \leq k} V_{i j k}+\ldots$.
3A coordinates in
r-space

Bottom line:
$2^{A} \times \frac{A!}{N!Z!}$ Coupled second order differential equations in 3A dimension

$$
\begin{gathered}
96 \text { for }{ }^{4} \mathrm{He} \\
17,920 \text { for }{ }^{8} \mathrm{Be} \\
3,784,704 \text { for }{ }^{12} \mathrm{C}
\end{gathered}
$$

Very challenging problem!!!

## Ab initio Methods: HH and QMC

Hyperspherical Harmonics $(\mathrm{HH})$ expansion for $\mathrm{A}=3$ and 4 bound and continuum states

$$
|\Psi\rangle=\sum_{\mu} c_{\mu} \underbrace{\left|\Phi_{\mu}\right\rangle}_{\text {HH basis }} \quad c_{\mu} \quad \text { from } \quad E=\frac{\langle\Psi| H|\Psi\rangle}{\langle\Psi \mid \Psi\rangle}
$$

$$
\text { Kievsky et al., JPG: NPP 35, } 063101 \text { (2008) }
$$

Quantum Monte Carlo (QMC) methods encompass a large family of computational methods whose common aim is the study of complex quantum systems


## QMC: Variational Monte Carlo (VMC)

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

Minimize the expectation value of $H$ :

$$
E_{T}=\frac{\left\langle\Psi_{T}\right| H\left|\Psi_{T}\right\rangle}{\left\langle\Psi_{T} \mid \Psi_{T}\right\rangle} \geq E_{0}
$$

Trial wave function (involves variational parameters):

$$
\left|\Psi_{T}\right\rangle=\left[1+\sum_{i<j<k} U_{i j k}\right]\left[S \prod_{i<j}\left(1+U_{i j}\right)\right]\left|\Psi_{J}\right\rangle
$$

$\left|\Psi_{J}\right\rangle=\left[\prod_{i<j} f_{c}\left(r_{i j}\right)\right]\left|\Phi\left(J M T T_{z}\right)\right\rangle$ (s-shell nuclei): Jastrow wave function, fully antisymmetric
$S \prod_{i<j}$ : represents a symmetrized product
$U_{i j}=\sum_{p=2,6} u_{p}\left(r_{i j}\right) O_{i j}^{p}:$ pair correlation operators
$U_{i j k}=\sum_{x} \epsilon_{x} V_{i j k}^{x}$ : three-body correlation operators
$\left|\Psi_{T}\right\rangle$ are spin-isospin vectors in 3A dimension with $2^{A}\binom{A}{Z}$

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

## QMC: Diffusion Monte Carlo (DMC)

## J. Carlson et al., Rev. Mod. Phys. 87, 1067 (2015)

The diffusion Monte Carlo (DMC) method (ex. GFMC or AFDMC) overcomes the limitations of VMC by using a projection technique to determine the true ground-state

The method relies on the observation that $\Psi_{T}$ can be expanded in the complete set of eigenstates of the Hamiltonian according to

$$
\begin{array}{ll}
\left|\Psi_{T}\right\rangle=\sum_{n} c_{n}\left|\Psi_{n}\right\rangle & H\left|\Psi_{n}\right\rangle=E_{n}\left|\Psi_{n}\right\rangle \\
\\
\lim _{\tau \rightarrow \infty}|\Psi(\tau)\rangle=\lim _{\tau \rightarrow \infty} e^{-\left(H-E_{0}\right) \tau}\left|\Psi_{T}\right\rangle=c_{0}\left|\Psi_{0}\right\rangle & |\Psi(\tau=0)\rangle=\left|\Psi_{T}\right\rangle
\end{array}
$$

where $\tau$ is the imaginary time
The evaluation of $\Psi(\tau)$ is done stochastically in small time steps $\Delta \tau(\tau=\mathrm{n} \Delta \tau)$ using a Green's function formulation


## Spectra of Light Nuclei

## Objectives:

- Study the spectra of light-nuclei: theory confronts experiment
- Validate theoretical framework used to derive nuclear interactions


## Accomplishments:

- GFMC calculations of the spectra of nuclei up to $A=12$ using Delta-full local chiral interactions (red) compared with the ones obtained using AV18+IL7 (cyan) and


The rms from experiment is 0.72 MeV for NV2+3-la compared to 0.80 MeV for $\mathrm{AV} 18+\mathrm{IL} 7$

## Equation of State of Pure Neutron Matter in $\chi$ EFT

The EoS of pure neutron matter (PNM): neutrons stars


- Compact objects: $\mathrm{R} \sim 10 \mathrm{~km}, M_{\mathrm{max}}^{\text {obs }} \sim 2 M_{\odot}$
- Composed predominantly of neutrons between the inner crust and the outer core
- NS from gravitational collapse of a massive star after a supernova explosion

AFDMC: Preliminary study



Cutoff sensitivity: modest in NV2 models; large in NV2+3 models

## Beyond Energy Calculations

Electroweak structure and reactions: Electroweak form factors
Magnetic moments and radii
Electroweak Response functions
Radiative/weak captures
G.T. matrix elements involved in beta decays

Inputs besides nuclear interactions:
Electroweak current operators:

$$
j^{\mathrm{EW}}=\sum_{i=1}^{A} j_{i}+\sum_{i<j=1}^{A} j_{i j}+\sum_{i<j<k=1}^{A} j_{i j k}+\ldots
$$



Current operators constructed in correspondence to the phenomenological interactions based on meson-exchange approach Marcucci et al. PRC 72, 014001 (2005)

Current operators derived in $\chi$ EFT: Pastore et al. PRC 78, 064002 (2008), PRC 80, 034004 (2009); Piarulli et al. PRC 87, 014006 (2013), Baroni et al. PRC 93, 015501 (2016); Kölling et al. PRC 86, 047001 (2012), Krebs et al., Ann. Phys. 378, 317 (2017)

## Objectives:

- Understand electromagnetic properties and transition rates of light-nuclei
- Test nuclear interactions and electromagnetic currents, including complete two-body terms

Pastore et al. PRC 87, 035503 (2013) PRC 90, 024321 (2014)

## Accomplishments:

- GFMC calculations of magnetic moments (right panel) and electromagnetic decays (left panel) using AV18+IL7 and only one-body currents (blue) disagrees with experiment (black)
- Including two-body currents based on effective field theory (red) improves all predictions


Electromagnetic data are explained when twobody correlations and currents are accounted for!

## Conclusions

We are testing our models of $N N+3 N$ interactions with $\Delta$-isobar based on chiral EFT framework in both light-nuclei and infinite nuclear matter

We mainly focused our attention on studying the static and dynamic properties of nuclei up to $A=12$ and EoS of infinite neutron matter

We are interested in studying the model-dependence of the nuclear observables by exploring different cutoffs and range of energies used to fit the NN interactions as well as analyzing different strategies fo fit the TNI

It looks like that the formulation of the TNI with only $c_{D}$ and $c_{E}$ terms is too simplistic if we want to have a good descriptions of spectra, properties of light-nuclei, infinite nuclear matter, three-body observables with a certain degree of accuracy

We are investigating the effect of subleading 3 N contact interactions in light-nuclei (we will do so also for infinite nuclear matter)

## 

## 5 <br> <br> Washington <br> <br> Washington University University inSt.Louis

 inSt.Louis}Theory Alliance


Alessandro Baroni, University of South Carolina, USA Luca Girlanda, University of Salento, Italy Alejandro Kievsky, INFN-Pisa, Italy Alessandro Lovato, INFN-Trento, Italy Laura E. Marcucci, INFN-Pisa, University of Pisa, Italy Saori Pastore,Washington University in St. Louis, USA Steven Pieper**, Argonne National Lab, USA (**deceased)
 Rocco Schiavilla, Old Dominion University/Jefferson Lab, USA Michele Viviani, INFN-Pisa, Italy Robert Wiringa, Argonne National Lab, USA

