Advances in Quantum Monte Carlo Studies of Nuclear Systems with Chiral Effective Field Theory Interactions

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The Atomic Nucleus



An artist's impression of a beryllium atom. The nucleus, with its four protons and five neutrons, is surrounded by a cloud of electrons.

Credit: https://www.sciencephoto.com/media/2075/view

Atomic nuclei are complex quantum many-body systems of strongly interacting fermions (nucleons, p and n), held together by the nuclear force

Nuclei display interesting properties: shell structure, pairing, deformation, strong clustering, etc... that characterize the complexity of matter

Their structure and scattering by electrons and neutrinos are at the forefront of the nuclear physics and high-energy physics in many worldwide research programs







Understanding Nuclei through Scattering and Electroweak Observables







Nuclei as a Testbed for Standard Model and Beyond



Nuclei are utilized in precision testing of the SM as well as in the search for physics BSM.

To untangle new physics from many-body nuclear effects, a precise understanding of nuclear structure and dynamics throughout a wide range of energy and momentum transferred is necessary.

This can be done by investigating the role of manybody correlations and currents in selected nuclear electroweak observables at different kinematics.

The emphasis will be on light nuclei (A \leq 12) that can be treated in Quantum Monte Carlo methods, able to retain many-body effects while delivering precise calculations of the order of a few percents.









The Role of Quantum Chromodynamics in Nuclear Forces

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?

Quantum Chromodynamcs







Atomic nuclei and nucleonic matter





The Role of Quantum Chromodynamics in Nuclear Forces

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?



This is not a trivial problem due to the nonperturbative nature of QCD at low energy

Strong interaction is weak at short distance or high energy (asymptotic freedom) but strong at long-distance or low energy leading to the confinement of quarks into colorless objects the hadron

QCD allows for a perturbative analysis at large energies, while it is highly non-perturbative in the lowenergy regime

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Nuclear few and manybody problem



... Nevertheless Lattice QCD

Lattice Quantum Chromodynamcs









Atomic nuclei and nucleonic matter







The Microscopic Model of Nuclear Theory



- Goal: develop a predictive understanding of nuclei in terms of the interactions between individual nucleons and external probes
- **Definition**: *ab-initio* methods seek to solve the non-relativistic Schrödinger equation for all constituent nucleons and the forces between them
 - 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 β -decay, EDMs, νA xsec, etc,...

The Microscopic Model of Nuclear Theory

• What do we need?

Two and many-body interactions:







one-body

two-body (NN)

three-body (3N)





Electroweak current operators:



one-body

two-body

three-body





The Microscopic Model of Nuclear Theory

<u>Ab-initio methods:</u> Several approaches in nuclear physics: QMC, NCSM, CC, ...



Hergert Front. Phys., Volume 8 - 2020

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

• What do we need?

- Increased many-body capability, algorithms under control
 - Remarkable agreement between different ab initio many-body methods for the structure of nuclei





The Nuclear Many-Body Problem

Many-body Schrödinger equation:

 $H\Psi(\mathbf{r}_1,\mathbf{r}_2,\ldots,\mathbf{r}_A;s_1,s_2,\ldots,s_A;t_1,t_2,\ldots,t_A)$

= $E \Psi(\mathbf{r}_1, \mathbf{r}_2, \dots, \mathbf{r}_A; s_1, s_2, \dots, s_A; t_1, t_2, \dots, t_A)$

where \mathbf{r}_i , s_i , and t_i are the nucleon coordinates, spins, and isospins, respectively

This corresponds to solve

96 for ⁴He 17,920 for ⁸Be 3,784,704 for ¹²C



Erwin Schrödinger

$2^A \times \begin{pmatrix} A \\ 7 \end{pmatrix}$ coupled second-order differential equations in 3A dimensions

This is a challenging many-body problem!



Nuclear Quantum Monte Carlo Methods





Nuclear Quantum Monte Carlo Methods

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



Work with bare interactions but local r-space representation of the Hamiltonian

$$\mathbf{k} = \mathbf{p}' - \mathbf{p} \qquad \mathbf{I}$$

$$\mathbf{k} = (\mathbf{p}' + \mathbf{p})/2 \qquad \mathbf{N}$$

Stochastic method: based on recursive sampling of a probability density, statistical errors quantifiable and systematically improvable

FDMC			
	(C)VMC GFMC AFDMC	light systems	$A \leq 12$
	CVMC AFDMC	light to medium- heavy nuclei	$A\sim 50$
E ₀ ation	AFDMC	infinite matter	$A \to \infty$

- Local Carlson et al., RMP. 87, 1067 (2015); Gandolfi, MP et. al., Front.in Phys. 8 (2020) 117 Non-Local





Variational Monte Carlo Method

In variational Monte Carlo, one minimize the expe

One assumes a suitable form for the trial wave function (involves variational parameters):

$$|\Psi_V
angle = \left[S \prod_{i < j} (1 + \frac{U_{ij}}{U_{ij}} + \sum_{k \neq i, j} \frac{U_{ijk}}{U_{ijk}}) \right] |\Psi_J
angle$$

$$U_{ij} = \sum_{p=2,6} u_p(r_{ij}) O_{ij}^p$$
;

Functions $f_c(r_{ij})$ and $u_p(r_{ij})$ obtained with coupled differential equations with v_{ij}

ectation value of *H*:
$$E_V = \frac{\langle \Psi_V | H | \Psi_V \rangle}{\langle \Psi_V | \Psi_V \rangle} \ge E_0$$

$$|\Psi_J\rangle = \left[\prod_{i < j} f_c(r_{ij})\right] |\Phi_A(JMTT_3)\rangle$$

 $|\Phi_d(1100)\rangle = \mathcal{A}|\uparrow p\uparrow n\rangle \; ; \; |\Phi_\alpha(0000)\rangle = \mathcal{A}|\uparrow p\downarrow p\uparrow n\downarrow n\rangle$

$$U_{ijk} = -\epsilon V_{ijk}(\tilde{r}_{ij}, \tilde{r}_{jk}, \tilde{r}_{ki})$$

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



Diffusion Monte Carlo Method



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

 $|\Psi_T\rangle = \sum$ $\lim_{\tau \to \infty} |\Psi(\tau)\rangle$

GFMC propagated energy vs imaginary time propagation for first 3 states in 6Li • g.s (1⁺) & 3⁺ stable after $\tau = 0.2 \, {\rm MeV^{-1}}$ • 2⁺ (a broad resonance) never stabledecaying to separate $\alpha + d$ • $E(\tau = 0.2)$ is best GFMC estimate of

- resonance energy

J. Carlson et al., RMP. 87, 1067 (2015); S. Gandolfi, MP et. al., Front.in Phys. 8 (2020) 11

$$\sum_{n} c_{n} |\Psi_{n}\rangle \qquad H |\Psi_{n}\rangle = E_{n} |\Psi_{n}\rangle$$
$$= \lim_{\tau \to \infty} e^{-(H - E_{0})\tau} |\Psi_{T}\rangle = c_{0} |\Psi_{0}\rangle \quad |\Psi(\tau = 0)\rangle = |\Psi_{T}\rangle$$



Hamiltonian and electroweak currents







State-of-the art Chiral EFT interactions



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 electroweak sector very challenging to achieve
- More LECs appearing at higher orders; challenging optimization problem



Many-body Nuclear Interactions

Many-body Nuclear Hamiltonian



In our Quantum Monte Carlo calculations we use: • AV18+UIX; AV18+IL7 phenomenological models (1983); S. Pieper et al. PRC 64, 014001 (2001)

• chiral $\pi N\Delta$ N3LO+N2LO Norfolk models

052503 (2018); A. Baroni, MP et al.PRC 98, 044003 (2018)

- Accurate understanding of the interactions/ correlations between nucleons in pairs, triplets,.. (v_{ij}) and V_{iik} are the two- and three-nucleon forces)
- Operators constrained by experimental data; fitted parameters encode underlying QCD dynamics

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Wiringa, Stoks, Schiavilla PRC 51, 38 (1995); J. Carlson et al. NP A401, 59
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MP et al. PRC 91, 024003 2015; PRC 94, 054007 2016; MP et al. PRL 120,
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Three-body LECs and N3LO-CT



The NV2+3s model fits *c* using strong interaction data only

The NV2+3s* model fits *c* with strong and weak interaction data

A. Baroni, **MP** et al. PRC 98, 044003 (2018)



$\mathbf{j}_{5,a}^{\mathrm{N3LO}}(\mathbf{q};\mathrm{CT}) = \mathbf{z_0}\mathcal{O}_{ij}(\mathbf{q})$ $z_0 \propto (c_D + \text{known LECs})$

 $E_0(^{3}\text{H}) = -8.482 \,\text{MeV}$ $^{2}a_{nd} = (0.645 \pm 0.010) \,\mathrm{fm}$

 $E_0(^{3}\text{H}) = -8.482 \,\text{MeV}$ GT m.e. in ³H β -decay



Many-body Nuclear Electroweak Currents

Electroweak structure and reactions:



- Two-body currents are a manifestation of two-body correlations
- Electromagnetic two-body currents are required to satisfy current conservation

$$\mathbf{q} : \mathbf{j} = [H, \rho] \rho = [t_i + W_{ijk}, \rho] V_{ijk}, \rho]$$

- Meson exchange currents: Schiavilla et al., PRC 45, 2628 (1992), Marcucci et al. PRC 72, 014001 (2005), Marcucci et al., PRC 78, 065501 (2008),...
- (2017),....,



• Chiral EFT currents: Park et al. NPA 596, 515 (1996); 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); Phillips et al. PRC 72, 014006 (2005), Kölling et al. PRC 80, 045502 (2009), PRC 84, 054008, PRC 86, 047001 (2012); Krebs et al., Ann. Phys. 378, 317

Selected Properties in Light Nuclei



Understanding Light Nuclei Through Binding Energy and Charge Radii Calculations



MP et al. Phys.Rev.C 91 (2015) 2, 024003

$$\langle r_{\rm ch}^2 \rangle = \langle r_{\rm pt}^2 \rangle + \langle R_p^2 \rangle + \frac{A - Z}{Z} \langle R_n^2 \rangle + \frac{3\hbar^2}{4M_p^2 c^2}$$

q · j = Gandolfi, MP, et al. Front.in Phys. 8 (202)



Probing Nuclear Structure: Insights from Single-Nucleon Densities

In QMC methods, single-nucleon densities are calculate



ed as:
$$\rho_N(r) = \frac{1}{4\pi r^2} \left\langle \Psi \left| \sum_i P_{N_i} \delta \left(r - |\mathbf{r}_i - \mathbf{R}_{cm}| \right) \right. \right.$$

For symmetric nuclei N = Z nuclei, proton and neutron densities are the same

s-shell nuclei (A \leq 4) exhibit large peaks at small separation, while the p-shell nuclei (A \geq 6) are much reduced at small r and more spread out

Densities are not observables but single-nucleon density can be related to longitudinal (charge) form factor physical quantity experimentally accessible via electron-nucleus scattering processes

MP et al. Phys.Rev.C 107 (2023) 1,014314











Analyzing Charge Form Factors in Light Nuclei



Inclusion of the 1b relativistic corrections and 2b corrections is in progress!

 $Q_{\rm el}^2 = q^2 - \omega_{\rm el}^2$ $\omega_{\rm el} = \sqrt{q^2 + m_A^2 - m_A}$ $G_F^N(Q^2)$: electric nucleonic form factor

Gandolfi, MP, et al. Front.in Phys. 8 (2020) 11







Probing Nuclear Structure: Insights from Two-Nucleon Densities



MP et al. Phys.Rev.C 107 (2023) 1,014314

distributions in different combinations of ST are available <u>online</u>









Magnetic Structure: Two-body Currents

Non-minimal (NM) contact term should naively be suppressed by Q^3

It is in fact order ~ $Q^{1.5}$, resulting in larger-thanexpected N3LO contribution

Summed contributions agree with data, but power counting is not converging order-by-order

$$\mu^{2b} = \int dr_{ij} \, 4\pi \, r_{ij}^2 \, \rho_M^{2b}(r_{ij})$$

Chambers-Wall, **MP** et al. e-Print: 2407.03487, e-Print: 2407.04744

NV2+3-IIb*



Magnetic Structure: Form Factors

NV2+3-IIb* is able to capture the shape of magnetic form factor

In some cases, good quantitative agreement at large momentum transfer

Two-body effects ~20% to 50% at large momentum transfer in various nuclei

Chambers-Wall, MP et al. e-Print: 2407.03487, e-Print: 2407.04744

predictions



Insights from (

Calculations with compared to AV18-



Correlations provide bulk of quenching

Two-body almost always enhances



Baroni, **MP** et al. PRC **93**, 015501 (2016)



King, MP et al. PRC 102, 025501 (2020)



Partial Muon Capture in Light Nuclei



Validation of vector and axial currents at q ~ 100 MeV

Same momentum transfer as neutrinoless double beta decay





Partial Muon Capture Rates

QMC rate for ${}^{3}\text{He}(1/2+;1/2) \rightarrow {}^{3}\text{H}(1/2+;1/2)$

$$\Gamma_{VMC} = 1512 \text{ s}^{-1} \pm 32 \text{ s}^{-1}$$

$$\Gamma_{GFMC} = 1476 \text{ s}^{-1} \pm 43 \text{ s}^{-1}$$

$$\Gamma_{expt} = 1496.0 \text{ s}^{-1} \pm 4.0 \text{ s}^{-1}$$

[Ackerbauer et al. Phys. Lett. B417 (1998)]

The inclusion of 2b electroweak currents increase the rate by about 9% to 16%. uncertainty estimates:

Cutoff: 8 s⁻¹ (0.5%)Energy range of fit: $11 \text{ s}^{-1}(0.7\%)$ Three-body fit: 27 s⁻¹ (1.8%) Systematic: 9 s⁻¹ (0.6%)



King, **MP** et al. PRC 105 (2022) 4, L042501

Partial Muon Capture Rates

QMC rate for ${}^{6}\text{Li}(1+;0) \rightarrow {}^{6}\text{He}(0+;1)$

 $\Gamma_{\rm VMC} = 1243 \, {\rm s}^{-1} \pm 59 \, {\rm s}^{-1}$ $\Gamma_{\rm GFMC} = 1056 \, {\rm s}^{-1} \pm 180 \, {\rm s}^{-1}$ $\Gamma_{\text{expt}} = 1600 \text{ s}^{-1} + 300/-129 \text{ s}^{-1}$ Deutsch et al. Phys. Lett. B26 (1968)

The inclusion of 2b electroweak currents increase the rate by about 3% to 7%.

uncertainty estimates:

Cutoff: $36 \text{ s}^{-1}(2.9\%)$ Energy range of fit: $36 \text{ s}^{-1}(2.9\%)$ Three-body fit: $30 \text{ s}^{-1}(2.4\%)$ Systematic: 8 s⁻¹ (0.6%)



King, MP et al. PRC 105 (2022) 4, L042501



Working on Theoretical UQ



Next-Generation χ **EFT Interactions**

We are interested in calibrating the next generation of EFT nucleon-nucleon interactions.

These models should have robust uncertainty quantification:

- Parametric uncertainty
- Truncation uncertainty

Incorporating these uncertainties into our model calibration we aim to better understand and predict nuclear phenomena based on microscopic interactions of nucleons.



Bayes' Theorem

For a model calibration problem in a Bayesian approach, we have

Posterior

 $\mathbf{pr}(\vec{\mathbf{y}} \mid \vec{\mathbf{a}}) \sim e^{-\sum_{i} \left(y_{\exp}^{(i)} - y_{th}^{(i)}(\vec{a}) \right)^{2} / 2\sigma_{i}^{2}}$

What the prior does for us is encode any previous information that we may know.

• Ex: LECs are natural, i.e., order $1 \rightarrow$

$pr(\vec{a} | \vec{y}, I) \propto pr(\vec{y} | \vec{a}) pr(\vec{a} | I)$

Likelihood Prior The likelihood can be formulated as it is in standard model fitting for uncorrelated data

$$= e^{-\chi^2/2}$$

$$\operatorname{pr}(\vec{a} | \mathbf{I}) \sim \mathcal{N}\left(\vec{0}, \Sigma_{\mathrm{pr}}\right)$$

Modeling the Model

Since our model is a perturbative series, we can write an observable as such (BUQEYE framework)*:

$$y_{\text{th}}(x) = y_{\text{ref}}(x) \sum_{n=0}^{\infty} c_n(x)Q^n(x), \quad Q \equiv \frac{\max[p_{soft}, p]}{\Lambda_b},$$

scale, and c_n are the natural coefficients.

This series follows the truncation scheme of the EFT: $y_{\text{th}}(x) = y_{\text{ref}}(x) \sum_{n=1}^{k} c_n(x)Q^n(x) + y_{\text{ref}}(x)$ n=0

where $y_{ref}(x)$ sets a reference scale for the observable y_{th} , Λ_b is the EFT breakdown

$$\sum_{n=k+1}^{\infty} c_n(x)Q^n(x) = y_{\text{th}}^{(k)}(x) + \delta y_{\text{th}}^{(k)}(x).$$

*R. J. Furnstahl et. al. Phys. Rev. C 92, 024005

Truncation Errors

From the neglected terms, we have

$$\delta y_{\rm th}^{(k)}(x) = y_{\rm ref}$$

Under the assumption that the truncation error is uncorrelated across orders, this is a geometric series in Q, so we can find*

 $\delta y_{\rm th}^{(k)}(x) =$

Where we assume that $c_n | \bar{c} \sim \mathcal{N}(0, \bar{c}^2)$.



$$=\frac{y_{\text{ref}}\,\bar{c}\,Q^{(k+1)}}{1-Q},$$

*J.A. Melendez et. al. Phys. Rev. C 100, 044001



Additional Parameters

In this process, we have introduced two new parameters: \bar{c} and Λ_{h} .

This changes the posterior we need to fi $pr(\vec{a}, \vec{c}^2, \Lambda_b | \vec{y}_{exp}, I) \propto pr(\vec{y}_{exp} | \vec{a}, \Sigma, I) I$

Total posterior

Likelihood for \vec{a} P

We can find a closed form of $pr(\bar{c}^2 | \Lambda_b, \bar{a}, I)$ and $pr(\Lambda_b | \bar{a}, I)$.

ind:

$$pr(\vec{a}|I) \quad pr(\vec{c}^2|\Lambda_b, \vec{a}, I) \quad pr(\Lambda_b|\vec{a}, I)$$

Prior for \vec{a} Posterior for \vec{c}^2 Posterior for Λ_b

*J.A. Melendez et. al. Phys. Rev. C 100, 044001

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Posterior Distributions: Pionless Interaction



\bar{c} and Λ_b Posteriors: Pionless Interaction





Bub, **MP** et al. e-Print: 2408.02480 [nucl-th]



Progress/Needs:

- (*Progress*): Tremendous progress in ab-initio theory: i) algorithms and interactions; ii) increased algorithm efficiency; iii) computational resources; iv) successful algorithm benchmarks; v) advent of EFTs and UQ
- with experiment
- (*Progress*): Possibility to perform consistent calculations for nuclei and infinite matter, connecting nuclei observables to astrophysical quantities and observations (not discussed in this talk!)

- which observables to use? In which mass range? Uncertainty quantification?
- A>12)
- within QMC)

• (*Progress*): Microscopic description of nuclei represent a powerful tool to elucidate the role of two-body effects in nuclear interactions and currents: two- and many-body effects can be sizable and improve the agreement of theory

• (*Needs*): New protocols to build realistic nuclear interactions: improvements in the formulation of the 3NFs;

• (Needs): Developments in ab-initio methods to go to larger and larger nuclei (effort also within QMC to go above

• (*Needs*): Developments in ab-initio methods to tackle connect bound states with continuum states (effort also



