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Canada's national laboratory for particle and nuclear physics Laboratoire national canadien pour la recherche en physique nucléaire et en physique des particules

Ab initio calculations in nuclear physics

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Outline

- What is meant by *ab initio* in nuclear physics
- Ab initio nuclear structure and reaction approaches
 - Exact few-body calculations (A=3,4)
 - Quantum Monte Carlo (A≤12)
 - Nuclear Lattice EFT (A=4,8,12,16, 20, 24, 28)
 - Coupled Cluster Method (A≤132, magic, semi-magic)
 - In-medium Similarity Renormalization Group (A≤90, open shells)
 - Self-Consistent Green's Function Method (A≤78, open shells)
- No-core shell model (A≤26, hypernuclei)
- Including the continuum with the resonating group method
 - NCSM/RGM
 - NCSM with continuum
- Outlook









What is meant by ab initio in nuclear physics?

- First principles for Nuclear Physics:
 QCD
 - Non-perturbative at low energies
 - Lattice QCD in the future

Degrees of freedom: NUCLEONS

- Nuclei made of nucleons
- Interacting by nucleon-nucleon and three-nucleon potentials
 - Ab initio
 - \diamond All nucleons are active
 - \diamond Exact Pauli principle
 - \diamond Realistic inter-nucleon interactions
 - \diamond Accurate description of NN (and 3N) data
 - \diamond Controllable approximations



Chiral Effective Field Theory

- First principles for Nuclear Physics: QCD
 - Non-perturbative at low energies
 - Lattice QCD in the future
- For now a good place to start:
- Inter-nucleon forces from chiral effective field theory
 - Based on the symmetries of QCD
 - Chiral symmetry of QCD $(m_u \approx m_d \approx 0)$, spontaneously broken with pion as the Goldstone boson
 - Degrees of freedom: nucleons + pions
 - Systematic low-momentum expansion to a given order (Q/Λ_x)
 - Hierarchy
 - Consistency
 - Low energy constants (LEC)
 - Fitted to data
 - Can be calculated by lattice QCD



 Λ_{χ} ~1 GeV : Chiral symmetry breaking scale



The NN interaction from chiral EFT

PHYSICAL REVIEW C 68, 041001(R) (2003)

Accurate charge-dependent nucleon-nucleon potential at fourth order of chiral perturbation theory

D. R. $Entem^{1,2,*}$ and R. Machleidt^{1,†}



Phase Shift (deg)

-10

-20

-30

0

- 24 LECs fitted to the *np* scattering data and the deuteron properties
 - Including c_i LECs (i=1-4) from pion-nucleon Lagrangian



Determination of NNN LECs c_D and c_E from the triton binding energy and the half life

- **Chiral EFT**: *c*_D also in the two-nucleon contact vertex with an external probe
- Calculate $\langle E_1^A \rangle = |\langle^3 \text{He}||E_1^A||^3 \text{H} \rangle|$
 - Leading order GT
 - N²LO: one-pion exchange plus contact
- A=3 binding energy constraint: $c_{\rm D}$ =-0.2±0.1 $c_{\rm E}$ =-0.205±0.015





Exact few-body calculations (A=3,4) Proton-³He elastic scattering with χ EFT NN+NNN

- Hypherspherical-harmonics variational calculations
 - M. Viviani, L. Girlanda, A. Kievski, L. E. Marcucci, and S. Rosati, EPJ Web Conf. 3 (2010) 05011; Few Body Syst. 54 (2013) 885
- A_v puzzle (almost) resolved with the chiral N³LO NN plus local chiral N²LO NNN
 - used with the NCSM and other methods

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Quantum Monte Carlo

Variational Monte Carlo (VMC): construct Ψ_V that

- Are fully antisymmetric and translationally invariant
- Have cluster structure and correct asymptotic form
- Contain non-commuting 2- & 3-body operator correlations from v_{ij} & V_{ijk}
- Are orthogonal for multiple J^{π} states
- Minimize $E_V = \langle \Psi_V | H | \Psi_V \rangle \geq E$ integrating by Metropolis Monte Carlo

These are $\sim 2^A \binom{A}{Z}$ component (270,336 for ¹²C) spin-isospin vectors in 3A dimensions

Green's function Monte Carlo (GFMC): project out the exact eigenfunction

- $\Psi(\tau) = \exp[-(H E_0)\tau]\Psi_V = \sum_n \exp[-(E_n E_0)\tau]a_n\Psi_n \Rightarrow \Psi_0$ at large τ
- Propagation done stochastically in small time slices $\Delta \tau$
- Exact $\langle H \rangle$ for local potentials; mixed estimates for other $\langle O \rangle$
- Constrained-path propagation controls fermion sign problem for $A \ge 8$
- Multiple excited states for same J^{π} stay orthogonal

Many tests demonstrate 1–2% accuracy for realistic $\langle H \rangle$

Wiringa, Pieper, Carlson, & Pandharipande, PRC **62**, 014001 (2000) Pieper, Varga, & Wiringa, PRC **66**, 044310 (2002) Pieper, Wiringa, & Carlson, PRC **70**, 054325 (2004) Pieper, NPA **751**, 516c (2005)

Quantum Monte Carlo: Eigenenergies of light nuclei



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Quantum Monte Carlo: Magnetic moments and transitions light nuclei









PHYSICAL REVIEW C 87, 035503 (2013)



Quantum Monte Carlo calculations of electromagnetic moments and transitions in $A \leq 9$ nuclei with meson-exchange currents derived from chiral effective field theory



Nuclear Lattice Effective Field Theory Calculations E. Epelbaum, H. Krebs, T. Lahde, D. Lee, U.-G. Meissner

Discretized version of chiral EFT for nuclear dynamics

Gautam Rupak

 $\left[\left(\sum_{i=1}^{A}\frac{-\vec{\nabla}_{i}^{2}}{2m_{N}}+\mathcal{O}(m_{N}^{-3})\right)+\underbrace{V_{2N}+V_{3N}+V_{4N}+\dots}\right]|\Psi\rangle=E|\Psi\rangle$



Timo A. Lähde^{a,*}, Evgeny Epelbaum^b, Hermann Krebs^b, Dean Lee^c, Ulf-G. Meißner^{a,d,e},





Nuclear Lattice Effective Field Theory Calculations E. Epelbaum, H. Krebs, T. Lahde, D. Lee, U.-G. Meissner



Epelbaum, Krebs, Lee, Meissner, PRL 106, 192501 (2011)



Coupled-Cluster Method

• exponential Ansatz for wave operator $|\Psi
angle=e^{\hat{T}}|\Phi_0
angle$

• CCSD: truncate \hat{T} at the 2p2h excitation level, $\hat{T} = \hat{T}_1 + \hat{T}_2$



$$\hat{T}_n = \frac{1}{(n!)^2} \sum_{\substack{ijk...\\abc...}} t^{abc...}_{ijk...} \{ \hat{a}^{\dagger}_a \hat{a}^{\dagger}_b \hat{a}^{\dagger}_c \dots \hat{a}_k \hat{a}_j \hat{a}_i \}$$

• effects of T_3 clusters included approximately in ground-state calculations via $\Lambda CCSD(T)$ or CR-CC(2,3) method

State-of-the-art: Λ -CCSD(T) with 3N interaction

Coupled-Cluster calculations for heavy nuclei with chiral interactions



- current chiral Hamiltonians capable of describing the experimental trend of binding energies
- systematic overbinding indicates that there are still deficiencies
 consistent 3N interaction at N³LO, and 4N interactions

• charge radii are considerably too small



Coupled-cluster effective interactions (CCEI) for the shell model

G. R. Jansen, J. Engel, G. Hagen, P. Navratil, A. Signoracci, Phys. Rev. Lett. 113, 142502 (2014).

- Start from chiral NN(N3LO_{EM}) + 3NF(N2LO) interactions
- Solve for A+1 and A+2 using CC. Project A+1 and A+2 CC wave functions onto the *s-d* model space using Lee-Suzuki similarity transformation.
- Spectra of oxygen isotopes computed with coupled-cluster effective interaction (CCEI), and compared to experimental data and the phenomenological USD shell model interaction.



In-medium SRG approach: Application to Oxygen isotopes



 $E_{
ho}-E_{h},E_{
ho
ho'}-E_{hh'}: ext{ approx. 1p1h, 2p2h excitation energies}$

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Magic, semi-magic and open-shell nuclei

In-medium SRG approach: Application to Ca and Ni isotopes



IM-SRG calculations for A~100 are routine, tin isotopes in progress

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- controlled uncertainties & consistent results for different abintio methods
- systematic overbinding due to current chiral Hamiltonians results for new generation of chiral Hamiltonians soon

Self-Consistent Green's Function Method: Oxygen, Fluorine, Nitrogen isotopes



→ 3NF crucial for reproducing binding energies and driplines around oxygen → $d_{3/2}$ raised by genuine 3NF

Green's functions in medium-mass nuclei

Gorkov GF go beyond standard expansion schemes and are not limited to doubly closed-shells

- \circ Expansion around a Bogoliubov vacuum
- From few tens to hundreds of medium-mass open-shell systems (→ complete chains)



→ Systematic overbinding of medium-mass nuclei (in agreement with other ab initio methods)

- \rightarrow initial (full) 3NF are necessary to reproduce relative trends
- \rightarrow Relative energies (S_{2n}) well reproduced

No-core shell model

- No-core shell model (NCSM)
 - A-nucleon wave function expansion in the harmonic-oscillator (HO) basis
 - short- and medium range correlations
 - Bound-states, narrow resonances



NCSM calculations for light nuclei and hypernuclei

Flexible approach capable performing exact calculations for few-nucleon systems and accurate calculations for nuclei with A≤24 & hypernuclei

(a)

-25

-35

E [MeV]

 E^* [MeV]

8

Nmax

⁶Li



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Testing chiral LO NY potentials with Λ - Σ mixing included

...outperform the Julich '04 **YN** potential



No-core shell model with continuum

No-core shell model (NCSM)

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- A-nucleon wave function expansion in the harmonic-oscillator (HO) basis
- short- and medium range correlations
- Bound-states, narrow resonances
- NCSM with Resonating Group Method (NCSM/RGM)
 - cluster expansion
 - proper asymptotic behavior
 - long-range correlations
 - NCSM with continuum (NCSMC)
 - unified description of bound and unbound states

$$N = N_{\max} + 1$$

$$N = 1$$

$$N = 0$$

$$M =$$



$$\Psi^{A} = \sum_{N=0} \sum_{i} c_{Ni} \Phi_{N}^{A}$$

$$\Psi^{A} = \sum_{\nu} \int d\vec{r} \varphi_{\nu}(\vec{r}) \mathcal{A}_{\nu} \Phi_{1\nu}^{(A-a)} \Phi_{2\nu}^{(a)} \delta(\vec{r} - \vec{r}_{A-a,a})$$



S. Baroni, P. N., and S. Quaglioni, PRL 110, 022505 (2013); PRC 87, 034326 (2013).



Coupled NCSMC equations



Scattering matrix (and observables) from matching solutions to known asymptotic with microscopic *R*-matrix on Lagrange mesh



n-⁴He & *p*-⁴He scattering within NCSMC



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NCSM/RGM calculations of transfer reactions

$$\int dr r^{2} \left[\begin{pmatrix} \mathbf{r} \\ \mathbf{n} \\ \mathbf{n} \end{pmatrix} \hat{A}_{1}(H-E) \hat{A}_{1} \\ \mathbf{n} \\ \mathbf{n} \\ \mathbf{n} \end{pmatrix} \hat{A}_{2}(H-E) \hat{A}_{1} \\ \mathbf{n} \\ \mathbf{n} \\ \mathbf{n} \end{pmatrix} \hat{A}_{2}(H-E) \hat{A}_{1} \\ \mathbf{n} \\ \mathbf{n} \\ \mathbf{n} \end{pmatrix} \hat{A}_{2}(H-E) \hat{A}_{2} \\ \mathbf{n} \\ \mathbf{n$$

Straightforward to couple different mass partitions in the NCSM/RGM formalism

Applications to (d,p) and (d,n) reactions Example: ³He(d,p)⁴He

> Work in progress: ⁷Li(d,p)⁸Li & ⁸Li(d,p)⁹Li



Ab Initio Many-Body Calculations of the ${}^{3}H(d, n){}^{4}He$ and ${}^{3}He(d, p){}^{4}He$ Fusion Reactions

Petr Navrátil^{1,2} and Sofia Quaglioni²



Solar *p-p* chain



^{[®]TRIUMF ³He(⁴He,γ)⁷Be & ⁷Be(*p*,γ)⁸B radiative capture}

- NCSMC & NCSM/RGM calculations
 - Soft NN potential (chiral SRG-N³LO with with $\Lambda = 2.1$ fm⁻¹ & $\Lambda = 1.86$ fm⁻¹)





NCSM with continuum: ⁷He \leftrightarrow ⁶He+*n*



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Structure of ⁹Be: bound states and resonances



⁹Be is a stable nucleus ... but all its excited states unbound A proper description requires to include effects of continuum

Three-nucleon interaction *and* continuum improve agreement with experiment for negative parity states

Continuum crucial for the description of positive-parity states

J. Langhammer, P. N., G. Hupin, S. Quaglioni, A. Calci, R. Roth, in preparation

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p+¹⁰C scattering: structure of ¹¹N resonances

¹¹N from chiral NN+3N within NCSMC

¹¹N Expt. (TUNL evaluation)

– Preliminary

	J ^π .	Т	E _{res} [MeV]	E _x [Me	eV] F [keV]
	1/2+	3/2	1.35	0	"4100"
✓	1/2-	3/2	1.94	0.59	580
\checkmark	3/2-	3/2	4.69	3.34	280
	5/2+	3/2	4.75	3.40	1790
	3/2+	3/2	4.95	3.60	"4760"
	5/2⁻	3/2	5.95	4.60	470
	3/2-	3/2	7.68	6.33	620

$E_{\rm res}$ (MeV \pm keV)	$E_{\rm x}$ (MeV \pm keV)	$J^{\pi}; T$	Γ (keV)
1.49 ± 60	0	$\frac{1}{2}^+; \frac{3}{2}$	830 ± 30
2.22 ± 30	0.73 ± 70	$\frac{1}{2}^{-}$	600 ± 100
3.06 ± 80	(1.57 ± 80)		< 100
3.69 ± 30	2.20 ± 70	$\frac{5}{2}^{+}$	540 ± 40
4.35 ± 30	2.86 ± 70	$\frac{3}{2}^{-}$	340 ± 40
5.12 ± 80	(3.63 ± 100)	$(\frac{5}{2}^{-})$	< 220
5.91 ± 30	4.42 ± 70	$(\frac{5}{2}^{-})$	
6.57 ± 100	5.08 ± 120	$(\frac{3}{2}^{-})$	100 ± 60



$$\Gamma = \left. \frac{2}{\partial \delta(E_{kin}) / \partial E_{kin}} \right|_{E_{kin} = E_R}$$

Negative parity 1/2⁻ and 3/2⁻ resonances in a good agreement with the current evaluation

Positive parity resonances too broad - N_{max} convergence

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p+¹⁰C scattering: structure of ¹¹N resonances

¹¹N from chiral NN+3N within NCSMC

¹¹N Expt. (TUNL evaluation)

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No candidate for 3.06 MeV resonance

We predict only one 5/2⁻ resonance below the 3/2⁻₂

Calculations suggest that either 5.12 MeV or 5.91 MeV resonance might be 3/2⁺ instead

NCSMC resonance predictions more in line with assignments in ¹¹Be





NCSM/RGM for three-body clusters: Structure of ⁶He



⁵H \approx ⁴He + *n* + *n* in progress

Conclusions and Outlook

- Ab initio calculations of nuclear structure & reactions is a dynamic field with rapid advances
- Several exact methods applicable to few-nucleon systems (A=3,4)
- Significant progress in *ab initio* approaches for *p*-shell nuclei
- New very successful approaches to medium mass nuclei
- We developed a new unified approach to nuclear bound and unbound states
 - Merging of the NCSM and the NCSM/RGM = NCSMC
- Outlook:
 - Applications to astrophysics
 - nuclear reactions important for astrophysics (and fusion energy generation)
 - equation of state, symmetry energy
 - Neutrino physics
 - neutrino-nucleus cross sections
 - double beta decay nuclear matrix elements
 - Fundamental symmetries
 - nuclear corrections (CKM unitarity...)
 - Strangeness
 - hypernuclei