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From *ab initio* no-core shell model to a unified approach to nuclear structure and reactions

The 80th Jubilee of Professor James P. Vary Institute of Modern Physics, Chinese Academy of Sciences in Lanzhou, China (online)

5th June 2023

Petr Navratil

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Discovery, accelerate

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Outline

- Introduction to *ab initio* no-core shell model (NCSM)
- Parity-violating moments within *ab initio* NCSM
- Unified description of bound and unbound states ab initio NCSM with Continuum
- ⁷Li(p,e⁺e⁻)⁸Be pair production & the X17 boson within NCSMC

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Ab initio no-core shell model (NCSM)



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Ab Initio No-Core Shell Model (NCSM)

Review

Ab initio no core shell model

Bruce R. Barrett^a, Petr Navrátil^b, James P. Vary^{c,*}



 $N = N_{\max} + 1$ N = 1 N = 0 $\Delta E = N_{\max} \hbar \Omega$ N = 0

- Basis expansion method
 - Harmonic oscillator (HO) basis truncated in a particular way (N_{max})
 - Why HO basis?
 - Lowest filled HO shells match magic numbers of light nuclei (2, 8, 20 – ⁴He, ¹⁶O, ⁴⁰Ca)
 - Equivalent description in relative-coordinate and Slater determinant basis
- Short- and medium range correlations
- Bound-states, narrow resonances



Ab Initio No-Core Shell Model (NCSM)

Basis expansion method

• Why HO basis?

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Ab Initio No-Core Shell Model (NCSM)

Basis expansion method

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 $\hbar\Omega$ $\Delta \dot{E} = N_{\max} \hbar \Omega$ N =N =





determinant basis

(2, 8, 20 – ⁴He, ¹⁶O, ⁴⁰Ca)

Bound-states, narrow resonances

$$\Psi^{A} = \sum_{N=0}^{N_{\text{max}}} \sum_{i} c_{Ni} \Phi_{Ni}^{HO}(\vec{\eta}_{1}, \vec{\eta}_{2}, ..., \vec{\eta}_{A-1})$$

$$\Psi_{SD}^{A} = \sum_{N=0}^{N_{max}} \sum_{j} c_{Nj}^{SD} \Phi_{SDNj}^{HO}(\vec{r}_{1}, \vec{r}_{2}, ..., \vec{r}_{A}) = \Psi^{A} \varphi_{000}(\vec{R}_{CM})$$

• Harmonic oscillator (HO) basis truncated in a particular way (N_{max})

Lowest filled HO shells match magic numbers of light nuclei

Equivalent description in relative-coordinate and Slater



Ab Initio No-Core Shell Model (NCSM) early development – personal notes

- For myself, a key development was the confirmation that NCSM calculations of the ³H gs energy reproduce Faddeev method results
- Later, the NCSM ⁴He gs energy prediction with the CD-Bonn potential was confirmed by Faddeev-Yakubovsky calculations
 - Jacobi-coordinate HO basis
 - Okubo-Lee-Suzuki effective interaction





Ab Initio No-Core Shell Model (NCSM) early development – personal notes

- Breakthrough paper on the structure of ¹²C
 - Energies of states and other properties of a complex nucleus can be predicted from an *ab initio* approach
 - Slater-Determinant HO basis
 - Okubo-Lee-Suzuki effective interaction





Ab Initio No-Core Shell Model (NCSM) early development – personal notes

- Other notable early papers
 - 0⁺ and 2⁺ intruder states in ⁸Be not 100% confirmed but a significant experimental evidence
 - Impact of a genuine 3N force on electroweak transitions in ¹²C, spectra of ^{10,11}B, ¹³C & on the ¹⁴C lifetime



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Novel chiral Hamiltonian and observables in light and medium-mass nuclei

V. Somà,^{1,*} P. Navrátil¹,^{2,†} F. Raimondi,^{3,4,‡} C. Barbieri¹,^{4,§} and T. Duguet^{1,5,∥}

Input for *ab initio* calculations: Nuclear forces from chiral Effective Field Theory

- Quite reasonable description of binding energies across the nuclear charts becomes feasible
 - The Hamiltonian fully determined in A=2 and A=3,4 systems
 - Nucleon–nucleon scattering, deuteron properties, ³H and ⁴He binding energy, ³H half life
 - Light nuclei NCSM
 - Medium mass nuclei Self-Consistent Green's Function method

NN N³LO (Entem-Machleidt 2003) 3N N²LO w local/non-local regulator



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 - Light nuclei NCSM
 - Heavy nuclei HF-MBPT(3)



SRG renormalization - 3N-induced interaction



NN N³LO (Entem-Machleidt 2003) 3N N²LO w local/non-local regulator 11

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Parity-violating moments within *ab initio* NCSM



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Why to investigate the parity violating moments - the anapole moment and the electric dipole moment (EDM)?

- Parity violation in atomic and molecular systems sensitive to a variety of "new physics"
 - Probes electron-quark electroweak interaction
 - Best limits on the Z' boson parity violating interaction with electrons and nucleons
- The EDM is a promising probe for CP violation beyond the standard model as well as CP violating QCD $\bar{\theta}$ parameter
 - Nuclear structure can enhance the EDM
 - Nuclear EDMs can be measured in storage rings (CERN feasibility study: arXiv:1912.07881)

Nuclear spin dependent parity violating effects in light polyatomic molecules

- Experiments proposed for ⁹BeNC, ²⁵MgNC
- To extract the underlying physics, atomic, molecular and nuclear structure effects must be understood
 - Ab initio calculations

- Spin dependent PV
 - Z-boson exchange between nucleon axialvector and electron-vector currents (b)
 - Electromagnetic interaction of atomic electrons with the nuclear anapole moment (c)



Parity violating nucleon-nucleon interaction and the nuclear anapole moment

- Parity violating (non-conserving) V_{NN}^{PNC} interaction
 - Conserves total angular momentum I
 - Mixes opposite parities
 - Has isoscalar, isovector and isotensor components
 - Admixes unnatural parity states in the ground state

$$\psi_{\rm gs} I\rangle = |\psi_{\rm gs} I^{\pi}\rangle + \sum_{j} |\psi_{j} I^{-\pi}\rangle$$
$$\times \frac{1}{E_{\rm gs} - E_{j}} \langle \psi_{j} I^{-\pi} | V_{\rm NN}^{\rm PNC} | \psi_{\rm gs} I^{\pi} \rangle$$

Anapole moment operator dominated by spin contribution

$$oldsymbol{a} = -\pi \int d^3 r \, r^2 \, oldsymbol{j}(oldsymbol{r})$$

$$\hat{\boldsymbol{a}}_{s} = \frac{\pi e}{m} \sum_{i=1}^{A} \mu_{i} (\boldsymbol{r}_{i} \times \boldsymbol{\sigma}_{i})$$
$$\mu_{i} = \mu_{p} (1/2 + t_{z,i}) + \mu_{n} (1/2 - t_{z,i})$$

$$a_s = \langle \psi_{\rm gs} \ I \ I_z = I | \hat{a}_{s,0}^{(1)} | \psi_{\rm gs} \ I \ I_z = I \rangle$$

Here is what we want to calculate:

$$\kappa_{A} = \frac{\sqrt{2}e}{G_{F}}a_{s} \qquad \qquad \kappa_{A} = -i4\pi \frac{e^{2}}{G_{F}}\frac{\hbar}{mc}\frac{(II10|II)}{\sqrt{2I+1}} \sum_{j} \langle\psi_{\rm gs} \ I^{\pi}||\sqrt{4\pi/3}\sum_{i=1}^{A}\mu_{i}r_{i}[Y_{1}(\hat{r}_{i})\sigma_{i}]^{(1)}||\psi_{j} \ I^{-\pi}\rangle \frac{1}{E_{\rm gs}-E_{j}}\langle\psi_{j} \ I^{-\pi}|V_{\rm NN}^{\rm PNC}|\psi_{\rm gs} \ I^{\pi}\rangle$$

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$$\begin{split} |\psi_{\rm gs} I\rangle &= |\psi_{\rm gs} I^{\pi}\rangle + \sum_{j} |\psi_{j} I^{-\pi}\rangle \\ \times \frac{1}{E_{\rm gs} - E_{j}} \langle \psi_{j} I^{-\pi} | V_{\rm NN}^{\rm PNC} | \psi_{\rm gs} I^{\pi} \rangle \end{split}$$

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Ab initio calculations of electric dipole moments of light nuclei

Paul Froese^{*} TRIUMF, 4004 Wesbrook Mall, Vancouver, British Columbia V6T 2A3, Canada and Department of Physics and Astronomy, University of British Columbia, Vancouver, British Columbia V6T 1Z1, Canada

> Petr Navrátil 01 TRIUMF, 4004 Wesbrook Mall, Vancouver, British Columbia V6T 2A3, Canada

N_{max} convergence for ³He N³LO NN



³He EDM Benchmark Calculation

Discrepancy between calculations?

	PLB 665:165-172 (2008) (NN EFT)	PRC 87:015501 (2013)	PRC 91:054005 (2015)	Our calculation (NN EFT)
\overline{G}_{π}^{0}	0.015	(x 1/2)	(x 1/2)	0.0073 (x 1/2)
\overline{G}_{π}^{1}	0.023	(x 1/2)	(x 1/2)	0.011 (x 1/2)
\overline{G}_{π}^{2}	0.037	(x 1/5)	(x 1/2)	0.019 (x 1/2)
$\overline{G}^0_ ho$	-0.0012	(x 1/2)	(x 1/2)	-0.00062 (x 1/2)
$\overline{G}^1_ ho$	0.0013	(x 1/2)	(x 1/2)	0.00063 (x 1/2)
$\overline{G}_{ ho}^2$	-0.0028	(x 1/5)	(x 1/2)	-0.0014 (x 1/2)
\overline{G}^0_ω	0.0009	(x 1/2)	(x 1/2)	0.00042 (x 1/2)
\overline{G}^1_ω	-0.0017	(x 1/2)	(x 1/2)	-0.00086 (x 1/2)

Our results confirm those of Yamanaka and Hiyama, PRC 91:054005 (2015)

Editors' Suggestion

Nuclear spin-dependent parity-violating effects in light polyatomic molecules

Yongliang Hao[®],¹ Petr Navrátil[®],² Eric B. Norrgard[®],³ Miroslav Iliaš[®],⁴ Ephraim Eliav,⁵ Rob G. E. Timmermans[®],¹ Victor V. Flambaum[®],⁶ and Anastasia Borschevsky[®],^{*} 18

Nuclear spin-dependent parity-violating effects from NCSM

Contributions from nucleon axial-vector and the anapole moment

	⁹ Be	¹³ C	14 N	15 N	²⁵ Mg
I^{π}	$3/2^{-}$	$1/2^{-}$	1+	$1/2^{-}$	$5/2^{+}$
$\mu^{ ext{exp.}}$	-1.177^{a}	0.702 ^b	0.404 ^c	-0.283^{d}	-0.855^{e}
		NCSM	calculations		
μ	-1.05	0.44	0.37	-0.25	-0.50
κ_{A}	0.016	-0.028	0.036	0.088	0.035
$\langle s_{p,z} \rangle$	0.009	-0.049	-0.183	-0.148	0.06
$\langle s_{n,z} \rangle$	0.360	-0.141	-0.1815	0.004	0.30
$\kappa_{\rm ax}$	0.035	-0.009	0.0002	0.015	0.024
К	0.050	-0.037	0.037	0.103	0.057

$$\kappa_{ax} \simeq -2C_{2p} \langle s_{p,z} \rangle - 2C_{2n} \langle s_{n,z} \rangle \simeq -0.1 \langle s_{p,z} \rangle + 0.1 \langle s_{n,z} \rangle$$
$$\langle s_{\nu,z} \rangle \equiv \langle \psi_{gs} I^{\pi} I_z = I | \hat{s}_{\nu,z} | \psi_{gs} I^{\pi} I_z = I \rangle$$
$$C_{2p} = -C_{2n} = g_A (1 - 4 \sin^2 \theta_W) / 2 \simeq 0.05$$



Calculated EDMs of selected stable nuclei

Ab initio calculations of electric dipole moments of light nuclei Paul Froese*







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Ab initio no-core shell model with continuum (NCSMC)



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Ab Initio Calculations of Structure, Scattering, Reactions Unified approach to bound & continuum states

No-Core Shell Model with Continuum (NCSMC)

$$\Psi^{(A)} = \sum_{\lambda} c_{\lambda} \left| {}^{(A)} \mathfrak{B}, \lambda \right\rangle + \sum_{\nu} \int d\vec{r} \, \gamma_{\nu}(\vec{r}) \, \hat{A}_{\nu} \left| \mathfrak{B}_{(A-a)}^{\vec{r}} \mathfrak{B}_{(a)}, \nu \right\rangle$$

Ab Initio Calculations of Structure, Scattering, Reactions

Unified approach to bound & continuum states

No-Core Shell Model with Continuum (NCSMC)

$$\Psi^{(A)} = \sum_{\lambda} c_{\lambda} | \stackrel{(A)}{\Longrightarrow}, \lambda \rangle + \sum_{\nu} \int d\vec{r} \gamma_{\nu}(\vec{r}) \hat{A}_{\nu} | \stackrel{\vec{r}}{\Longrightarrow}_{(A-a)} (a), \nu \rangle$$

$$N = N_{\max} + 1 \stackrel{\vec{h}\Omega}{\longrightarrow}_{N=1} \Delta E = N_{\max} \hbar \Omega$$

$$N = 0$$

Static solutions for aggregate system, describe all nucleons close together

Ab Initio Calculations of Structure, Scattering, Reactions

Unified approach to bound & continuum states

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Static solutions for aggregate system, describe all nucleons close together

Coupled NCSMC equations

$$H \Psi^{(A)} = E \Psi^{(A)} \qquad \Psi^{(A)} = \sum_{\lambda} c_{\lambda} |^{(A)} \mathfrak{D}, \lambda \rangle + \sum_{\nu} \int d\vec{r} \gamma_{\nu}(\vec{r}) \hat{A}_{\nu} |_{(A-a)}^{\vec{r}} \mathfrak{D}, \nu \rangle$$

$$E_{\lambda}^{NCSM} \mathfrak{D}_{\lambda r} \qquad (A \mathfrak{D} H \hat{A}_{\nu} | \mathfrak{D}_{a}, r) \qquad (A \mathfrak{D} H \hat{A}_{\nu} | \mathfrak{D}_{\mu}, r) \qquad (A \mathfrak{D} H \hat{A}_{$$

Physica Scripta doi:10.1088/0031-8949/91/5/053002

Petr Navrátil¹, Sofia Quaglioni², Guillaume Hupin^{3,4}, Carolina Romero-Redondo² and Angelo Calci¹

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⁷Li(p,e⁺e⁻)⁸Be pair production & X17 boson within NCSMC



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NCSMC calculations of ⁸Be structure and ⁷Li+p scattering and capture

Wave function ansatz

$$\Psi_{\mathsf{NCSMC}}^{(8)} = \sum_{\lambda} c_{\lambda} \left| {}^{8}\mathrm{Be}, \lambda \right\rangle + \sum_{\nu} \int \mathrm{d}r \gamma_{\nu}(r) \hat{A}_{\nu} \left| {}^{7}\mathrm{Li} + p, \nu \right\rangle + \sum_{\mu} \int \mathrm{d}r \gamma_{\mu}(r) \hat{A}_{\mu} \left| {}^{7}\mathrm{Be} + n, \mu \right\rangle$$

- 3/2⁻, 1/2⁻, 7/2⁻, 5/2⁻, 5/2⁻ ⁷Li and ⁷Be states in cluster basis
- 15 positive and 15 negative parity states in ⁸Be composite state basis



TUNL Nuclear Data Evaluation Project

NCSMC calculations of ⁸Be structure and ⁷Li+p scattering and capture

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$$\Psi_{\mathsf{NCSMC}}^{(8)} = \sum_{\lambda} c_{\lambda} \left| {}^{8}\mathrm{Be}, \lambda \right\rangle + \sum_{\nu} \int \mathrm{d}r \gamma_{\nu}(r) \hat{A}_{\nu} \left| {}^{7}\mathrm{Li} + p, \nu \right\rangle + \sum_{\mu} \int \mathrm{d}r \gamma_{\mu}(r) \hat{A}_{\mu} \left| {}^{7}\mathrm{Be} + n, \mu \right\rangle$$

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Novel chiral Hamiltonian and observables in light and medium-mass nuclei

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Convergence of ground-state energies of ⁷Li, ⁷Be, ⁸Be

Chiral EFT NN+3N interaction from PRC **101**, 014318 (2020) Low-energy constants determined in *A*=2,3,4 systems



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Convergence of NCSM excitation energies of ⁷Li, ⁷Be, ⁸Be

Chiral EFT NN+3N interaction from PRC **101**, 014318 (2020) Low-energy constants determined in *A*=2,3,4 systems



⁸Be structure

Calculated ⁸Be bound states w.r.t. ⁷Li + p threshold ($N_{max} = 8/9$)

State	Energy [MeV]		Excitation Energy [MeV]	
	NCSMC	Expt.	NCSMC	Expt.
0^+	-16.13	-17.25	0.00	0.00
2^+	-12.72	-14.23	3.41	3.03
4^+	-4.31	-5.91	11.82	11.35
2^+	-0.10	-0.63	16.03	16.63
2^+	+0.31	-0.33	16.44	16.92

Matches experiment well, except the 3rd 2^+ is slightly above the $^7\text{Li} + p$ threshold.





3.0

⁸Be structure – calculated positive-parity eigenphase shifts



- Motivated by ATOMKI experiments (Firak, Krasznahorkay et al., EPJ Web of Conferences 232, 04005 (2020))
- No-core shell model with continuum (NCSMC) with wave function ansatz

Z.Phys.A 351 229-236 (1995)

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⁷Li $(p, e^+e^-)^8$ Be; $E_{kin} = 0.9$ MeV

Preliminar

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NCSMC: $d\Gamma(E1.M1)$ NCSMC: $d\Gamma(M1)$

NCSMC: $d\Gamma(E1)$ ATOMKI 2016

 10^{-1}

 10^{-2}

ATOMKI 2019

X17 boson?

140

160

120

100

Angle between e- and e+

 Θ [deg]

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$$\Psi_{\mathsf{NCSMC}}^{(8)} = \sum_{\lambda} c_{\lambda} \left| {}^{8}\mathrm{Be}, \lambda \right\rangle + \sum_{\nu} \int \mathrm{d}r \gamma_{\nu}(r) \hat{A}_{\nu} \left| {}^{7}\mathrm{Li} + p, \nu \right\rangle + \sum_{\mu} \int \mathrm{d}r \gamma_{\mu}(r) \hat{A}_{\mu} \left| {}^{7}\mathrm{Be} + n, \mu \right\rangle$$

Internal electron-positron pair conversion correlation Assuming $J=1 \rightarrow 0^+$ bound-to-bound like decay rate IPCC (relative units) ψ_f 10^{-2} NCSMC matched to data at 65°

NCSMC IPCC results consistent with LANL R-matrix phenomenology arXiv: 2106.06834; Phys. Rev. C 105, 055502 (2022)

 e^{-}



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Internal electron-positron pair conversion correlation





P. Navratil. K. Kravvaris, P. Gysbers et al., arXiv: 2212.00160; P. Gysbers, PhD Thesis; P. Gysbers et al., in preparation

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⁷Li $(p, e^+e^-)^8$ Be; $E_{kin} = 0.9$ MeV Internal electron-positron pair conversion correlation ••••• NCSMC: dT NCSMC: $d\sigma$ Relative Counts/(10 degrees) Preliminary Calculating properly the pair production cross section ATOMKI 2016 **ATOMKI 2019** with the interference of different multipoles $\cdot 10^{-1}$ Following formalism by Viviani et al. $\psi_{F}^{(A)}$ $\psi_P^{(a)}$ Phys. Rev. C 105, 014001 (2022) X17 boson? 10^{-2} 10^{-2} NCSMC matched to data at 65° 80 100 120140160 6040 $\psi_T^{(A-a)}$ Θ [deg] NCSMC pair production cross section slightly closer to ATOMKI SM background data Angle between e- and e+

P. Navratil. K. Kravvaris, P. Gysbers et al., arXiv: 2212.00160; P. Gysbers, PhD Thesis; P. Gysbers et al., in preparation

Conclusions and outlook

- Ab initio nuclear theory
 - Makes connections between the low-energy QCD and many-nucleon systems
 - Applicable to nuclear structure, reactions including those relevant for astrophysics, electroweak processes, tests of fundamental symmetries
- *Ab initio* no-core shell model is one of the pioneering methods with impact beyond light nuclei

In synergy with experiments, ab initio nuclear theory is the right approach to understand low-energy properties of atomic nuclei

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Congratulations, James!

Recent NCSM and NCSMC collaborators:

S. Quaglioni (LLNL), G. Hupin (Orsay), K. Kravvaris (LLNL), C. Hebborn (MSU/LLNL), M. Atkinson (LLNL), M. Vorabbi (Surrey), M. Gennari (TRIUMF/UVic), P. Gysbers (TRIUMF)

Thank you!



Discovery, accelerated