Prospects for the No Core Shell Model

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Arizona's First University.

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OUTLINE

I. Brief Overview of the No Core Shell Model (NCSM)

II. Applications of the NCSM

III. Approaches for Extending the NCSM to Heavier Mass Nuclei

IV. Summary and Outlook

MICROSCOPIC NUCLEAR-STRUCTURE **THEORY**

1. Start with the bare interactions among the nucleons

2. Calculate nuclear properties using nuclear many body theory

No Core Shell Model

"Ab Initio" approach to microscopic nuclear structure calculations, in which all \underline{A} nucleons are treated as being active.

Want to solve the A-body Schrödinger equation

$$
H_A \Psi^A = E_A \Psi^A
$$

R P. Navrátil, J.P. Vary, B.R.B., PRC 62, 054311 (2000) P. Navratil, et al., J. Phys. G: Nucl. Part. Phys. 36, 083101 (2009)

From few-body to many-body

No-Core Shell-Model Approach

• Start with the purely intrinsic Hamiltonian

$$
H_A = T_{rel} + \mathcal{V} = \frac{1}{A} \sum_{i < j = 1}^{A} \frac{(\vec{p}_i - \vec{p}_j)^2}{2m} + \sum_{i < j = 1}^{A} V_{NN} \left(+ \sum_{i < j < k}^{A} V_{ijk}^{3b} \right)
$$

Note: There are **no** phenomenological s.p. energies!

Can use any NN potentials Coordinate space: Momentum space: Argonne V8', AV18 Nijmegen I, II CD Bonn, EFT Idaho

No-Core Shell-Model Approach

• Next, add CM harmonic-oscillator Hamiltonian

$$
H_{CM}^{HO} = \frac{\vec{P}^2}{2Am} + \frac{1}{2}Am\Omega^2 \vec{R}^2; \quad \vec{R} = \frac{1}{A} \sum_{i=1}^{A} \vec{r}_i, \quad \vec{P} = Am\vec{R}
$$

To H_A, yielding

$$
H_A^{\Omega} = \sum_{i=1}^{A} \left[\frac{\vec{p}_i^2}{2m} + \frac{1}{2} m \Omega^2 \vec{r}_i^2 \right] + \sum_{i < j = 1}^{A} \left[V_{NN} (\vec{r}_i - \vec{r}_j) - \frac{m \Omega^2}{2A} (\vec{r}_i - \vec{r}_j)^2 \right]
$$

Defines a basis (*i.e.* HO) for evaluating *V ij*

$$
H\Psi_{\alpha} = E_{\alpha}\Psi_{\alpha} \quad \text{where} \quad H = \sum_{i=1}^{A} t_i + \sum_{i \leq j}^{A} v_{ij}.
$$

$$
\mathcal{H}\Phi_{\beta} = E_{\beta}\Phi_{\beta}
$$

$$
\Phi_{\beta} = P\Psi_{\beta}
$$

 P is a projection operator from S into S

$$
\langle \tilde{\Phi}_{\gamma} | \Phi_{\beta} \rangle = \delta_{\gamma \beta}
$$

$$
\mathcal{H} = \sum_{\beta \in \mathcal{S}} |\Phi_{\beta} \rangle E_{\beta} < \tilde{\Phi}_{\beta}
$$

- **NCSM** convergence test
	- Comparison to other methods

P. Navratil, INT Seminar, November 13, 2007, online

P. Navrátil and E. Caurier, Phys. Rev. C **69**, 014311 (2004)

II. Applications of the NCSM

H. Kamada, *et al.*, *Phys. Rev. C* 64, 044001 (2001)

PHYSICAL REVIEW C, VOLUME 64, 044001

Benchmark test calculation of a four-nucleon bound state

In the past, several efficient methods have been developed to solve the Schrödinger equation for fournucleon bound states accurately. These are the Faddeev-Yakubovsky, the coupled-rearrangement-channel Gaussian-basis variational, the stochastic variational, the hyperspherical variational, the Green's function Monte Carlo, the no-core shell model, and the effective interaction hyperspherical harmonic methods. In this article we compare the energy eigenvalue results and some wave function properties using the realistic AV8' NN interaction. The results of all schemes agree very well showing the high accuracy of our present ability to calculate the four-nucleon bound state.

H. Kamada, *et al.*, *Phys. Rev. C* 64, 044011 (2001)

Figure 2. NCSM and GFMC NN pair density in ⁴He.

Stetcu, Barrett, Navratil, Vary, Phys. Rev. C 71, 044325 (2005)

- small model space: expect larger renormalization
- large variation with the model space
- three-body forces: might be important, but not the issue
- $a \rightarrow A$ for fixed model space;
- $P \rightarrow \infty$ for fixed cluster.

Range dependence

Stetcu, Barrett, Navratil, Vary, Phys. Rev. C 71, 044325 (2005)

Longitudinal-longitudinal distribution function

$$
\rho_{LL}(q)=\frac{1}{4Z}\sum_{j\neq i}(1+\tau_z(i))(1+\tau_z(j))\langle g.s.|j_0(q|\vec{r_i}-\vec{r_j}|)|g.s. \rangle
$$

Stetcu, Barrett, Navratil, Vary, nucl-th/0601076

Model space independence at high momentum transfer: good renormalization at the two-body cluster level

PHYSICAL REVIEW C 79, 044606 (2009)

Ab initio many-body calculations of nucleon-nucleus scattering

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We develop a new *ab initio* many-body approach capable of describing simultaneously both bound and scattering states in light nuclei, by combining the resonating-group method with the use of realistic interactions, and a microscopic and consistent description of the nucleon clusters. This approach preserves translational symmetry and the Pauli principle. We outline technical details and present phase-shift results for neutron scattering on ³H, ⁴He, and ¹⁰Be and proton scattering on ^{3,4}He, using realistic nucleon-nucleon (NN) potentials. Our $A = 4$ scattering results are compared to earlier *ab initio* calculations. We find that the CD-Bonn NN potential in particular provides an excellent description of nucleon-⁴He S-wave phase shifts. In contrast, the experimental nucleon- 4 He P-wave phase shifts are not well reproduced by any NN potential we use. We demonstrate that a proper treatment of the coupling to the n -¹⁰Be continuum is successful in explaining the parity-inverted ground state in ¹¹Be.

DOI: 10.1103/PhysRevC.79.044606

PACS number(s): 21.60.De, 25.10. $+s$, 27.10. $+h$, 27.20. $+n$

S. Quaglioni and P. Navratil, Phys. Rev. Lett. 101, 092501 (2008)

long range (continuum)

PHYSICAL REVIEW C 81, 021301(R) (2010)

Ab initio nuclear structure simulations: The speculative ¹⁴F nucleus

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We present results from *ab initio* no-core full configuration simulations of the exotic proton-rich nucleus ¹⁴F, whose first experimental observation is expected soon. Calculations with the JISP16 NN interaction are performed up to the $N_{\text{max}} = 8$ basis space. The binding energy is evaluated using an extrapolation technique. This technique is generalized to excitation energies, verified in calculations of ⁶Li, and applied to ¹⁴F and ¹⁴B, the ¹⁴F mirror, for which some data are available.

DOI: 10.1103/PhysRevC.81.021301

PACS number(s): 21.60.De, 21.10.Dr, 27.20.+n

Origin of the Anomalous Long Lifetime of ¹⁴C

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We report the microscopic origins of the anomalously suppressed beta decay of ${}^{14}C$ to ${}^{14}N$ using the *ab initio* no-core shell model with the Hamiltonian from the chiral effective field theory including threenucleon force terms. The three-nucleon force induces unexpectedly large cancellations within the p shell between contributions to beta decay, which reduce the traditionally large contributions from the nucleonnucleon interactions by an order of magnitude, leading to the long lifetime of ¹⁴C.

DOI: 10.1103/PhysRevLett.106.202502

PACS numbers: 21.10.Tg, 21.60.De, 23.40 -s, 27.20.+n

 III. Extending the NCSM to Heavier Mass Nuclei

P. Navrátil, J. P. Vary and B. R. B., Phys. Rev. C 62, 054311 (2000)

 Beyond the No Core Shell Model 1. The ab initio Shell Model with a Core

- 2. Importance Truncation
- 3. The NCSM in an Effective Field Theory (EFT) Framework
- 4. MC-NCSM (U of Tokyo/Iowa State U)
- 5. Other approaches

1. The *ab initio* Shell Model with a Core

PHYSICAL REVIEW C 78, 044302 (2008)

Ab-initio shell model with a core

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We construct effective two- and three-body Hamiltonians for the p-shell by performing $12\hbar\Omega$ ab initio no-core shell model (NCSM) calculations for $A = 6$ and 7 nuclei and explicitly projecting the many-body Hamiltonians onto the $0\hbar\Omega$ space. We then separate these effective Hamiltonians into inert core, one- and two-body contributions (also three-body for $A = 7$) and analyze the systematic behavior of these different parts as a function of the mass number A and size of the NCSM basis space. The role of effective three- and higher-body interactions for $A > 6$ is investigated and discussed.

DOI: 10.1103/PhysRevC.78.044302

PACS number(s): 21.10 . Hw, 21.60 . Cs, 23.20 . Lv, $27.20 + n$

2-body Valence Cluster **approximation for A=6**

2-body Valence Cluster approximation for A=7

3-body Valence Cluster approximation for A>6

 P¹ + Q1 = P; P¹ Construct 3-body interaction in terms of 3-body matrix elements: Yes

$$
V_3^{A,7} = \mathcal{H}_{A,7}^{0,N_{\rm max}} - \mathcal{H}_{A,6}^{0,N_{\rm max}}\bigg]
$$

FIG. 9. Comparison of spectra for ⁸He, ⁹He, and ¹⁰He from SSM calculations using the effective 2BVC and 3BVC Hamiltonians and from exact NCSM calculation for $N_{\text{max}} = 6$ and $\hbar \Omega = 20$ MeV using the CD-Bonn interaction.

FIG. 6: The quadrupole moment of the ground state for ⁶Li $(1^+(T = 0))$ is shown in terms of one- and two-body contributions as a function of increasing model space size.

2. Importance Truncation

The idea of Importance Truncation

Formalism of Importance truncation.

• First order multi-configurational perturbation theory gives...

$$
|\Psi^{(1)}\rangle = -\sum_{\nu \notin \mathcal{M}_{ref}} \frac{\langle \Phi_{\nu} | W | \Psi_{ref} \rangle}{\epsilon_{\nu} - \epsilon_{ref}} | \Phi_{\nu} \rangle
$$

$$
= -\sum_{\nu \notin \mathcal{M}_{ref}} \frac{\langle \Phi_{\nu} | H | \Psi_{ref} \rangle}{\epsilon_{\nu} - \epsilon_{ref}} | \Phi_{\nu} \rangle.
$$

$$
W = H - H_0
$$

Importance truncation schematically

Corrections to the energy

• 2nd order perturbation theory gives you an estimate of the correction to the energy from the discarded state. The first order result is equal to zero.

$$
\Delta_{\text{excl}}(\kappa_{\text{min}}) = -\sum_{\nu \notin \mathcal{M}(\kappa_{\text{min}})} \frac{|\langle \Phi_{\nu} | H | \Psi_{\text{ref}} \rangle|^2}{\epsilon_{\nu} - \epsilon_{\text{ref}}}
$$

⁸He: IT started at N max = 6, final space Nmax = 8

Interaction: ⁸He SRG N3LO

3. The NCSM in an Effective Field Theory (EFT) Framework

Available online at www.sciencedirect.com

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www.elsevier.com/locate/physletb

No-core shell model in an effective-field-theory framework

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Abstract

We present a new approach to the construction of effective interactions suitable for many-body calculations by means of the no-core shell model (NCSM). We consider an effective field theory (EFT) with only nucleon fields directly in the NCSM model spaces. In leading order, we obtain the strengths of the three contact interactions from the condition that in each model space the experimental ground-state energies of ${}^{2}H$. ${}^{3}H$ and ${}^{4}He$ be exactly reproduced. The first $(0^+; 0)$ excited state of ⁴He and the ground state of ⁶Li are then obtained by means of NCSM calculations in several spaces and frequencies. After we remove the harmonic-oscillator frequency dependence, we predict for ⁴He an energy level for the first $(0^+;0)$ excited state in remarkable agreement with the experimental value. The corresponding ⁶Li binding energy is about 70% of the experimental value, consistent with the expansion parameter of the EFT.

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Effective interactions for light nuclei: an effective (field theory) approach

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Abstract

One of the central open problems in nuclear physics is the construction of effective interactions suitable for many-body calculations. We discuss a recently developed approach to this problem, where one starts with an effective field theory containing only fermion fields and formulated directly in a no-core shell-model space. We present applications to light nuclei and to systems of a few atoms in a harmonic-oscillator trap. Future applications and extensions, as well as challenges, are also considered.

Why $EFT + NCSM$?

EFT:

1. Captures the relevant degrees of freedom/symmetries

- 2. Builds in the correct long-range behavior
- 3. Has a systematic way for including the short-range behavior/order by order
- 4. Many-body and two-body interactions treated in the same framework
- 5. Explains naturally the hierarchy of the (many-body) forces

NCSM:

- 1. Flexible many-body method/easy to implement
- 2. Equivalent SD and Jacobi formulations
- 3. Can handle both NN and NNN interactions
- 4. In principle applies to any nucleus/extensions to heavier nuclei

Effective Field Theory (1/3)

i) Separation of scale:

 $M_{\text{QCD}} \sim 1$ GeV (mass of nucleon) $M_{\text{nucl}} \sim 100$ MeV (typical momentum in a nucleus) $M_{\text{struct}} \sim 10$ MeV (binding energy of a nucleon in a nucleus)

-> details of physics at short distance (high energy) are irrelevant for low energy physics.

-> in EFT low energy degrees of freedom are explicitly included (high momenta are integrated out).

ii) The Lagrangian / potential consistent with symmetries is expanded as a Taylor Series:

$$
V(\vec{p}', \vec{p}) = \sum_{i,j} C_{i,j} (\vec{p})^i (\vec{p}')^j
$$

Effective Field Theory (2/3)

iii) Regularization and renormalization:

-> cut-off Λ (separation between low and high energy physics)

$$
V(\vec{p}', \vec{p}) = \sum_{i,j} C_{i,j}(\Lambda)(\vec{p})^i (\vec{p}')^j
$$

-> no dependence on cut-off for observables (for a high enough cut-off), dependence absorbed by coupling constants (fitted with observables).

Effective Field Theory (3/3)

iv) Find the power counting ("truncation of the Taylor series"):

-> hierarchy between the different contributions

-> results improvable order by order (Leading Order, Next-to-Leading-Order, Next-to-Next-to-Leading-Order......)

Pionless EFT for nuclei within the NCSM: Without pions--> Breakdown momentum roughly 100 MeV/c

$$
H = \frac{1}{2m_N A} \sum_{[i < j]} (\vec{p}_i - \vec{p}_j)^2 + C_0^1 \sum_{[i < j]} \delta(\vec{r}_i - \vec{r}_j) + C_0^0 \sum_{[i < j]} \delta(\vec{r}_i - \vec{r}_j) + D_0 \sum_{[i < j < k]} \delta(\vec{r}_i - \vec{r}_j) \delta(\vec{r}_j - \vec{r}_k),
$$
\nt. al., 2007

Stetcu e

-> calculation at Leading order: two N-N contact interactions in the ${}^{3}S_{1}$ ¹S₀ channel and a threebody contact interaction in the 3nucleon $S_{1/2}$ channel

-> coupling constants fitted to the binding energy of the deuteron, triton and ⁴He

Difficulties:

fixing the couplings to few-body states is cumbersome HO: bound states only no immediate connection to the scattering observables

Question : How to construct an EFT within a bound many-body model space beyond Leading-Order?

Answer: by trapping nuclei in a harmonic potential

T. Busch, et al., Found. Phys. 28, 549 (1998)

$$
\frac{\Gamma\left(\frac{3}{4} - \frac{E}{2\hbar\omega}\right)}{\Gamma\left(\frac{1}{4} - \frac{E}{2\hbar\omega}\right)} = -\frac{bk}{2} \cot \delta
$$
\nenergy in the trap (bound state physics) phase shift (scattering physics)\n
\n
$$
k \cot \delta = -\frac{1}{a_2} + \frac{1}{2}r_2k^2 + \dots,
$$
\nEffective Range Expansion

J. Rotureau, ORNL, March 2011

3 nucleons at Leading-Order in the trap coupled to $J^{\pi} = \frac{3}{2}^{+}$

for a fixed two-body cutoff (N_2) , the size of the model space (N_a) is increased until convergence

-> convergence of energy as the two-body cutoff $N₂$ increases -> as expected no need for a three body force at Leading Order. J. Rotureau, ORNL, March 2011

SUMMARY

The NCSM is an *ab initio* method for calculating nuclear structure.

It has been applied to nuclei throughout the 0p-shell, where it has been able:

- a.) to predict new results, e.g., the spectrum of 14-F,
- b.) to explain previously non-understood observations, e.g., the lifetime of 14-C by including three nucleon forces,
- c.) to describe the binding energies, low-lying spectra and other observables for 0p-shell nuclei,
- d.) to serve as input for *ab initio* nuclear reaction calculations, *etc.*

But there are challenges and much else still to do.

SOME REMAINING CHALLENGES

- 1. Understanding the fundamental interactions among the nucleons in terms of QCD, e.g., NN, NNN,
- 2. Determination of the mean field (the monopole effect).
- 3. Microscopic calculations of medium- to heavy-mass nuclei:
	- a.) How to use the advances for light nuclei to develop techniques for heavier nuclei.
	- b.) Building in more correlations among the nucleons in small model spaces, e.g., effective interactions for heavier nuclei.
- 4. Further extensions of these microscopic advances for nuclear structure to nuclear reactions.

COLLABORATORS

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A. SchwenkWeinberg, van Kolck, Kaplan, Savage, Wise, Epelbaum, Meissner, Nogga, Machleidt,

- I. Forces among nucleons
- 1. QCD --> EFT --> CPT --> self-consistent nucleon interactions
- 2. Need NN and NNN and perhaps also NNNN interactions

P. Navratil and E. Caurier, Phys. Rev. C 69, 014311 (2004)

$$
H_{int} = \frac{1}{A} \sum_{i>j=1}^{A} \frac{(\vec{p}_i - \vec{p}_j)^2}{2m} + \sum_{i>j=1}^{A} V_{ij} + \sum_{i>j>k=1}^{A} V_{ijk} + \dots
$$

\n
$$
H = H_{int} + \frac{\vec{P}_{CM}^2}{2mA} + \frac{1}{2}mA\omega^2 \vec{R}_{CM}^2
$$

\n
$$
= \sum_{i=1}^{A} \left(\frac{p_i^2}{2m} + \frac{1}{2}m\omega^2 r_i^2\right) + \sum_{i
\n
$$
h_{12} = \frac{p_1^2}{2m} + \frac{1}{2}m\omega r_1^2 + \frac{p_2^2}{2m} + \frac{1}{2}m\omega r_2^2 + V_{12} - \frac{m\omega^2}{2A}(\vec{r}_1 - \vec{r}_2)^2
$$

\n
$$
h_{12} = h_{rel} + h_{CM}
$$

\nNCSM: unitary transformation h_{rel} Renormalization for trap $\Omega = \omega \sqrt{\frac{A-2}{A}}$
$$

I. Stetcu, TRIUMF, Feb. 2011

FOR TWO PARTICLES IN A T

Original motivation: to understand gross features of nuclear systems from a QCD perspective

At the heart of an effective theory: a truncation of the Hilbert space / all interactions allowed by symmetries are generated / power counting

$$
\frac{\Gamma(3/4 - \varepsilon/2)}{\Gamma(1/4 - \varepsilon/2)} = \frac{b}{2a_2}
$$

$$
\frac{\Gamma(3/4 - \varepsilon/2)}{\Gamma(1/4 - \varepsilon/2)} = -\frac{b}{2} \left(-\frac{1}{a_2} + \frac{r_2}{b^2} \varepsilon + \ldots \right)
$$

In finite model spaces:

$$
V_{LO}(\vec{p}, \vec{p}') = C_0
$$

\n
$$
V_{NLO}(\vec{p}, \vec{p}') = C_2(p^2 + p'^2)
$$

\n
$$
V_{N^2LO}(\vec{p}, \vec{p}') = C_4(p^2 + p'^2)^2
$$

 $C_0, C_2, C_4, ...$ Constants to be determined in each model space so that select observables are preserved

I. Stetcu, TRIUMF, Feb. 2011

RENORMALIZA

$$
\Psi(\vec{r}) = \sum_{n=0}^{N_{\text{max}}/2} A_n \varphi_n(\vec{r})
$$

RAPPED NUCLEONS

ν,

Triplet S NN phase shift

III. New Methods/Transformative Ideas (???)

- 1. "soft" NN interactions plus weak NNN interactions
- 2. Coupled Cluster calculations with NNN interactions
- 3. Universal Nuclear Energy Density Functional
- 4. Building more correlations into smaller model space: a) Fermionic Molecular Dynamics Approach (T. Neff, et al.) b) Extensions of the NCSM:
	- i) Projected NCSM/SSM
	- ii) Symplectic (3,R) NCSM (J. Draayer, et al.)
	- iii) Importance Truncated NCSM (Navratil and Roth)
	- iv) NCSM + Resonating Group Method (Navratil & Quaglioni)