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Nuclear structure and dynamics from chiral forces

Nuclear Theory in the Supercomputing Era – 2018 (NTSE-2018)

IBS Headquarters, Daejeon, Korea 29 October – 2 November 2018

Petr Navratil

TRIUMF

Collaborators: S. Quaglioni (LLNL), G. Hupin (Orsay), M. Vorabbi, A. Calci (TRIUMF), P. Gysbers (UBC/TRIUMF), M. Gennari (U Waterloo)



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- Nuclear structure and reactions from first principles
- New chiral NN N⁴LO + 3N
 - Beta decays of light nuclei in NCSM
 - Microscopic optical potentials from NCSM densities
- No-Core Shell Model with Continuum (NCSMC)
- N-⁴He scattering and polarized D+T fusion
- Structure of ⁷He
- ¹²N, ¹¹C(p,p) scattering and ¹¹C(p,γ)¹²N capture
 - Support of approved TRIUMF TUDA experiment

First principles or ab initio nuclear theory



First principles or *ab initio* nuclear theory – what we do at present



Ab initio

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- ♦ Degrees of freedom: Nucleons
- ♦ All nucleons are active
- ♦ Exact Pauli principle
- ♦ Realistic inter-nucleon interactions
 - ♦ Accurate description of NN (and 3N) data

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♦ Controllable approximations

Chiral Effective Field Theory

- 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_{χ})
 - Hierarchy
 - Consistency
 - Low energy constants (LEC)
 - Fitted to data
 - Can be calculated by lattice QCD

Λ_x~1 GeV : Chiral symmetry breaking scale



N³LO NN+N²LO 3N (NN+3N400, NN+3N500)

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N⁴LO500 NN + N²LO 3N

Currents in chiral EFT

Meson-exchange current



- weak axial current
 - one-body: LO Gamow-Teller

$$\boldsymbol{A}_{l} = -g_{A}\tau_{l}^{-}e^{-i\boldsymbol{q}\cdot\boldsymbol{r}_{l}}\left[\boldsymbol{\sigma}_{l} + \frac{2(\boldsymbol{\bar{p}}_{l}\boldsymbol{\sigma}_{l}\cdot\boldsymbol{\bar{p}}_{l} - \boldsymbol{\sigma}_{l}\boldsymbol{\bar{p}}_{l}^{2}) + i\boldsymbol{q}\times\boldsymbol{\bar{p}}_{l}}{4m_{N}^{2}}\right]$$

two-body: MEC

$$A_{12} = \frac{g_A}{2m_N f_\pi^2} \frac{1}{m_\pi^2 + k^2} \bigg[-\frac{i}{2} \tau_{\times} \boldsymbol{p}(\boldsymbol{\sigma}_1 - \boldsymbol{\sigma}_2) \cdot \boldsymbol{k} \\ + 4\hat{c}_3 \boldsymbol{k} \boldsymbol{k} \cdot (\tau_1^- \boldsymbol{\sigma}_1 + \tau_2^- \boldsymbol{\sigma}_2) + \left(\hat{c}_4 + \frac{1}{4}\right) \tau_{\times} \boldsymbol{k} \times [\boldsymbol{\sigma}_{\times} \times \boldsymbol{k}] \bigg] \\ + \frac{g_A}{m_N f_\pi^2} [2\hat{d}_1(\tau_1^- \boldsymbol{\sigma}_1 + \tau_2^- \boldsymbol{\sigma}_2) + \hat{d}_2 \tau_{\times}^a \boldsymbol{\sigma}_{\times}],$$



From QCD to nuclei



Conceptually simplest ab initio method: No-Core Shell Model (NCSM)

- 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

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

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





| | Progress in Particle and Nuclear Physics 69 (2013) 131-181 | |
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Review Ab initio no core shell model Bruce R. Barrett ^a, Petr Navrátil ^b, James P. Vary^{c,*}



³H and ⁴He with chiral EFT interactions up to N⁴LO

$^{3}H \rightarrow ^{3}He \beta decay$

$$\hat{O} = GT^{(1)} + MEC^{(2)} \rightarrow \hat{O}_{\alpha} = GT^{(1)} + GT^{(2)}_{\alpha} + MEC^{(2)}_{\alpha} + \dots$$

Operator:

Gamow-Teller (1-body) + chiral meson exchange current (2-body) Park (2003)

Potential: "N⁴LO NN"

- chiral NN @ N⁴LO, Machleidt PRC96 (2017), 500MeV cutoff
- LEC $c_D = -1.8$ determined



Original EM 2003 N³LO NN c_D=+0.8

(3N repulsive)



Applications to β decays in p-shell nuclei and beyond

- Does inclusion of the MEC explain g_A quenching?
- In light nuclei correlations present in *ab initio* (NCSM) wave functions explain almost all of the quenching compared to the standard shell model
 - MEC inclusion overall improves agreement with experiment
- The effect of the MEC inclusion is greater in heavier nuclei
- SRG evolved matrix elements used in coupled-cluster and IM-SRG calculations (up to ¹⁰⁰Sn)



P. Gysbers et al., "Quenching puzzle of beta decays," submitted.

Hollow symbols – GT Filled symbols – GT+MEC Both Hamiltonian and operators SRG evolved Hamiltonian and current consistent parameters



Microscopic optical potentials derived from *ab initio* translationally invariant nonlocal one-body densities

Microscopic optical potentials from NCSM densities

Michael Gennari[®] University of Waterloo, 200 University Avenue West Waterloo, Ontario N2L 3G1, Canada and TRIUMF, 4004 Wesbrook Mall, Vancouver, British Columbia V6T 2A3, Canada 14

Matteo Vorabbi,[†] Angelo Calci, and Petr Navrátil[‡] TRIUMF, 4004 Wesbrook Mall, Vancouver, British Columbia V6T 2A3, Canada

- Translationally-invariant non-local densities from NCSM calculations with chiral NN N⁴LO + 3N N²LO interactions
- High-energy proton-nucleus scattering with microscopic optical potentials from chiral N⁴LO NN interaction and NCSM densities



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Nuclear kinetic density from NCSM wave functions

- DFT calculations include kinetic density
 - Might contain center-of-mass contamination
- Can be calculated for light nuclei in NCSM
 - Translationally invariant





$$\tau_{\mathcal{N}}(\vec{r}) = \left[\vec{\nabla} \cdot \vec{\nabla}' \rho_{\mathcal{N}}(\vec{r}, \vec{r}')\right]_{\vec{r}=\vec{r}'}$$

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$$\tau_{\mathcal{N}}(\vec{r}) = \left[\vec{\nabla} \cdot \vec{\nabla}' \rho_{\mathcal{N}}(\vec{r}, \vec{r}')\right]_{\vec{r}=\vec{r}'}$$



| Nucleus | $N_{\rm max}$ | $\langle T_{int} \rangle$ | $\langle T_{wiCOM} \rangle$ | $\langle T_{DFT} \rangle$ |
|-------------------|---------------|---------------------------|-----------------------------|---------------------------|
| ⁴ He | 14 | 51.91 | 66.91 | 50.18 |
| ⁶ He | 12 | 78.26 | 93.26 | 77.72 |
| ⁸ He | 10 | 116.30 | 131.30 | 114.89 |
| $^{12}\mathrm{C}$ | 8 IT | 219.84 | 234.84 | 215.27 |
| ¹⁶ O | 8 IT | 301.69 | 316.69 | 296.90 |



Extending no-core shell model beyond bound states

Include more many nucleon correlations... $N_{\underline{\mathrm{max}}}$ $\Psi^A =$ $c_{Ni} \Phi^A_{Ni}$ NCSM N=0 i +(A-a)(a) $I_{A-a,a}$ + $\left(a_{2\mu}\right)$ $\vec{r}_{\mu 1}$ $a_{1\mu} + a_{2\mu} + a_{3\mu} = A$



...using the Resonating Group Method (RGM) ideas

• • •

+

 $(a_{1\mu})$

 $r_{\mu 2}$

 $\left(a_{3\mu}\right)$

Unified approach to bound & continuum states; to nuclear structure & reactions

- No-core shell model (NCSM)
 - A-nucleon wave function expansion in the harmonicoscillator (HO) basis
 - short- and medium range correlations
 - Bound-states, narrow resonances
- NCSM with Resonating Group Method (NCSM/RGM)
 - cluster expansion, clusters described by NCSM
 - proper asymptotic behavior
 - Iong-range correlations
- Most efficient: ab initio no-core shell model with continuum (NCSMC)



NCSM/RGM



Binary cluster basis



• Working in partial waves ($v = \{A - a \alpha_1 I_1^{\pi_1} T_1; a \alpha_2 I_2^{\pi_2} T_2; s\ell\}$)

$$\left|\psi^{J^{\pi}T}\right\rangle = \sum_{\nu} \hat{A}_{\nu} \left[\left(\left| A - a \; \alpha_{1} I_{1}^{\pi_{1}} T_{1} \right\rangle \left| a \; \alpha_{2} I_{2}^{\pi_{2}} T_{2} \right\rangle \right)^{(sT)} Y_{\ell}(\hat{r}_{A-a,a}) \right]^{(J^{\pi}T)} \frac{g_{\nu}^{J^{\pi}T}(r_{A-a,a})}{r_{A-a,a}}$$
Target
Projectile

• Introduce a dummy variable \vec{r} with the help of the delta function

$$\psi^{J^{\pi}T} \rangle = \sum_{v} \int \frac{g_{v}^{J^{\pi}T}(r)}{r} \hat{A}_{v} \left[\left(\left| A - a \, \alpha_{1} I_{1}^{\pi_{1}} T_{1} \right\rangle \right| a \, \alpha_{2} I_{2}^{\pi_{2}} T_{2} \right) \right]^{(sT)} Y_{\ell}(\hat{r}) \right]^{(J^{\pi}T)} \delta(\vec{r} - \vec{r}_{A-a,a}) \, r^{2} dr \, d\hat{r}$$

Allows to bring the wave function of the relative motion in front of the antisymmetrizer

$$\sum_{v} \int d\vec{r} \, \gamma_{v}(\vec{r}) \, \hat{A}_{v} \bigg| \underbrace{\overset{\vec{r}}{\overset{\mathbf{a}}{\Rightarrow}}}_{(A-a)} (a), v \bigg\rangle$$

Coupled NCSMC equations

$$H \Psi^{(A)} = E \Psi^{(A)} \qquad \Psi^{(A)} = \sum_{\lambda} c_{\lambda} [A] \otimes A + \sum_{\nu} \int d\vec{r} \gamma_{\nu}(\vec{r}) \hat{A}_{\nu} \Big|_{(A-a)}^{\vec{r}} \otimes A \Big|_{(A-a)}^{\vec{r}}$$

Solved by Microscopic R-matrix theory on a Lagrange mesh – efficient for coupled channels

Computational aspects of NCSMC

- NN matrix elements
 - Choice of various potentials chiral N³LO, LO-N⁴LO...
 - SRG (also for one and two-body operators)
 - Transformation to s.p. basis (up to N_{12max}~30)
 - ncsmv2b Fortran90 with OpenMP
- 3N matrix elements
 - Choice of various NN (chiral N³LO, LO-N⁴LO) and 3N (N²LO with local or local/non-local regulators, N⁴LO contacts) potentials
 - SRG (also for one, two- and three-body operators)
 - Transformation to s.p. basis (up to N_{123max}~17)
 - manyeff, v3trans (op3trans) Fortran90 with OpenMP
- NCSM diagonalization
 - NN, NN+3N or NN+3N(NO2b) interactions
 - Calculations of N_{max} sequence (0(1),2(3),...Nmax)
 - Importance truncation
 - ncsd Lanczosh algorithm, bit operations, hashing, partial or full storing of non-zero matrix elements, Fortran 90 with MPI, ~12,000 MPI tasks
- Transition densities and/or RGM and coupling kernels
 - One- and two-body transition densities for wave functions of the same or different nuclei (three- and four-body for A=3,4 nuclei)
 - Coordinate space local and nonlocal translationally invariant one-body densities
 - RGM and coupling kernel calculation for the NCSMC (including the 3N interaction)
 - Normal ordering of 3N interaction
 - trdens bit operations, hashing, Fortran90 with MPI, ~8,000 MPI tasks
- NCSMC calculation
 - RGM and coupling kernels either input or calculated from densities
 - Solves NCSMC coupled equations, calculates the S-matrix and scattering/reaction observables
 - ncsmc Fortran90 with OpenMP and MPI

n-⁴He scattering within NCSMC









n-⁴He scattering within NCSMC

n-⁴He scattering phase-shifts for chiral NN and NN+3N500 potential

Total *n*-⁴He cross section with NN and NN+3N potentials





3N force enhances 1/2⁻ ←→ 3/2⁻ splitting: Essential at low energies!

⁴He

PHYSICAL REVIEW C 88, 054622 (2013)

Ab initio many-body calculations of nucleon-⁴He scattering with three-nucleon forces Guillaume Hupin,^{1,*} Joachim Langhammer,^{2,†} Petr Navrátil,^{3,‡} Sofia Quaglioni,^{1,§} Angelo Calci,^{2,∥} and Robert Roth^{2,¶}
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 Physics Gorge

 Phys. Bio 10 (2016) (2020) (2016)
 Invited Comment

 Unified ab initio approaches to nuclear structure and reactions

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

p-⁴He scattering within NCSMC





PHYSICAL REVIEW C 90, 061601(R) (2014)

Predictive theory for elastic scattering and recoil of protons from ⁴He

Guillaume Hupin,^{1,*} Sofia Quaglioni,^{1,†} and Petr Navrátil^{2,‡}

Predictive power in the 3/2⁻ resonance region: Applications to material science

Deuterium-Tritium fusion

- The $d+^{3}H \rightarrow n+^{4}He$ reaction
 - The most promising for the production of fusion energy in the near future
 - Used to achieve inertial-confinement (laser-induced) fusion at NIF, and magnetic-confinement fusion at ITER
 - With its mirror reaction, ${}^{3}\text{He}(d,p){}^{4}\text{He}$, important for Big Bang nucleosynthesis







n-⁴He scattering and ³H+d fusion within NCSMC





FY: Faddeev-Yakubovsky method - Rimantas Lazauskas

The d-³H fusion takes place through a transition of d+³H is *S*-wave to n+⁴He in *D*-wave: Importance of the **tensor and 3N force**



 $S(E) = E\sigma(E) \exp[2\pi\eta(E)]$ $\eta(E) = Z_{A-a}Z_a e^2 / \hbar v_{A-a,a}$





 $S(E) = E\sigma(E) \exp[2\pi\eta(E)]$ $\eta(E) = Z_{A-a}Z_a e^2 / \hbar v_{A-a,a}$

Ab initio predictions for polarized DT thermonuclear fusion

31

Nature Communications (accepted); arXiv:1803.11378 Guillaume Hupin^{1,2,3}, Sofia Quaglioni³ and Petr Navrátil⁴

³H(d,n)⁴He with chiral NN+3N500 interaction

 2.10^{1}

 5.10^{0}

 2.10^{0}

 5.10^{-1}

 10^{-}

 5.10^{-1}

 10^{-}

 5.10°

 10^{-3}

 5.10^{-4}

 10^{-1}

 $\frac{\partial \sigma}{\partial \theta} \left[\mathrm{b.sr}^{-1} \right]$

 5.10^{0}

AR52, CO52, AR54 KO66, JA84, BR87

NCSMC - pheno

 2.10^{1}

 5.10^{-2} 10^{-1}

 5.10^{1}

 $E_{\rm c.m.}$ [keV]

 10^{2}

VCSMC – pheno

 5.10^{-1}

 10^{0}

NCSMC

 $E_{\rm c.m.}$ [MeV]

NCSMC 10¹

S-factor [b.MeV]



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AR52, CO52, AR54 KO66, JA84, BR87

NCSMC - pheno

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 5.10^{1}

NCSMC

 $E_{\rm c.m.}$ [MeV]

 $E_{\rm c.m.}$ [keV]

NCSMC 10¹

S-factor [b.MeV]



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



r

 6 He + n

⁶He

Experimental controversy: Existence of low-lying 1/2⁻ state ... not seen in these calculations 33

⁷He unbound

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

p+¹¹C scattering and ${}^{11}C(p,\gamma){}^{12}N$ capture

¹¹C(p,γ)¹²N capture relevant in hot *p*-*p* chain: Link between pp chain and the CNO cycle - bypass of slow triple alpha capture ⁴He(αα,γ)¹²C



 ${}^{3}He(\alpha,\gamma){}^{7}Be(\alpha,\gamma){}^{11}C(p,\gamma){}^{12}N(p,\gamma){}^{13}O(\beta^{+},\nu){}^{13}N(p,\gamma){}^{14}O(\beta^{+},\nu){}^{14}$

 ${}^{3}He(\alpha,\gamma){}^{7}Be(\alpha,\gamma){}^{11}C(p,\gamma){}^{12}N(\beta^{+},\nu){}^{12}C(p,\gamma){}^{13}N(p,\gamma){}^{14}O$ ${}^{11}C(\beta^{+}\nu){}^{11}B(p,\alpha){}^{8}Be({}^{4}He,{}^{4}He)$

p+¹¹C scattering and ¹¹C(p,γ)¹²N capture

- Measurement of ¹¹C(p,p) resonance scattering planned at TRIUMF
 - TUDA facility
 - ¹¹C beam of sufficient intensity produced
 - Experiment approved with high priority
- NCSMC calculations of ¹¹C(p,p) with chiral NN+3N under way
- Obtained wave functions will be used to calculate ¹¹C(p,γ)¹²N capture relevant for astrophysics

p+¹¹C scattering and ${}^{11}C(p,\gamma){}^{12}N$ capture

NCSMC calculations of ¹¹C(p,p) with chiral NN+3N under way

- ¹¹C: 3/2⁻, 1/2⁻, 5/2⁻, 3/2⁻ NCSM eigenstates
- ¹²N: $\geq 6 \pi = +1$ and $\geq 4 \pi = -1$ NCSM eigenstates





NCSMC calculations to be validated by measured cross sections and applied to calculate the ${}^{11}C(p,\gamma){}^{12}N$ capture

$p+^{11}C$ scattering and $^{11}C(p,\gamma)^{12}N$ capture

NCSMC calculations of ¹¹C(p,p) with chiral NN+3N under way

- ¹¹C: 3/2⁻, 1/2⁻, 5/2⁻, 3/2⁻ NCSM eigenstates
- ¹²N: $\geq 6 \pi = +1$ and $\geq 4 \pi = -1$ NCSM eigenstates





NCSMC calculations to be validated by measured cross sections and applied to calculate the ${}^{11}C(p,\gamma){}^{12}N$ capture

Conclusions

- Ab initio calculations of nuclear structure and reactions with predictive power becoming feasible beyond the lightest nuclei
- Ab initio structure calculations can even reach (selected) medium
 & medium-heavy mass nuclei
- These calculations make connections between the low-energy QCD, many-body systems, and nuclear astrophysics

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Thank you! <mark>Merci!</mark> 고맙습니다

