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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

Calculations with chiral forces in no-core shell model with continuum

RIBF ULIC Symposium on Perspective in Isospin Physics

 Role of non-central interactions in structure and dynamics of unstable nuclei ~
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Connection

to

Astrophysics

Outline

Ab initio calculations of nuclear structure and reactions



Connection to QCD

- Chiral forces
- No-core shell model, NCSM/RGM
 - Neutron rich He isotopes, N-⁴He scattering, ¹²C structure
- No-core shell model with continuum (NCSMC):
 - Unbound ⁷He



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

Determination of NNN constants 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



No-core shell model combined with the resonating group method (NCSM/RGM)

- **The NCSM:** An approach to the solution of the *A*-nucleon bound-state problem
 - Accurate nuclear Hamiltonian
 - Finite harmonic oscillator (HO) basis
 - Complete $N_{max} \hbar \Omega$ model space
 - Effective interaction due to the model space truncation
 - Similarity-Renormalization-Group evolved NN(+NNN) potential
 - Short & medium range correlations
 - No continuum

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$$\Psi^{A} = \sum_{N=0}^{N_{\text{max}}} \sum_{i} c_{Ni} \Phi^{A}_{Ni}$$

- **The RGM:** A microscopic approach to the A-nucleon scattering of clusters
 - Long range correlations, relative motion of clusters

$$\Psi^{(A)} = \sum_{\nu} \int d\vec{r} \, \varphi_{\nu}(\vec{r}) \, \hat{\mathcal{A}} \, \Phi^{(A-a,a)}_{\nu \vec{r}}$$

Ab initio NCSM/RGM: Combines the best of both approaches Accurate nuclear Hamiltonian, consistent cluster wave functions Correct asymptotic expansion, Pauli principle and translational invariance

⁴He from chiral EFT interactions: g.s. energy convergence

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The ab initio NCSM/RGM in a snapshot

• Ansatz: $\Psi^{(A)} = \sum_{ij} \int d\vec{r} \phi_{\nu}(\vec{r}) \hat{\mathcal{A}} \Phi^{(A-a,a)}_{\nu \vec{r}}$

Many-body Schrödinger equation:

NNN interaction effects in neutron rich nuclei: He isotopes

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⁸He

A=3 binding energy & half life constraint

c_D=-0.2, c_E=-0.205, Λ=500 MeV

- 3N matrix elements in coupled-J single-particle basis:
 - Introduced and implemented by Robert Roth et al.
 - Now also in my codes: Jacobi-Slater-Determinant transformation & NCSD code
 - Example: ⁶He, ⁸He NCSM calculations up to N_{max} =10 done with moderate resources

3N interaction effects in neutron rich nuclei: He isotopes

- ⁶He and ⁸He with SRG-evolved chiral N³LO NN + N²LO 3N
 - chiral N³LO NN: ⁴He underbound, ⁶He and ⁸He unbound
 - chiral N³LO NN + N²LO 3N(500): ⁴He OK, both ⁶He and ⁸He bound

A=3 binding energy & half life constraint $c_{\rm D}$ =-0.2, $c_{\rm E}$ =-0.205, Λ =500 MeV

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NNN interaction important to bind neutron rich nuclei

3N interaction effects in neutron rich nuclei: He isotopes

- ⁶He and ⁸He with SRG-evolved chiral N³LO NN + N²LO 3N
 - chiral N³LO NN: ⁴He underbound, ⁶He and ⁸He unbound
 - chiral N³LO NN + N²LO 3N(400): ⁴He fitted, ⁶He barely unbound, ⁸He unbound
 - describes quite well binding energies of ¹²C, ¹⁶O, ⁴⁰Ca, ⁴⁸Ca
 - chiral N³LO NN + N²LO 3N(500): ⁴He OK, both ⁶He and ⁸He bound
 - does well up to A=10, overbinds ¹²C, ¹⁶O, Ca isotopes
 - SRG-N³LO NN Λ=2.02 fm⁻¹: ⁴He OK, both ⁶He and ⁸He bound
 - ¹⁶O, Ca strongly overbound

⁴He binding energy & ³H half life constraint $c_{\rm D}$ =-0.2, $c_{\rm E}$ =+0.098, Λ =400 MeV

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A=3 binding energy & half life constraint $c_{\rm D}$ =-0.2, $c_{\rm E}$ =-0.205, Λ =500 MeV

NNN interaction important to bind neutron rich nuclei

Our knowledge of the 3N interaction is incomplete

По N-4 He scattering with NN+NNN interactions

G. Hupin, J. Langhammer, S. Quaglioni, P. Navratil, R. Roth, work in progress

⁴He(*n*,*n*)⁴He phase shifts

⁴He(*n*,*n*)⁴He phase shifts

Here:

 $n + {}^{4}\text{He}(g.s.)$, SRG-(N³LO *NN* + N²LO NNN) potential with (λ =2 fm⁻¹). Convergence with respect to HO basis size (N_{max})

Largest splitting between *P* waves obtained with NN+NNN. Need ⁴He exited states and study with respect to SRG λ

Neutron rich Carbon isotopes from chiral NN+NNN interactions (IT-NCSM, R. Roth *et al*.)

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M1 transitions in ¹²C sensitive to 3N interaction

Chiral 3N interaction changes occupations of the $p_{3/2}$ and $p_{1/2}$ orbits ("increases the gap" between them) Enhances the M1 transition from the g.s. to 1⁺ 1 state

Similar increase of the Gamow-Teller transition between g.s. of ¹²B(¹²N) and ¹²C

Tensor correlations and 3N effects in ground states of ⁴He and ¹²C

- Tensor correlations related to $\langle \vec{S}_p \cdot \vec{S}_n \rangle$ and $\langle \vec{S}_p \cdot \vec{S}_p + \vec{S}_n \cdot \vec{S}_n \rangle$ $- \vec{S}_p = \frac{1}{2} \sum_{i=1}^{A} (\frac{1}{2} + t_{z,i}) \vec{\sigma}_i$, $\vec{S}_n = \frac{1}{2} \sum_{i=1}^{A} (\frac{1}{2} - t_{z,i}) \vec{\sigma}_i$... spin operators
- Experiment: Atsushi Tamii et al.
- Ab initio NCSM:

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- ¹²C N_{max} =6 only

	$\left\langle \vec{S}_p \cdot \vec{S}_p + \vec{S}_n \cdot \vec{S}_n \right\rangle$	$\left< ec{S}_p \cdot ec{S}_n \right>$	$\left< ec{S}^2 \right>$
⁴ He Minnesota NN	0.04	-0.02	0
⁴ He chiral NN	0.19	0.04	0.27
⁴ He chiral NN+3N(500)	0.22	0.05	0.32
¹² C chiral NN	0.50	0.065	0.63
¹² C chiral NN+3N(400)	0.68	0.061	0.80
¹² C chiral NN+3N(500)	1.01	0.065	1.14

¹²C: chiral NN+3N(400) the best agreement with experiment

New developments: NCSM with continuum

NCSM.

 $\left|\Psi_{A}^{J^{\pi}T}\right\rangle = \sum_{Ni} c_{Ni} \left|ANiJ^{\pi}T\right\rangle$

New developments: NCSM with continuum

New developments: NCSM with continuum

NCSMC formalism

Start from

NCSM sector:

NCSM/RGM sector:

Coupling:

$$\begin{aligned} H_{NCSM} \quad \frac{\bar{h}}{\bar{\mathcal{H}}} \end{pmatrix} \begin{pmatrix} c \\ \chi \end{pmatrix} &= E \begin{pmatrix} 1 & \bar{g} \\ \bar{g} & 1 \end{pmatrix} \begin{pmatrix} c \\ \chi \end{pmatrix} \\ (H_{NCSM})_{\lambda\lambda'} &= \langle A\lambda J^{\pi}T | \hat{H} | A\lambda' J^{\pi}T \rangle = \varepsilon_{\lambda}^{J^{\pi}T} \delta_{\lambda\lambda'} \\ \overline{\mathcal{H}}_{\nu\nu'}(r,r') &= \sum_{\mu\mu'} \int \int dy dy' y^2 y'^2 \mathcal{N}_{\nu\mu}^{-\frac{1}{2}}(r,y) \mathcal{H}_{\mu\mu'}(y,y') \mathcal{N}_{\mu'\nu'}^{-\frac{1}{2}}(y'(\mathbf{r}')) \\ \bar{g}_{\lambda\nu}(r) &= \sum_{\nu'} \int dr' r'^2 \langle A\lambda J^{\pi}T | \hat{\mathcal{A}}_{\nu'} \Phi_{\nu'r'}^{J^{\pi}T} \rangle \ \mathcal{N}_{\nu'\nu}^{-\frac{1}{2}}(r',r) \\ \bar{h}_{\lambda\nu}(r) &= \sum_{\nu'} \int dr' r'^2 \langle A\lambda J^{\pi}T | \hat{H} \hat{\mathcal{A}}_{\nu'} | \Phi_{\nu'r'}^{J^{\pi}T} \rangle \ \mathcal{N}_{\nu'\nu}^{-\frac{1}{2}}(r',r) \end{aligned}$$

Orthogonalization: $N_{\nu r \nu' r'}^{\lambda \lambda'} = \begin{pmatrix} \delta_{\lambda \lambda'} & \bar{g}_{\lambda \nu'}(r') \\ \bar{g}_{\lambda' \nu}(r) & \delta_{\nu \nu'} \frac{\delta(r-r')}{rr'} \end{pmatrix} \quad \overline{H} = N^{-\frac{1}{2}} \begin{pmatrix} H_{NCSM} & \bar{h} \\ \bar{h} & \overline{\mathcal{H}} \end{pmatrix} N^{-\frac{1}{2}} \quad \begin{pmatrix} \bar{c} \\ \bar{\chi} \end{pmatrix} = N^{+\frac{1}{2}} \begin{pmatrix} c \\ \chi \end{pmatrix}$

Solve with generalized microscopic R-matrix

$$(\hat{\overline{H}} + \hat{L} - E) \begin{pmatrix} \bar{c} \\ \bar{\chi} \end{pmatrix} = \hat{L} \begin{pmatrix} \bar{c} \\ \bar{\chi} \end{pmatrix}$$

Bloch operator $\longrightarrow \hat{L}_{\nu} = \begin{pmatrix} 0 & 0 \\ 0 & \frac{1}{2}\delta(r-a)(\frac{d}{dr} - \frac{B_{\nu}}{r}) \end{pmatrix}$

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NCSM calculations of ⁶He and ⁷He energies

- N_{max} convergence OK
- Extrapolation feasible
 - ⁶He: E_{as}=-29.25(15) MeV (Expt. -29.269 MeV)
 - ⁷He: E_{as}=-28.27(25) MeV (Expt. -28.82(30) MeV)
- ⁷He unbound (+0.44(3) MeV), width 0.16(3) MeV
 - NCSM: no information about the width
- All ⁶He excited states above 2⁺₁ broad resonances or states in continuum 19

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

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

⁷He: NCSMC vs. NCSM/RGM vs. NCSM

Preliminary

J^{π}	experiment			NCSMC		NCSM/RGM		NCSM
	Ε	Γ	Ref.	Ε	Γ	Ε	Γ	Е
$3/2^{-}$	0.44(3)	0.16(3)	[29]	0.75	0.31	1.42	0.52	1.30
$5/2^{-}$	3.36(10)	2.2(3)	[30]	3.69	2.57	4.58	3.06	4.56
$1/2^{-}$	3.98	10	[42]	4.01	15.15	4.96	14.95	3.26
	3.48	2	[38]					

- NCSMC and NSCM/RGM energies from phase shifts at 90 degrees
- NCSMC and NSCM/RGM widths from the derivatives of phase shifts (preliminary)

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

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

Three-cluster NCSM/RGM

• Solves:

$$\sum_{a_2a_3vK} \int d\rho \ \rho^5 \Big[H_{a'v',av}^{K',K}(\rho',\rho) - E \ N_{a'v',av}^{K',K}(\rho',\rho) \Big] \ \rho^{-5/2} \chi_{vK}^{(A-a_{23},a_2,a_3)}(\rho) = 0$$

Where the hyperspherical coordinates are given by:

$$\rho = \sqrt{x^2 + y^2}, \quad \alpha = \arctan\left(\frac{y}{x}\right) \qquad \left(x = \rho \cos \alpha, \quad y = \rho \sin \alpha\right)$$

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First results for ⁶He ground state

S. Quaglioni, C. Romero-Redondo, P. Navratil, work in progress

- Preliminary NCSM/RGM results for up to N_{max} = 8 model space (hΩ=16 MeV)
 - $n+n+^{4}He(g.s.)$
 - SRG-NN chiral with λ =2.02 fm⁻¹
- Results compared with NCSM: Gain in binding due to the coupling to continuum
 - At N_{max}=8 ⁶He unbound within the NCSM, bound in the three-cluster NCSM/RGM by ~1 MeV
 - Extrapolated NCSM beyond N_{max}=12:
 ⁶He bound by ~ 1MeV

Structure of the exotic ⁹He nucleus

Conclusions and Outlook

- With the NCSM/RGM approach we are extending the *ab initio* effort to describe low-energy reactions and weakly-bound systems
- The first ${}^{7}Be(p,\gamma){}^{8}B$ ab initio S-factor calculation

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- Deuteron-projectile results with SRG-N³LO *NN* potentials:
 - d-⁴He scattering
 - First *ab initio* study of ${}^{3}H(d,n){}^{4}He \& {}^{3}He(d,p){}^{4}He$ fusion
- Under way:

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- *n*-⁸He scattering and ⁹He structure
- ³He-⁴He and ³He-³He scattering calculations
- Ab initio NCSM with continuum (NCSMC)
- Three-cluster NCSM/RGM and treatment of three-body continuum
- Inclusion of NNN force
- To do:
 - Alpha clustering: ⁴He projectile

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