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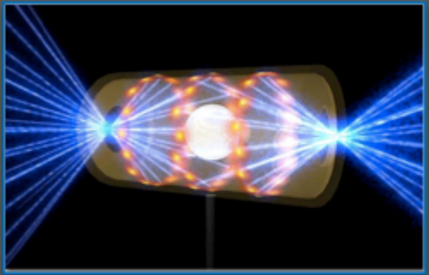
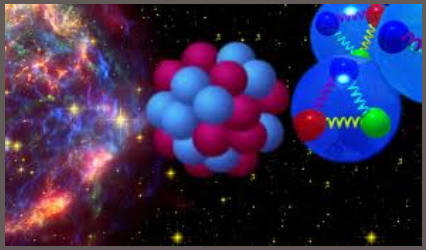
Canada's national laboratory for particle and nuclear physics
Laboratoire national canadien pour la recherche en physique nucléaire et en physique des particules

Ab initio calculations of nuclear structure and reactions

The 22nd European Conference on Few-Body Problems in Physics
Kraków, Poland,
9 - 13 September 2013

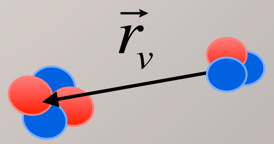
Petr Navratil | TRIUMF





Outline

- *Ab initio* nuclear structure and reaction methods
  - Exact few-body calculations
  - GFMC
  - Nuclear Lattice
  - CCM
  - In-medium SRG
  - SCGF
- No-core shell model
- Including the continuum with the resonating group method
  - NCSM/RGM
  - NCSMC
- Outlook



Ab initio Nuclear Structure & Reaction approaches

Ab initio

- ✧ All nucleons are active
- ✧ Exact Pauli principle
- ✧ Realistic inter-nucleon interactions
  - ✧ Accurate description of NN (and 3N) data
- ✧ Controllable approximations

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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_χ)
  - Hierarchy
  - Consistency
  - Low energy constants (LEC)
    - Fitted to data
    - Can be calculated by lattice QCD

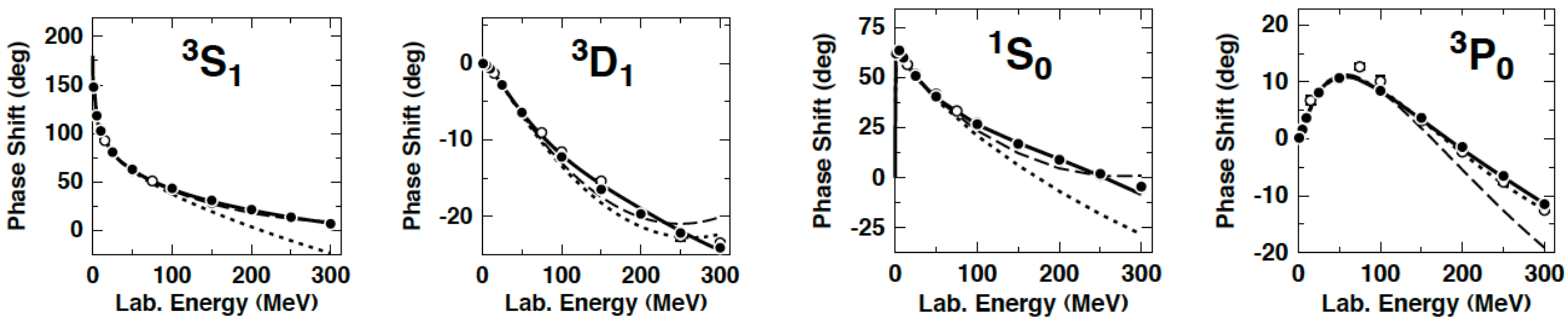
Λ_χ~1 GeV :
Chiral symmetry breaking scale

The NN interaction from chiral EFT

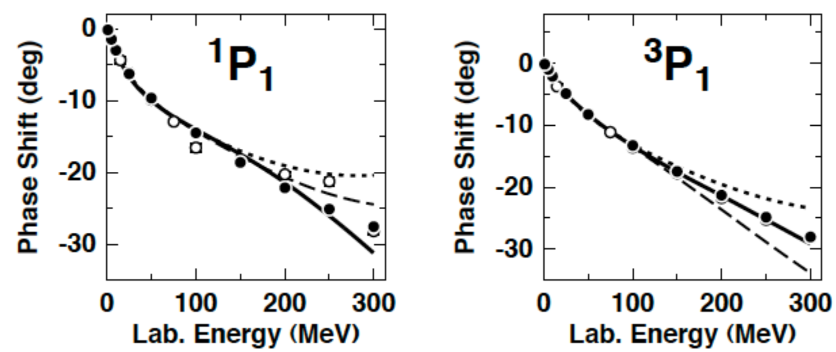
PHYSICAL REVIEW C **68**, 041001(R) (2003)

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

D. R. Entem[1,2,*] and R. Machleidt[1,†]



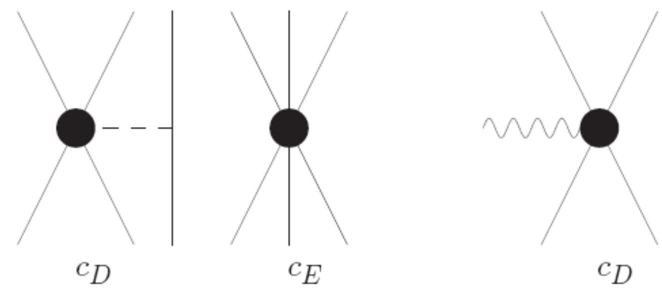
- 24 LECs fitted to the *np* scattering data and the deuteron properties
  - Including c_i LECs (i=1-4) from pion-nucleon Lagrangian

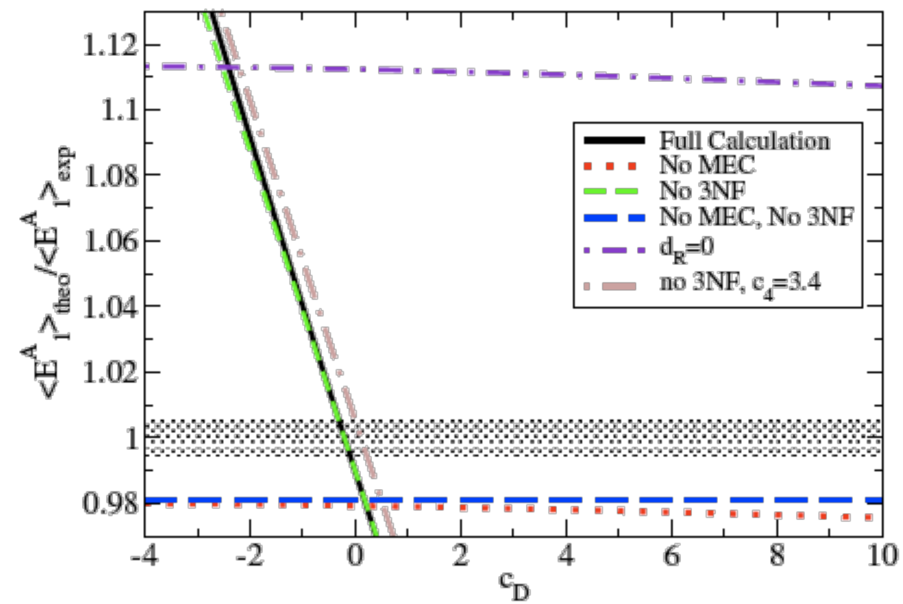


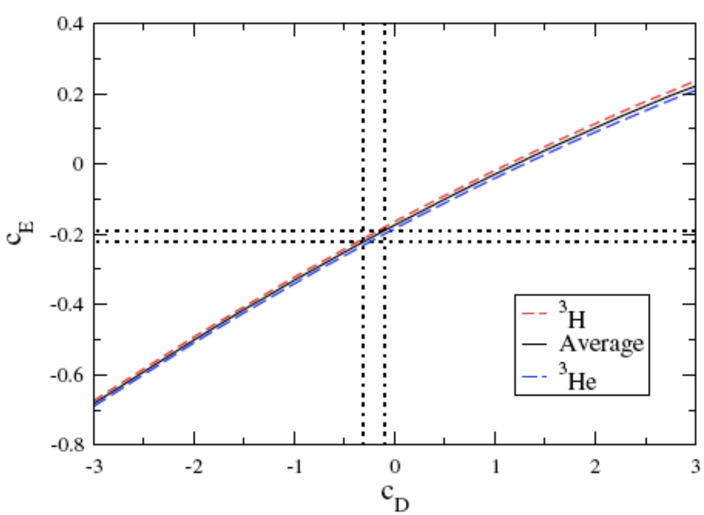
Determination of NNN LECs c_D and c_E from the triton binding energy and the half life

- **Chiral EFT**: c_D also in the two-nucleon contact vertex with an external probe
- Calculate $\langle E_1^A \rangle = |\langle {}^3\mathrm{He} \| E_1^A \| {}^3\mathrm{H} \rangle|$
  - Leading order GT
  - N^2LO: one-pion exchange plus contact
- A=3 binding energy constraint:

c_D=-0.2±0.1 c_E =-0.205±0.015







PRL **103**, 102502 (2009) PHYSICAL REVIEW LETTERS week ending 4 SEPTEMBER 2009

Three-Nucleon Low-Energy Constants from the Consistency of Interactions and Currents in Chiral Effective Field Theory

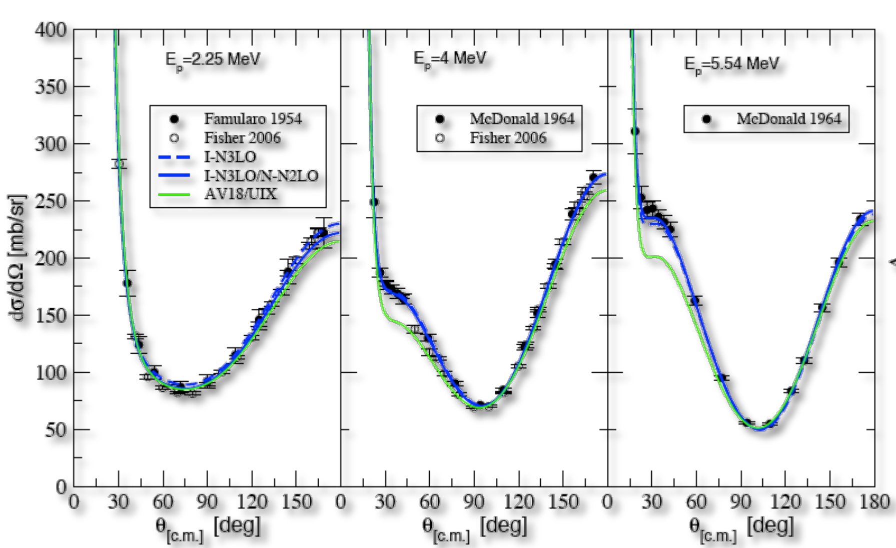
Doron Gazit
Institute for Nuclear Theory, University of Washington, Box 351550, Seattle, Washington 98195, USA

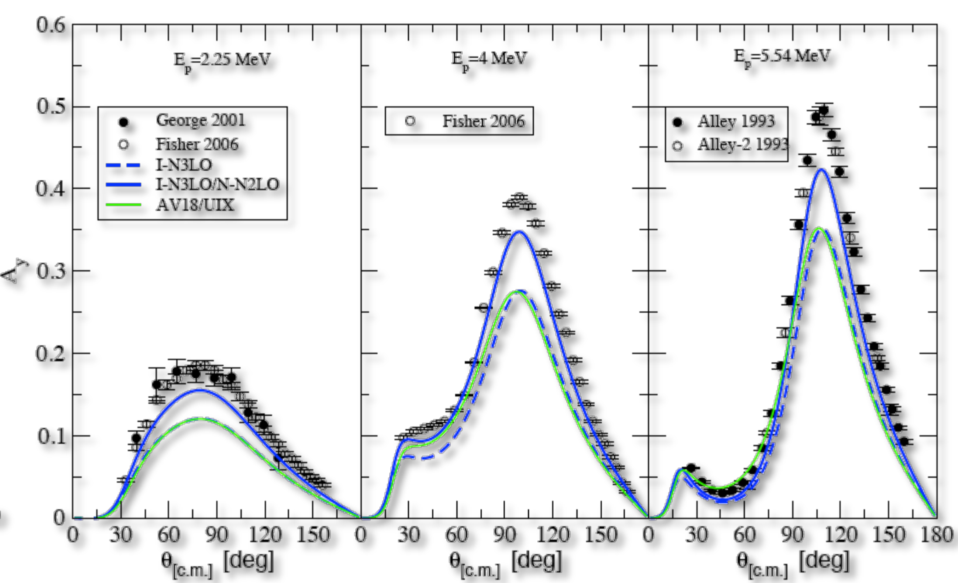
Sofia Quaglioni and Petr Navrátil
Lawrence Livermore National Laboratory, P.O. Box 808, L-414, Livermore, California 94551, USA

Proton-^{3}He elastic scattering with χEFT NN+NNN

- Hyphenspherical-harmonics variational calculations
  - M. Viviani, L. Girlanda, A. Kievski, L. E. Marcucci, and S. Rosati, arXiv:1004.1306
- ***A_y* puzzle (almost) resolved** with the chiral N^{3}LO NN plus **local chiral N^{2}LO NNN**
  - *used with the NCSM and other methods*

A=3 binding energy constraint, c_D=+1, c_E=-0.029, Λ=500 MeV

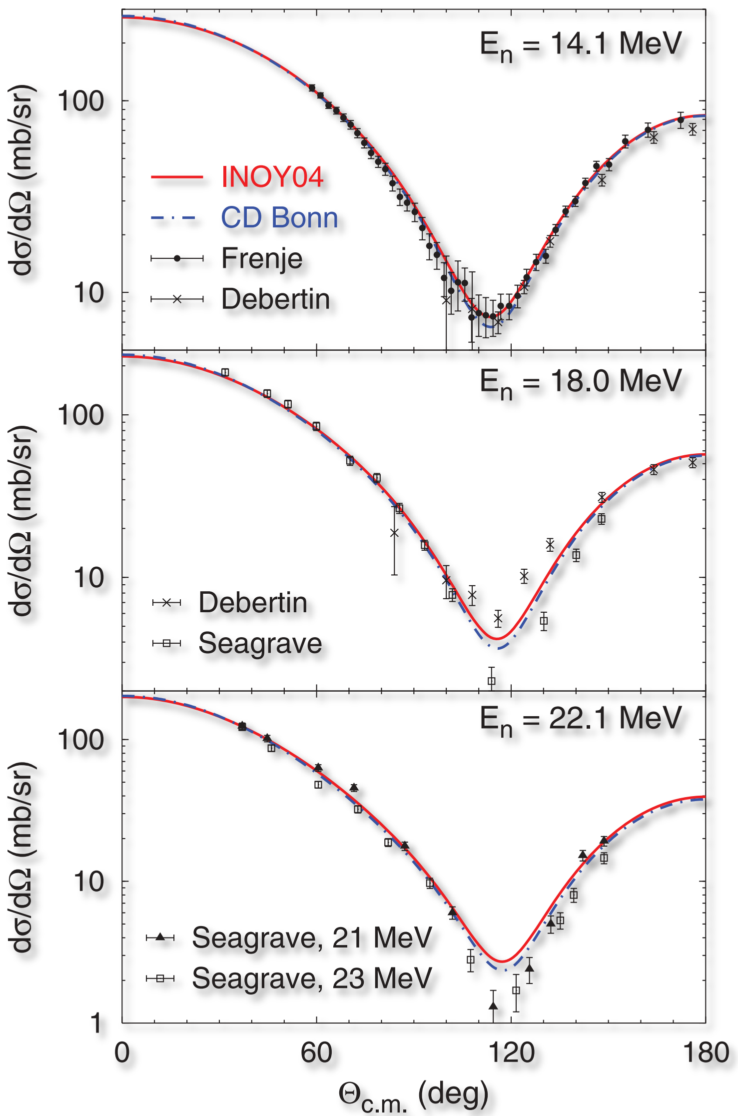




Chiral NN+NNN Hamiltonian provides the best agreement with the cross section and analyzing power data and with the new TUNL PSA analysis

Plenary talk by L. E. Marcucci, Wednesday 9:00

Ab initio calculations of n-^{3}H scattering



AGS equations

PHYSICAL REVIEW C **86**, 011001(R) (2012)

Neutron-^{3}H scattering above the four-nucleon breakup threshold

A. Deltuva and A. C. Fonseca

Plenary talk
by A. Deltuva,
Wednesday 9:35

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 ^{12}C) spin-isospin vectors in $3A$ dimensions

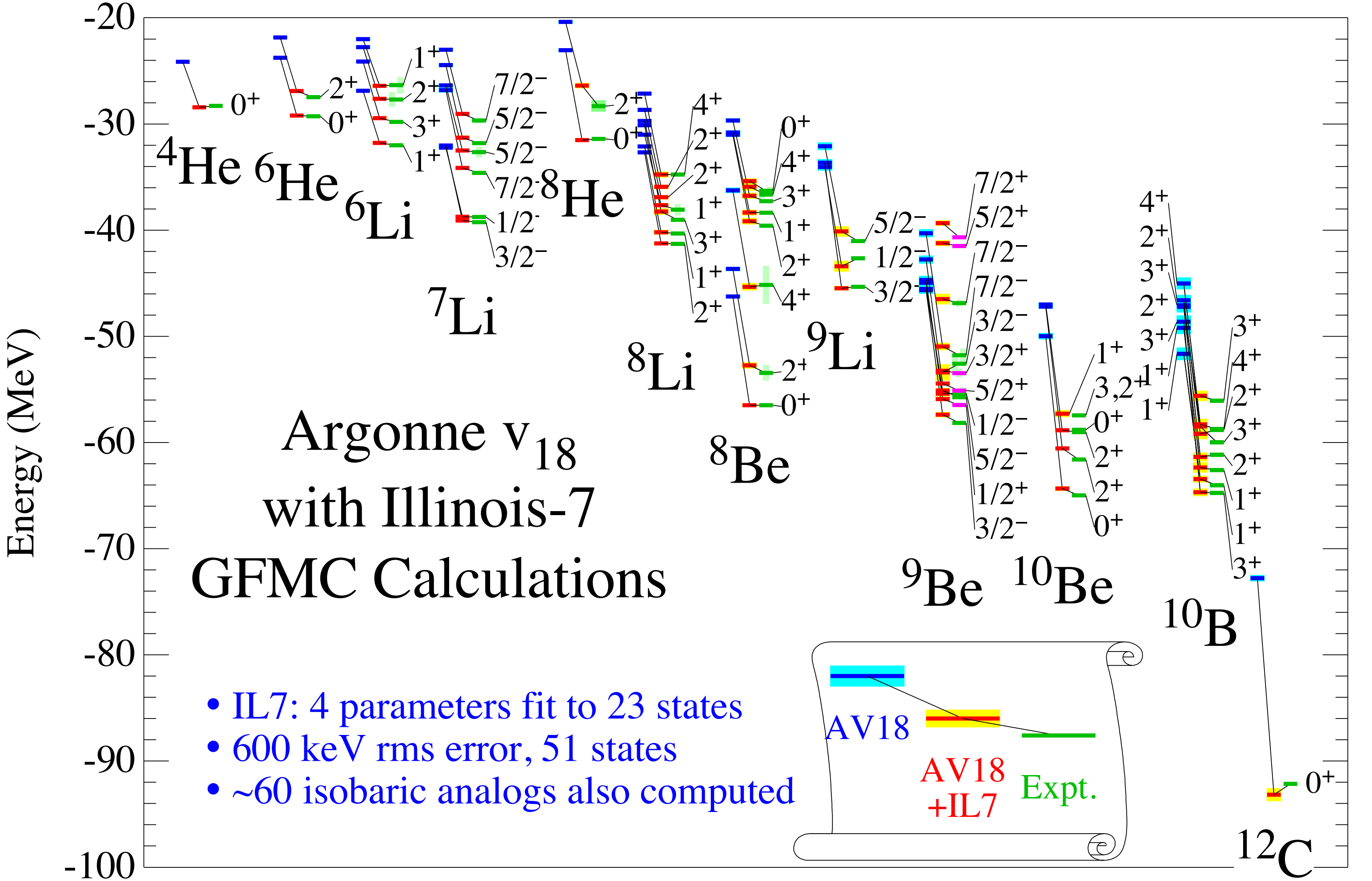
Green's function Monte Carlo (GFMC): project out the exact eigenfunction

- $\Psi(\tau) = \exp[-(H - E_0)\tau]\Psi_V = \sum_n \exp[-(E_n - E_0)\tau] a_n \Psi_n \Rightarrow \Psi_0$ 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 $A \geq 8$
- 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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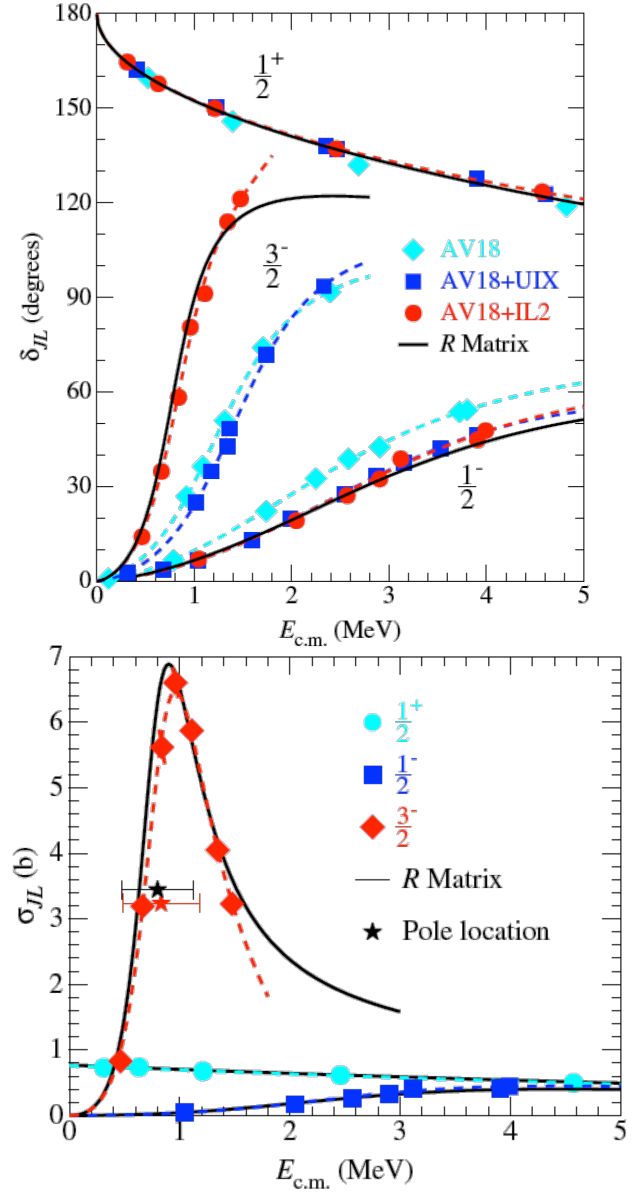
Quantum Monte Carlo Calculations of Neutron-^{4}He Scattering

- GFMC method generalized for scattering
  - Similar to GFMC for bound states
    - Essential difference: **boundary conditions**
- Realistic NN plus NNN interactions
  - Importance of the three-body force for *P*-waves

Method

- Pick a log derivative χ at the boundary (R >7 fm)
- Starting w.f.: VMC with scattering boundary χ
- Special method for propagation to preserve χ
- Finds E(R, χ)
- Repeat for many χ until δ(E) is mapped out

K. Nollett et al., PRL99, 022502 (2007)



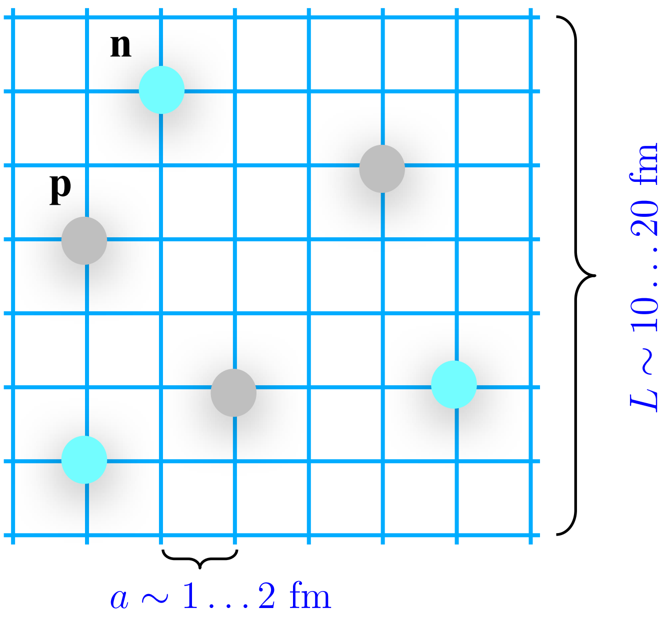
Nuclear Lattice Effective Field Theory Calculations

E. Epelbaum, H. Krebs, T. Lahde, D. Lee,U.-G. Meissner

Discretized version of chiral EFT for nuclear dynamics

$$\left[\left(\sum_{i=1}^{A}\frac{-\vec{\nabla}_i^2}{2m_N}+\mathcal{O}(m_N^{-3})\right)+\underbrace{V_{2N}+V_{3N}+V_{4N}+\ldots}_{\text{derivable within in ChPT}}\right]|\Psi\rangle = E|\Psi\rangle$$

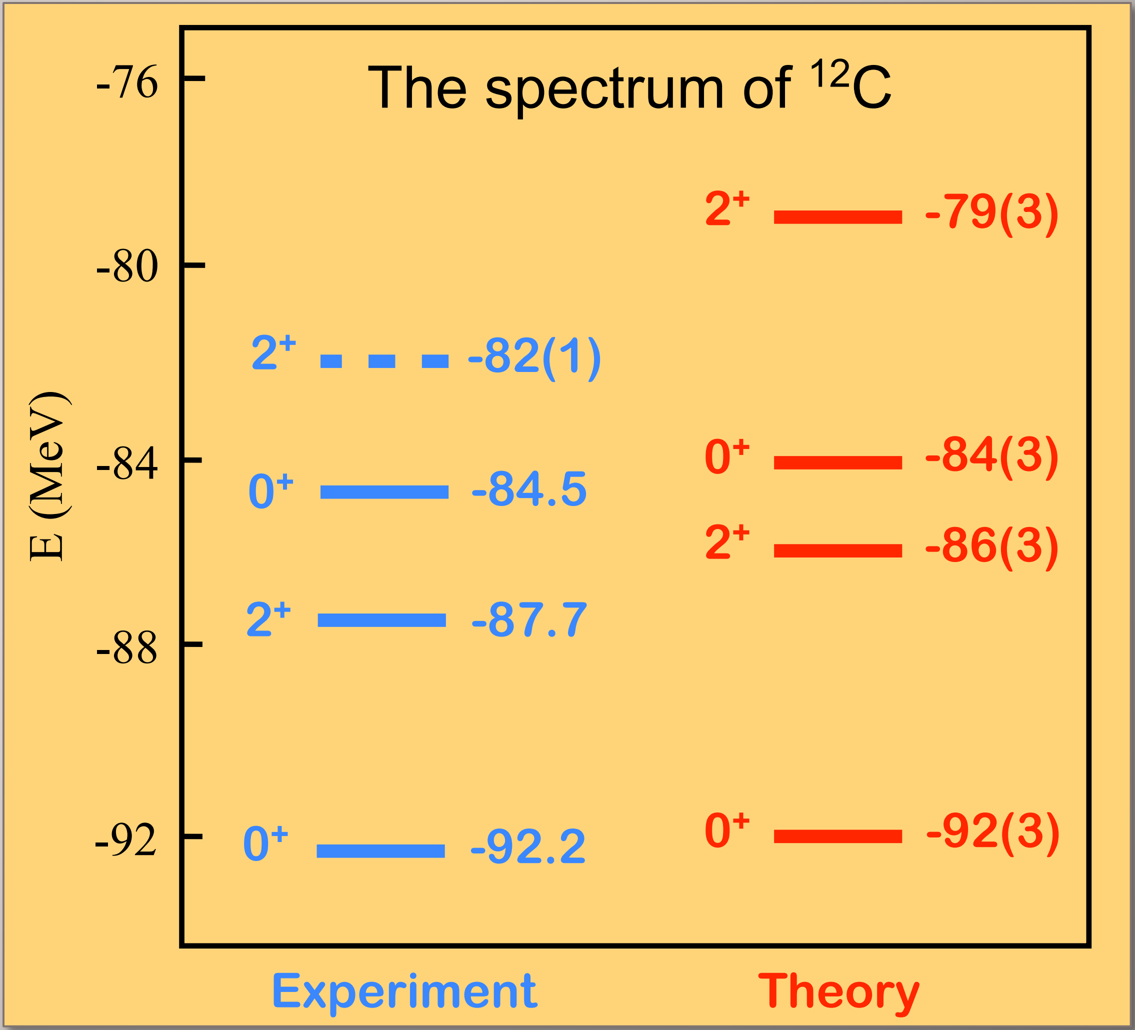
Borasoy, E.E., Krebs, Lee, Meißner, Eur. Phys. J. A31 (07) 105,
Eur. Phys. J. A34 (07) 185,
Eur. Phys. J. A35 (08) 343,
Eur. Phys. J. A35 (08) 357,
E.E., Krebs, Lee, Meißner, Eur. Phys. J A40 (09) 199,
Eur. Phys. J A41 (09) 125,
Phys. Rev. Lett 104 (10) 142501,
Eur. Phys. J. 45 (10) 335,
Phys. Rev. Lett. 106 (11) 192501



Nuclear Lattice Effective Field Theory Calculations

E. Epelbaum, H. Krebs, T. Lahde, D. Lee, U.-G. Meissner

The Hoyle state



Plenary talk
by Evgeny Epelbaum,
Tuesday 11:15

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

Coupled-Cluster Method

- **exponential Ansatz** for wave operator

$$|\Psi\rangle = \hat{\Omega}|\Phi_0\rangle = e^{\hat{T}_1+\hat{T}_2+\hat{T}_3+\cdots+\hat{T}_A}|\Phi_0\rangle$$

- $\hat{T}_n$: ***n*****p*****n*****h excitation** ("cluster") operators

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

- **similarity transformed** Schrödinger Eq.

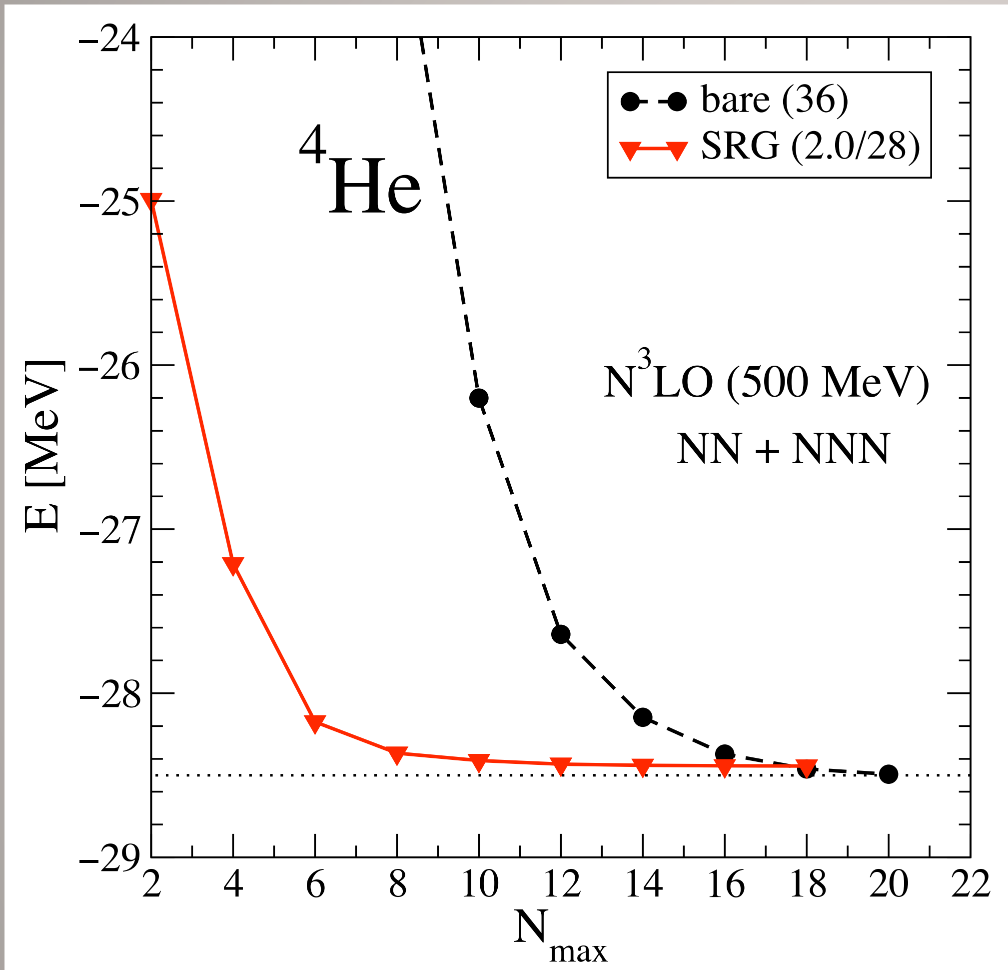
$$\hat{\mathcal{H}}|\Phi_0\rangle = \Delta E|\Phi_0\rangle \ , \quad \hat{\mathcal{H}} \equiv e^{-\hat{T}}\hat{H}_N e^{\hat{T}}$$

- $\hat{\mathcal{H}}$: non-Hermitian **effective Hamiltonian**

- **CCSD** : truncate $\hat{T}$ at **2p2h** level, $\hat{T} = \hat{T}_1 + \hat{T}_2$

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

Calculations with chiral 3N: SRG renormalization needed



PRL 103, 082501 (2009) PHYSICAL REVIEW LETTERS week ending 21 AUGUST 2009

Evolution of Nuclear Many-Body Forces with the Similarity Renormalization Group

E. D. Jurgenson,[1] P. Navrátil,[2] and R. J. Furnstahl[1]

A=3 binding energy and half life constraint
c_D=-0.2, c_E=-0.205, Λ=500 MeV

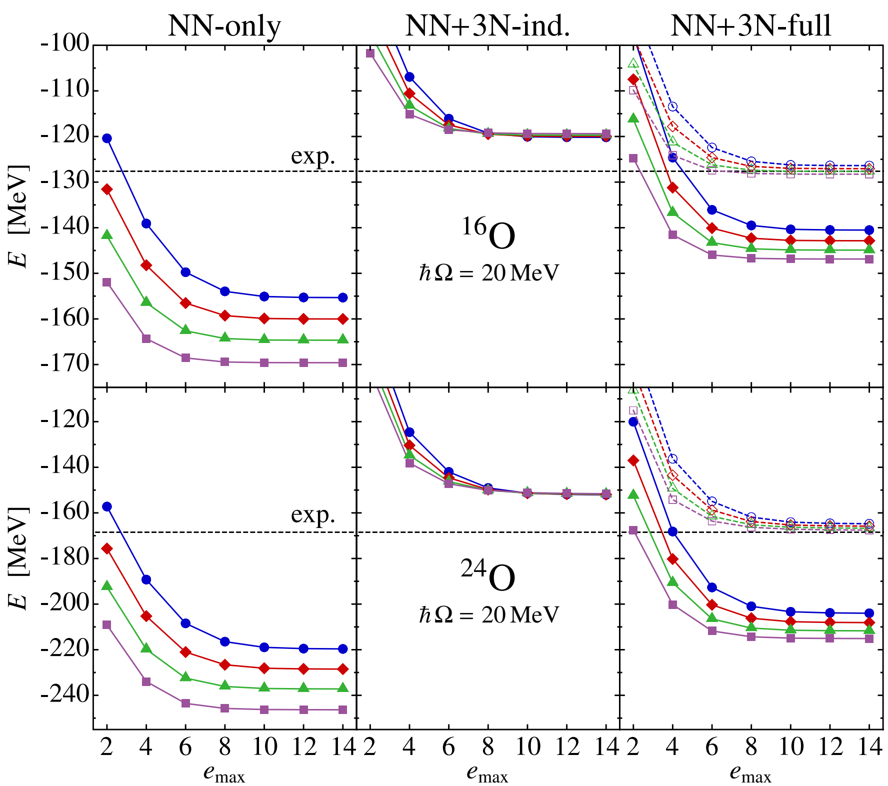
Chiral N^{3}LO NN plus N^{2}LO NNN potential

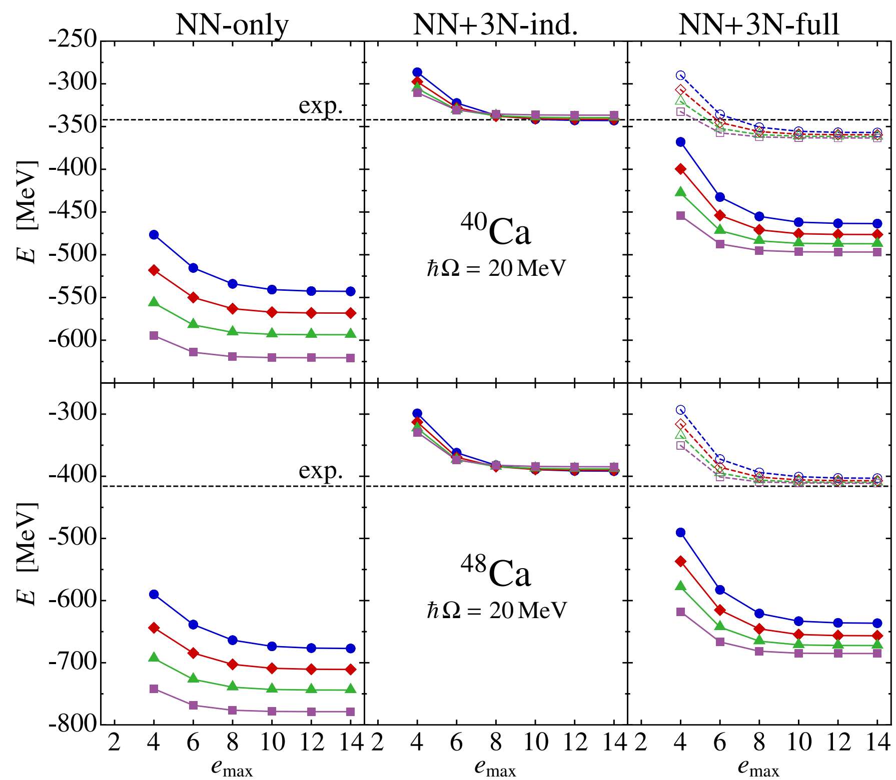
- Bare interaction (black line)
  - Strong short-range correlations
    - Large basis needed
- SRG evolved effective interaction (red line)
  - Unitary transformation

$$H_\alpha = U_\alpha H U_\alpha^+ \Rightarrow \frac{dH_\alpha}{d\alpha} = [[T, H_\alpha], H_\alpha] \quad \left(\alpha = 1/\lambda^4\right)$$

  - Two- plus *three*-body components, *four*-body omitted
  - Softens the interaction
    - Smaller basis sufficient

CCSD calculations with SRG evolved interactions





$\alpha = 0.04\,\text{fm}^4$	$\alpha = 0.05\,\text{fm}^4$	$\alpha = 0.0625\,\text{fm}^4$	$\alpha = 0.08\,\text{fm}^4$
$\Lambda = 2.24\,\text{fm}^{-1}$	$\Lambda = 2.11\,\text{fm}^{-1}$	$\Lambda = 2.00\,\text{fm}^{-1}$	$\Lambda = 1.88\,\text{fm}^{-1}$

PRL 109, 052501 (2012) PHYSICAL REVIEW LETTERS week ending 3 AUGUST 2012

Medium-Mass Nuclei with Normal-Ordered Chiral $NN + 3N$ Interactions

Robert Roth,[1,*] Sven Binder,[1] Klaus Vobig,[1] Angelo Calci,[1] Joachim Langhammer,[1] and Petr Navrátil[2]

- Significant 3N induced interaction
- 4N induced interaction when chiral 3N(500) included
- No 4N induced interaction when chiral 3N(400) included (dotted lines)

Plenary talk
by Robert Roth,
Friday 9:00

Photo-disintegration reactions

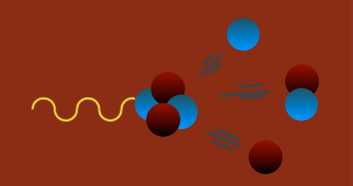
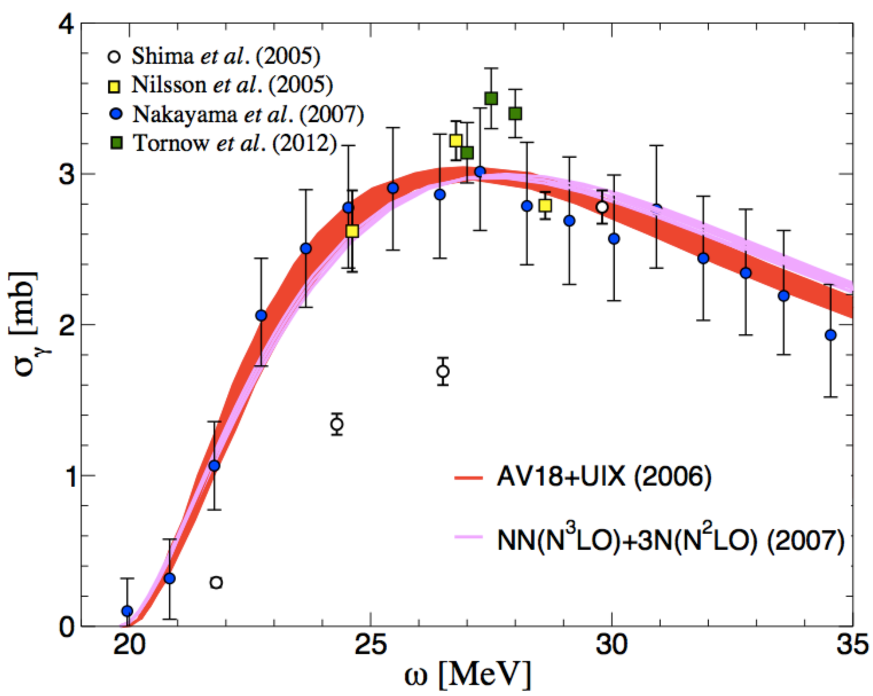


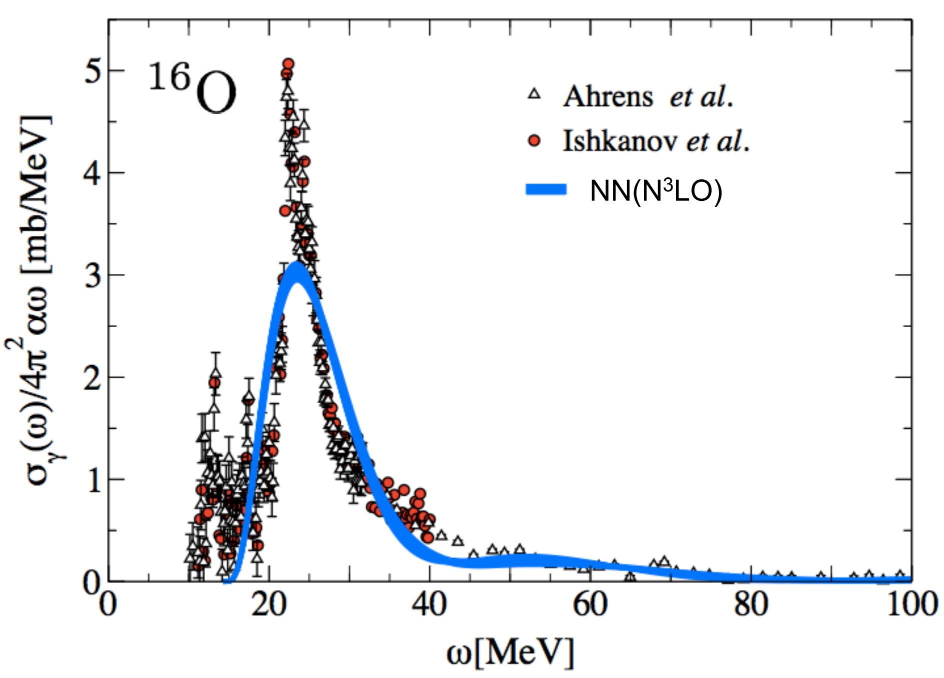
Photo-disintegration reactions can break the nucleus into many different clusters:
two-body clusters, three-body clusters, ..., A-nucleons → terribly complicated many-body continuum state

Ab initio approach: Lorentz Integral Transform Method → reduces the continuum problem to the solution of a bound-state equation which can be solved with any good bound-state technique



Hyperspherical Harmonics: Gazit, et al. PRL 96 112301 (2006)

NCSM: Quaglioni and Navratil PLB 652 (2007)



Coupled-Cluster Theory: Bacca et al., arXiv:1303.7446, to appear in PRL

Talk by G. Orlandiny, B3, Tuesday 14:30

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Elastic proton/neutron scattering on ^{40}Ca

G. Hagen and N. Michel Phys. Rev. C **86**, 021602(R) (2012).

Elastic scattering of a nucleon on a target nucleus can be computed from the one-nucleon overlap function.

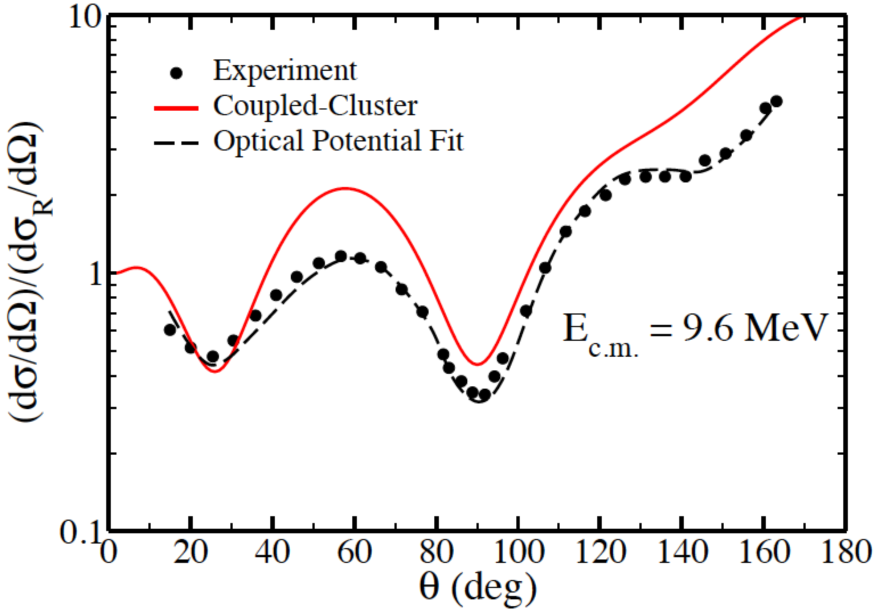
$$O_A^{A+1}(lj;kr) = \sum_n \left\langle A+1 \left\| \tilde{a}^\dagger_{nlj} \right\| A \right\rangle \phi_{nlj}(r).$$

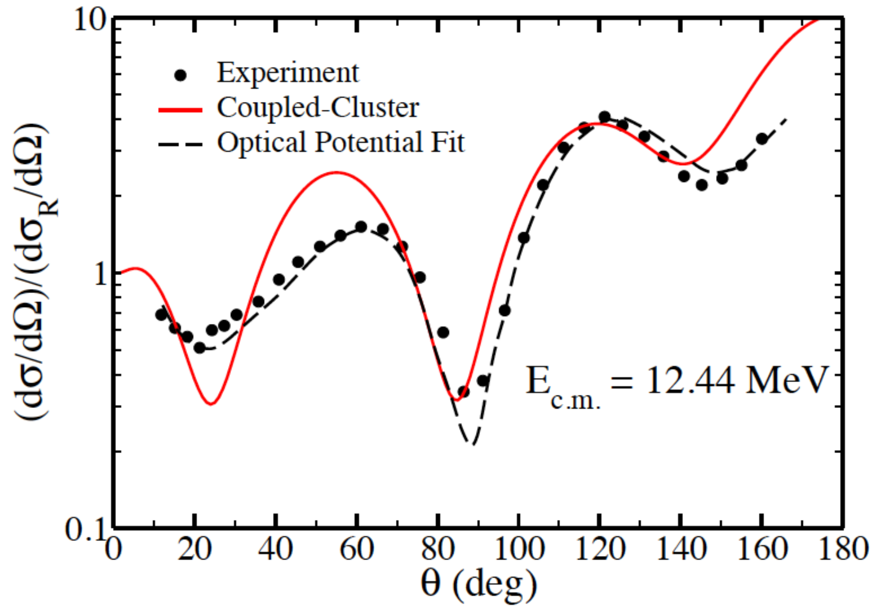
Beyond the range of the potential they are given by:

$$O_A^{A+1}(lj;kr) = C_{lj} \frac{W_{-\eta,l+1/2}(kr)}{r}, \quad k = i\kappa$$

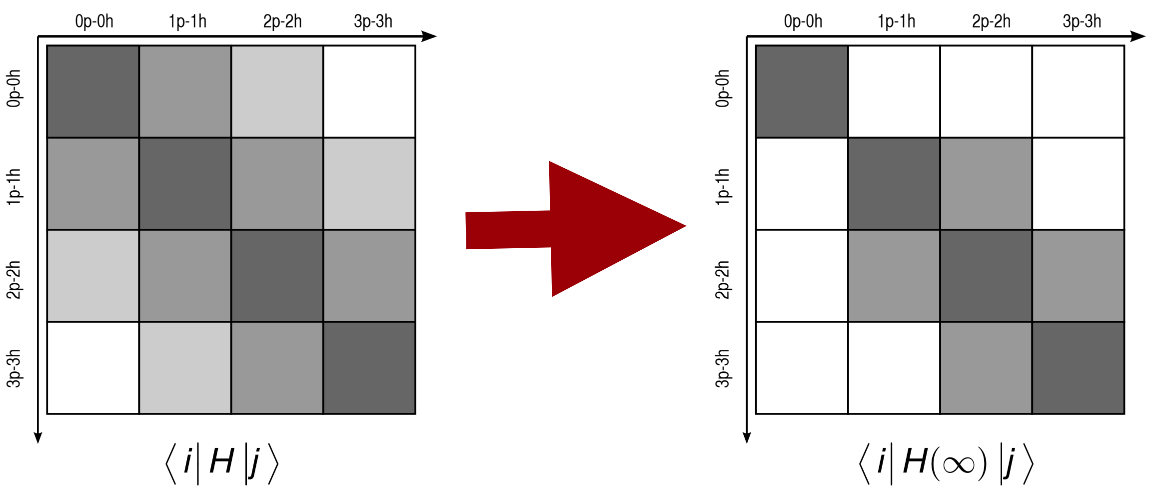
$$O_A^{A+1}(lj;kr) = C_{lj} \left[F_{\ell,\eta}(kr) - \tan\delta_l(k) G_{\ell,\eta}(kr) \right]$$

Using coupled-cluster theory to compute overlap functions we obtained cross sections at low-energy for elastic proton scattering on ^{40}Ca in fair agreement with experiment.





In-medium SRG approach: Application to Oxygen isotopes



aim: decouple reference state (0p-0h) from excitations

$$\frac{d}{ds}H(s) = \left[\eta(s), H(s)\right] , \quad \eta(s) = \frac{dU(s)}{ds}U^\dagger(s) = -\eta^\dagger(s)$$

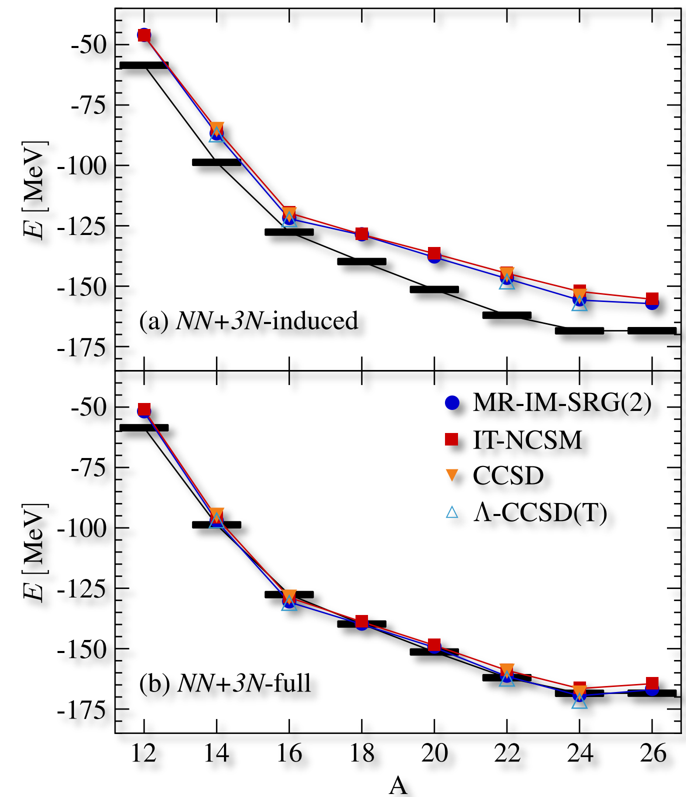
- Wegner

$$\eta^I = \left[H^d, H^{od}\right]$$

- White (J. Chem. Phys. 117, 7472)

$$\eta^{II} = \sum_{ph} \frac{f^p_h}{E_p - E_h} :A^p_h: + \sum_{pp'hh'} \frac{\Gamma^{pp'}_{hh'}}{E_{pp'} - E_{hh'}} :A^{pp'}_{hh'}: + \text{H.c.}$$

$E_p - E_h, E_{pp'} - E_{hh'}$: approx. 1p1h, 2p2h excitation energies



PRL 110, 242501 (2013) PHYSICAL REVIEW LETTERS week ending 14 JUNE 2013

***Ab Initio* Calculations of Even Oxygen Isotopes with Chiral Two-Plus-Three-Nucleon Interactions**

H. Hergert,[1,*] S. Binder,[2] A. Calci,[2] J. Langhammer,[2] and R. Roth[2]

Plenary talk by Robert Roth, Friday 9:00

Magic, semi-magic and open-shell nuclei

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

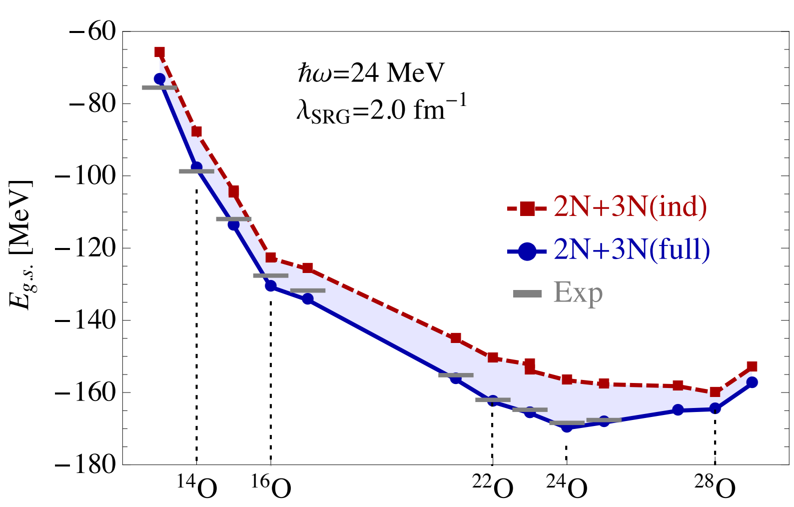
$$
g_{\alpha\beta}(\omega) = \sum_n \frac{\langle\Psi_0^A|c_\alpha|\Psi_n^{A+1}\rangle\langle\Psi_n^{A+1}|c_\beta^\dagger|\Psi_0^A\rangle}{\omega-\varepsilon_n^{A+1}+i\eta} + \sum_k \frac{\langle\Psi_0^A|c_\beta^\dagger|\Psi_k^{A-1}\rangle\langle\Psi_k^{A-1}|c_\alpha|\Psi_0^A\rangle}{\omega-\varepsilon_k^{A-1}-i\eta},
$$

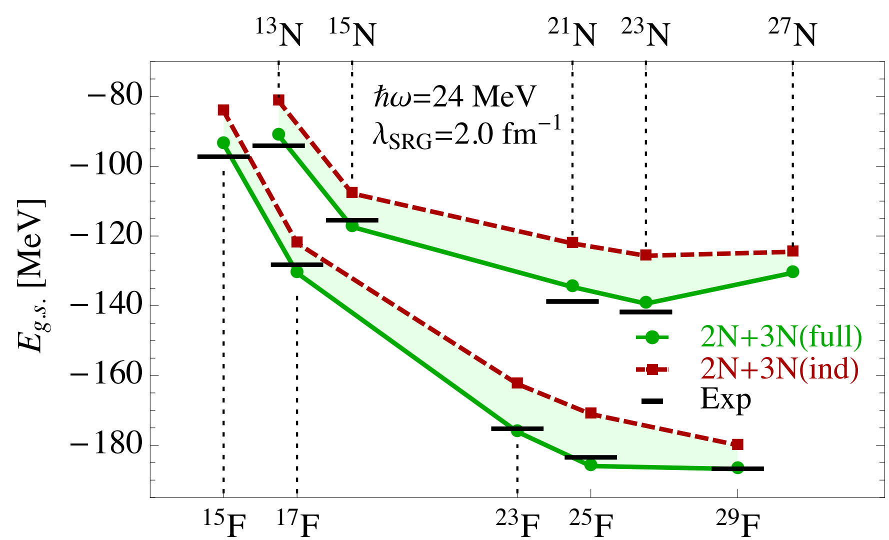
Magic and semi-magic nuclei

PRL 111, 062501 (2013) PHYSICAL REVIEW LETTERS week ending 9 AUGUST 2013

Isotopic Chains Around Oxygen from Evolved Chiral Two- and Three-Nucleon Interactions

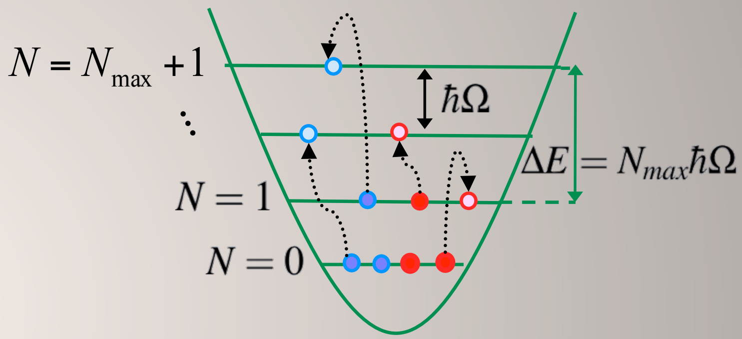
A. Cipollone,[1] C. Barbieri,[1,*] and P. Navrátil[2]



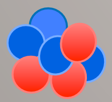


The *ab initio* no-core shell model (NCSM)

- The NCSM is a technique for the solution of the *A*-nucleon bound-state problem
- Realistic nuclear Hamiltonian
  - High-precision nucleon-nucleon potentials
  - Three-nucleon interactions
- Finite harmonic oscillator (HO) basis
  - *A*-nucleon HO basis states
  - complete $N_{max}\hbar\Omega$ model space
- ***Effective interaction tailored to model-space truncation*** for NN(+NNN) potentials
  - Okubo-Lee-Suzuki unitary transformation
- Or a **sequence of unitary transformations in momentum space**:
  - Similarity-Renormalization-Group (SRG) evolved NN(+NNN) potential



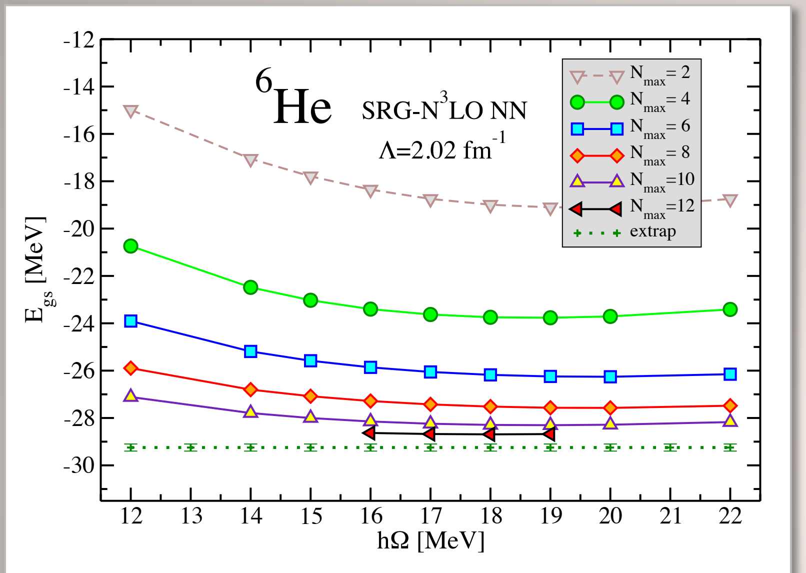
A

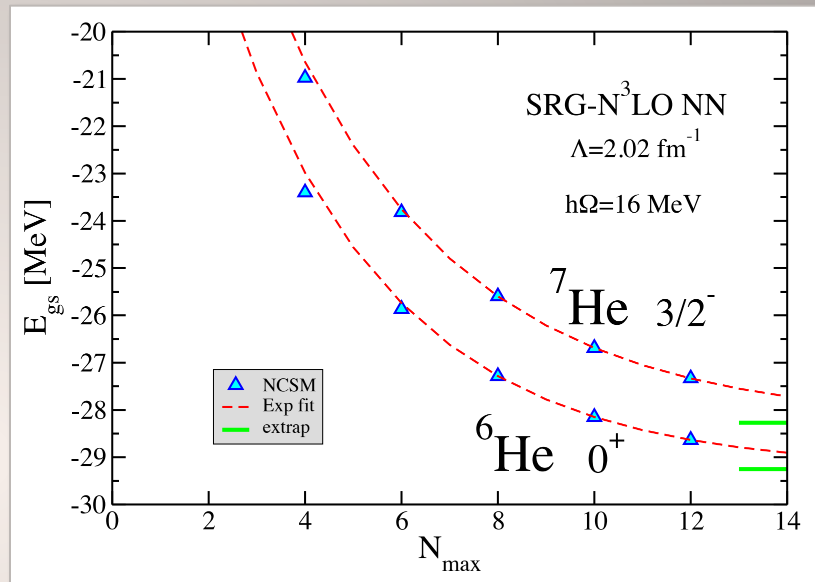


$$\Psi^A = \sum_{N=0}^{N_{\max}} \sum_i c_{Ni} \Phi_{Ni}^A$$

Convergence to exact solution with increasing $N_{\max}$ for bound states. No coupling to continuum.

NCSM calculations of ^{6}He and ^{7}He g.s. energies

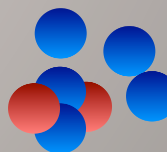




$E_{g.s.}$ [MeV]	^{4}He	^{6}He	^{7}He
NCSM N_{max}=12	-28.05	-28.63	-27.33
NCSM extrap.	-28.22(1)	-29.25(15)	-28.27(25)
Expt.	-28.30	-29.27	-28.84

- ✓ N_{max} convergence OK
- ✓ Extrapolation feasible
  - ^{6}He: E_{gs}=-29.25(15) MeV (Expt. -29.269 MeV)
  - ^{7}He: E_{gs}=-28.27(25) MeV (Expt. -28.84(30) MeV)
- ^{7}He unbound (+0.430(3) MeV), width 0.182(5) MeV
  - **NCSM: no information about the width**

^{7}He

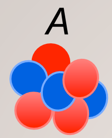


unbound

Extending no-core shell model beyond bound states

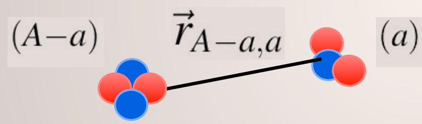
Include more many nucleon correlations…

NCSM →

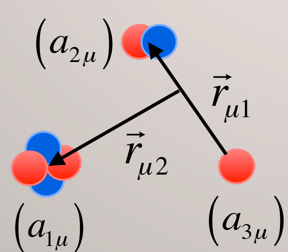


$$\Psi^A = \sum_{N=0}^{N_{\max}} \sum_i c_{Ni} \Phi_{Ni}^A$$

+



+



$$a_{1\mu} + a_{2\mu} + a_{3\mu} = A$$

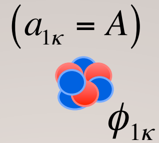
+

…

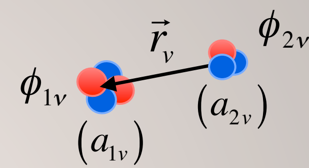
…using the Resonating Group Method (RGM) ideas

Trial function: generalized cluster wave function

$$\psi^{(A)} = \sum_{\kappa} c_\kappa \phi_{1\kappa}\left(\left\{\vec{\xi}_{1\kappa}\right\}\right)$$



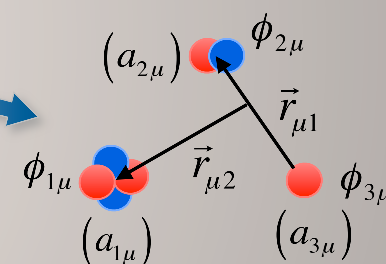
$$+\sum_{\nu} \hat{A}_\nu \phi_{1\nu}\left(\left\{\vec{\xi}_{1\nu}\right\}\right)\phi_{2\nu}\left(\left\{\vec{\xi}_{2\nu}\right\}\right) g_\nu(\vec{r}_\nu)$$



$$a_{1\nu} + a_{2\nu} = A$$

$$+\sum_{\mu} \hat{A}_\mu \phi_{1\mu}\left(\left\{\vec{\xi}_{1\mu}\right\}\right)\phi_{2\mu}\left(\left\{\vec{\xi}_{2\mu}\right\}\right)\phi_{3\mu}\left(\left\{\vec{\xi}_{3\mu}\right\}\right) G_\mu(\vec{r}_{\mu 1},\vec{r}_{\mu 2})$$

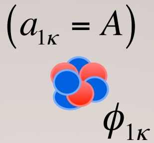
$$+\ \cdots$$



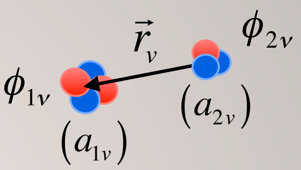
$$a_{1\mu} + a_{2\mu} + a_{3\mu} = A$$

Trial function: generalized cluster wave function

$$\psi^{(A)} = \sum_{\kappa} c_{\kappa} \phi_{1\kappa}\left(\left\{\vec{\xi}_{1\kappa}\right\}\right)$$



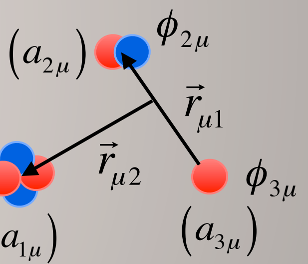
$$+ \sum_{\nu} \hat{A}_{\nu} \phi_{1\nu}\left(\left\{\vec{\xi}_{1\nu}\right\}\right) \phi_{2\nu}\left(\left\{\vec{\xi}_{2\nu}\right\}\right) g_{\nu}(\vec{r}_{\nu})$$



$$a_{1\nu} + a_{2\nu} = A$$

$$+ \sum_{\mu} \hat{A}_{\mu} \phi_{1\mu}\left(\left\{\vec{\xi}_{1\mu}\right\}\right) \phi_{2\mu}\left(\left\{\vec{\xi}_{2\mu}\right\}\right) \phi_{3\mu}\left(\left\{\vec{\xi}_{3\mu}\right\}\right) G_{\mu}(\vec{r}_{\mu 1}, \vec{r}_{\mu 2})$$

$$+ \cdots$$



$$a_{1\mu} + a_{2\mu} + a_{3\mu} = A$$

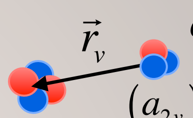
- ϕ : antisymmetric cluster wave functions
  - {ξ}: Translationally invariant internal coordinates

    (Jacobi relative coordinates)
  - These are known, they are an input

Trial function: generalized cluster wave function

$$\psi^{(A)} = \sum_{\kappa} c_\kappa \phi_{1\kappa}\left(\left\{\vec{\xi}_{1\kappa}\right\}\right)$$

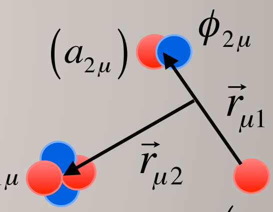
$$+ \sum_{\nu} \hat{A}_\nu \phi_{1\nu}\left(\left\{\vec{\xi}_{1\nu}\right\}\right)\phi_{2\nu}\left(\left\{\vec{\xi}_{2\nu}\right\}\right)g_\nu(\vec{r}_\nu)$$



$$a_{1\nu} + a_{2\nu} = A$$

$$+ \sum_{\mu} \hat{A}_\mu \phi_{1\mu}\left(\left\{\vec{\xi}_{1\mu}\right\}\right)\phi_{2\mu}\left(\left\{\vec{\xi}_{2\mu}\right\}\right)\phi_{3\mu}\left(\left\{\vec{\xi}_{3\mu}\right\}\right)G_\mu(\vec{R}_{\mu 1}, \vec{R}_{\mu 2})$$

$$+ \cdots$$



$$a_{1\mu} + a_{2\mu} + a_{3\mu} = A$$

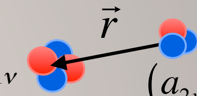
- A_ν, A_μ : intercluster antisymmetrizers
  - Antisymmetrize the wave function for exchanges of nucleons between clusters
  - Example:

$$a_{1\nu} = A-1,\ a_{2\nu} = 1 \quad \Rightarrow \quad \hat{A}_\nu = \frac{1}{\sqrt{A}}\left[1 - \sum_{i=1}^{A-1} \hat{P}_{iA}\right]$$

Trial function: generalized cluster wave function

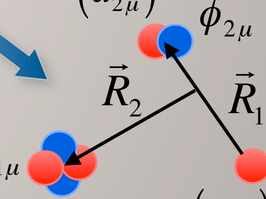
$$\psi^{(A)} = \sum_{\kappa} \boxed{c_\kappa} \phi_{1\kappa}\left(\left\{\vec{\xi}_{1\kappa}\right\}\right)$$

$$+ \sum_{\nu} \int \boxed{g_\nu(\vec{r}\,)}\, \hat{A}_\nu \left[\phi_{1\nu}\left(\left\{\vec{\xi}_{1\nu}\right\}\right)\phi_{2\nu}\left(\left\{\vec{\xi}_{2\nu}\right\}\right)\delta(\vec{r} - \vec{r}_\nu)\right] d\vec{r}$$



$$+ \sum_{\mu} \iint \boxed{G_\mu(\vec{R}_1, \vec{R}_2)}\, \hat{A}_\mu \left[\phi_{1\mu}\left(\left\{\vec{\xi}_{1\mu}\right\}\right)\phi_{2\mu}\left(\left\{\vec{\xi}_{2\mu}\right\}\right)\phi_{3\mu}\left(\left\{\vec{\xi}_{3\mu}\right\}\right)\delta(\vec{R}_1 - \vec{R}_{\mu 1})\delta(\vec{R}_2 - \vec{R}_{\mu 2})\right] d\vec{R}_1 d\vec{R}_2$$

$$+ \cdots$$

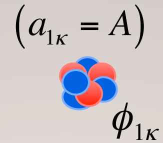


- ***c***, ***g*** and ***G***: discrete and continuous linear variational amplitudes
  - Unknowns to be determined

TRIUMF

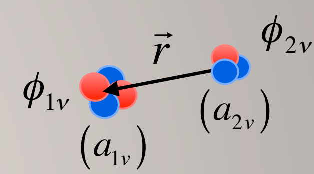
Trial function: generalized cluster wave function

$$\psi^{(A)} = \sum_{\kappa} c_{\kappa} \phi_{1\kappa}\left(\left\{\vec{\xi}_{1\kappa}\right\}\right)$$



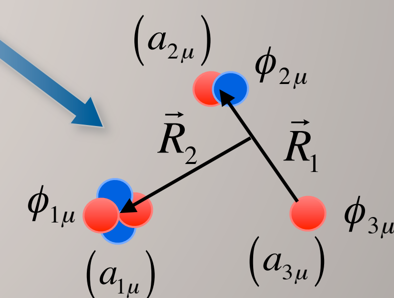
$$+ \sum_{\nu} \int g_{\nu}(\vec{r}\,)\ \hat{A}_{\nu}\left[\phi_{1\nu}\left(\left\{\vec{\xi}_{1\nu}\right\}\right)\phi_{2\nu}\left(\left\{\vec{\xi}_{2\nu}\right\}\right)\delta(\vec{r} - \vec{r}_{\nu})\right]d\vec{r}$$

$a_{1\nu} + a_{2\nu} = A$



$$+ \sum_{\mu} \iint G_{\mu}(\vec{R}_1, \vec{R}_2)\ \hat{A}_{\mu}\left[\phi_{1\mu}\left(\left\{\vec{\xi}_{1\mu}\right\}\right)\phi_{2\mu}\left(\left\{\vec{\xi}_{2\mu}\right\}\right)\phi_{3\mu}\left(\left\{\vec{\xi}_{3\mu}\right\}\right)\delta(\vec{R}_1 - \vec{R}_{\mu 1})\delta(\vec{R}_2 - \vec{R}_{\mu 2})\right]d\vec{R}_1 d\vec{R}_2$$

$$+ \cdots$$



$a_{1\mu} + a_{2\mu} + a_{3\mu} = A$

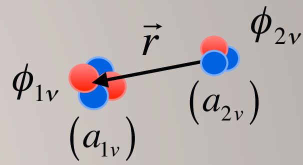
- Discrete and continuous set of basis functions
  - Non-orthogonal
  - Over-complete

Binary cluster wave function

$$\psi^{(A)} = \sum_{\kappa} c_{\kappa} \phi_{1\kappa}\left(\left\{\vec{\xi}_{1\kappa}\right\}\right)$$

$$+ \sum_{\nu} \int g_{\nu}(\vec{r}\,)\ \hat{A}_{\nu}\left[\phi_{1\nu}\left(\left\{\vec{\xi}_{1\nu}\right\}\right)\phi_{2\nu}\left(\left\{\vec{\xi}_{2\nu}\right\}\right)\delta(\vec{r} - \vec{r}_{\nu})\right] d\vec{r}$$

$$a_{1\nu} + a_{2\nu} = A$$



$$+ \sum_{\mu} \iint G_{\mu}(\vec{R}_1, \vec{R}_2)\ \hat{A}_{\mu}\left[\phi_{1\mu}\left(\left\{\vec{\xi}_{1\mu}\right\}\right)\phi_{2\mu}\left(\left\{\vec{\xi}_{2\mu}\right\}\right)\phi_{3\mu}\left(\left\{\vec{\xi}_{3\mu}\right\}\right)\delta(\vec{R}_1 - \vec{R}_{\mu 1})\delta(\vec{R}_2 - \vec{R}_{\mu 2})\right] d\vec{R}_1 d\vec{R}_2$$

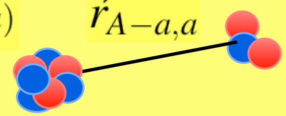
$$+ \cdots$$

- In practice: function space limited by using relatively simple forms of Ψ chosen according to physical intuition and energetical arguments
  - Most common: expansion over binary-cluster basis

The *ab initio* NCSM/RGM in a snapshot

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

$(A-a)$ $\quad \vec{r}_{A-a,a} \quad$ (a)



$\psi^{(A-a)}_{1\nu}\, \psi^{(a)}_{2\nu}\, \delta(\vec{r} - \vec{r}_{A-a,a})$

eigenstates of $H_{(A\text{-}a)}$ and $H_{(a)}$ in the *ab initio* NCSM basis

- Many-body Schrödinger equation:

$$H\Psi^{(A)} = E\Psi^{(A)}$$

$$T_{\rm rel}(r) + \mathcal{V}_{\rm rel} + \bar{V}_{\rm Coul}(r) + H_{(A-a)} + H_{(a)}$$

realistic nuclear Hamiltonian

$$\sum_\nu \int d\vec{r} \left[\mathcal{H}^{(A-a,a)}_{\mu\nu}(\vec{r}\,', \vec{r}) - E\, \mathcal{N}^{(A-a,a)}_{\mu\nu}(\vec{r}\,', \vec{r}) \right] \varphi_\nu(\vec{r}) = 0$$

$$\langle \Phi^{(A-a,a)}_{\mu\vec{r}\,'} | \hat{\mathcal{A}} H \hat{\mathcal{A}} | \Phi^{(A-a,a)}_{\nu\vec{r}} \rangle$$

Hamiltonian kernel

$$\langle \Phi^{(A-a,a)}_{\mu\vec{r}\,'} | \hat{\mathcal{A}}^2 | \Phi^{(A-a,a)}_{\nu\vec{r}} \rangle$$

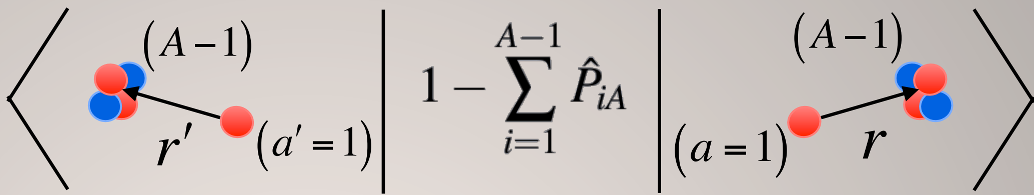
Norm kernel

TRIUMF

Norm kernel (Pauli principle)

Single-nucleon projectile

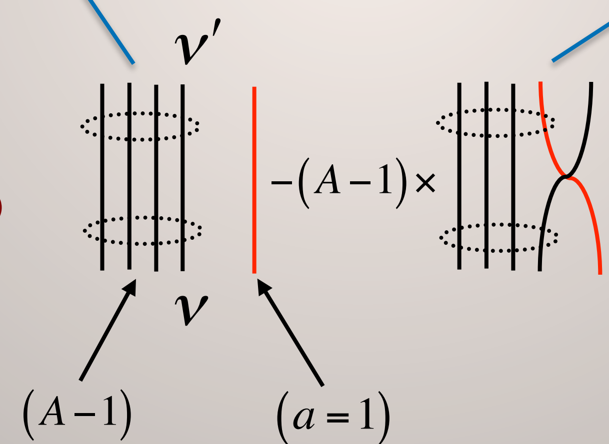
$$\left\langle \Phi^{J^\pi T}_{\nu' r'} \middle| \hat{A}_{\nu'} \hat{A}_{\nu} \middle| \Phi^{J^\pi T}_{\nu r} \right\rangle =$$



$$N^{J^\pi T}_{\nu'\nu}(r',r) = \delta_{\nu'\nu} \frac{\delta(r'-r)}{r'r} - (A-1) \sum_{n'n} R_{n'\ell'}(r') R_{n\ell}(r) \left\langle \Phi^{J^\pi T}_{\nu' n'} \middle| \hat{P}_{A-1,A} \middle| \Phi^{J^\pi T}_{\nu n} \right\rangle$$

$${}_{SD}\left\langle \psi^{(A-1)}_{\mu_1} \middle| a^+ a \middle| \psi^{(A-1)}_{\nu_1} \right\rangle_{SD}$$

Direct term:
Treated exactly!
(in the full space)

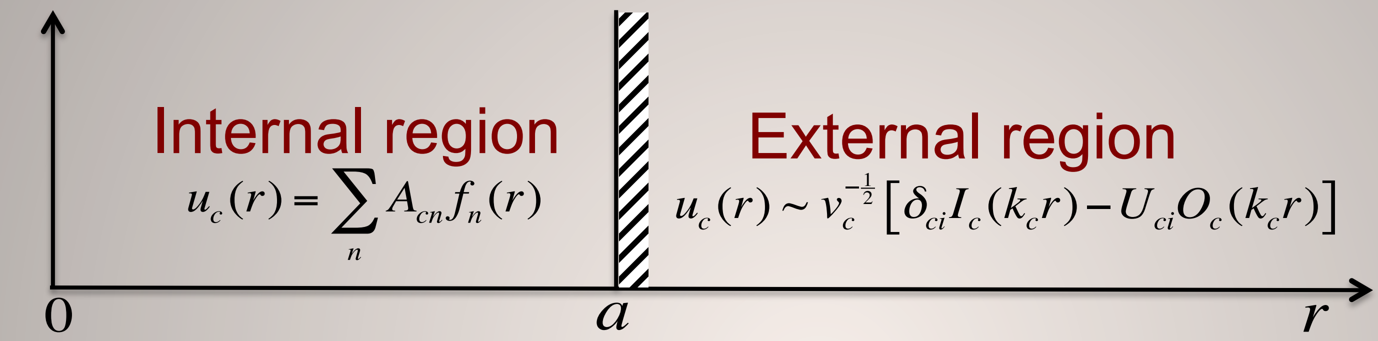


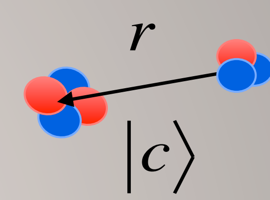
Exchange term:
Obtained in the model space!
(Many-body correction due to the exchange part of the inter-cluster antisymmetrizer)

$$\frac{\delta(r - r_{A-a,a})}{r\, r_{A-a,a}} = \sum_n R_{n\ell}(r) R_{n\ell}(r_{A-a,a})$$

Microscopic *R*-matrix on a Lagrange mesh

Separation into "internal" and "external" regions at the channel radius a





- This is achieved through the Bloch operator: $$L_c = \frac{\hbar^2}{2\mu_c} \delta(r-a) \left(\frac{d}{dr} - \frac{B_c}{r} \right)$$
- System of Bloch-Schrödinger equations:

$$\left[\hat{T}_{rel}(r) + L_c + \overline{V}_{Coul}(r) - (E - E_c) \right] u_c(r) + \sum_{c'} \int dr' \, r' W_{cc'}(r,r') u_{c'}(r') = L_c u_c(r)$$

$$u_c(r) = \sum_n A_{cn} f_n(r)$$

- Internal region: expansion on square-integrable Lagrange mesh basis
- External region: asymptotic form for large r

$$\{ a x_n \in [0,a] \}$$

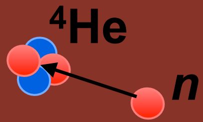
$$\int_0^1 g(x) dx \approx \sum_{n=1}^{N} \lambda_n g(x_n)$$

$$\int_0^a f_n(r) f_{n'}(r) dr \approx \delta_{nn'}$$

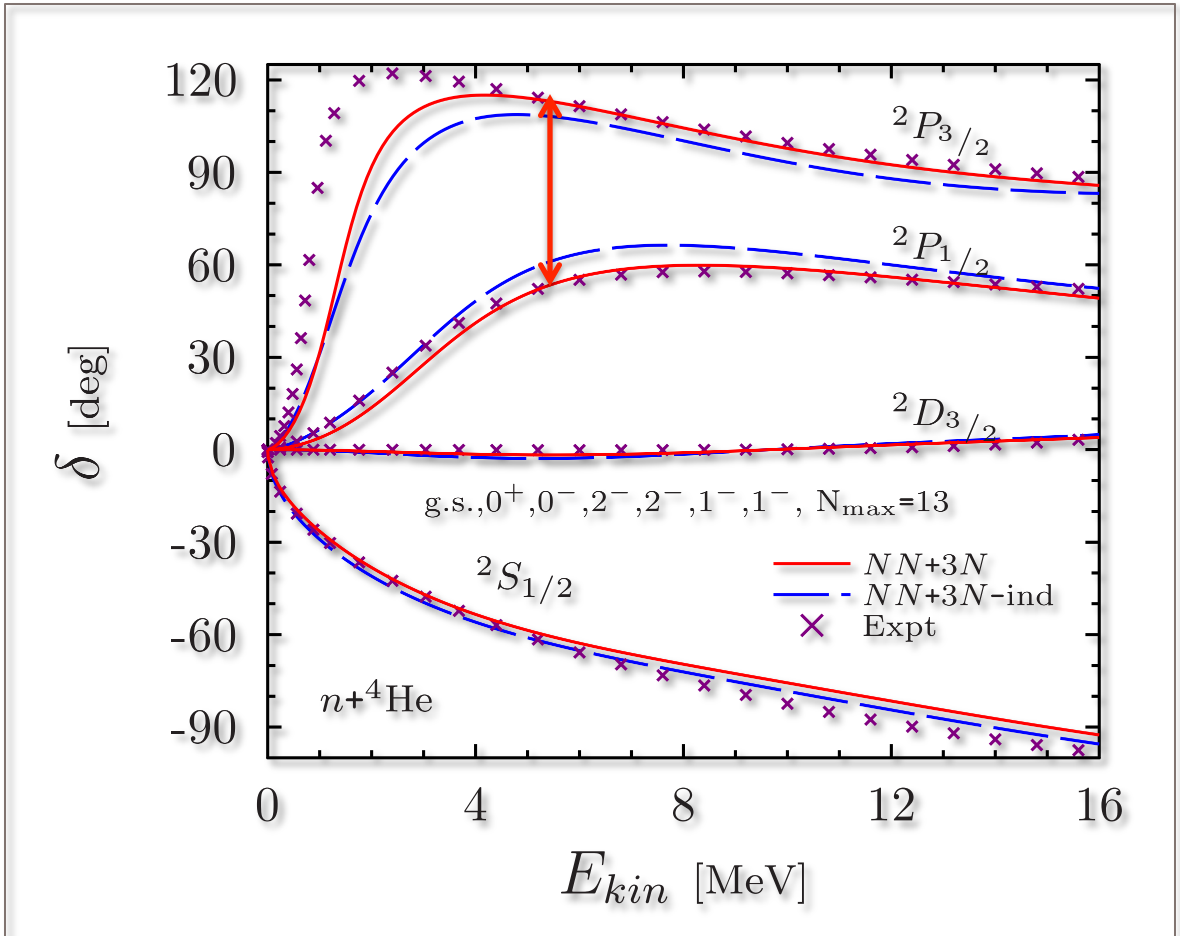
$$u_c(r) \sim C_c W(k_c r) \quad \text{or} \quad u_c(r) \sim v_c^{-\frac{1}{2}} \left[\delta_{ci} I_c(k_c r) - U_{ci} O_c(k_c r) \right]$$

Bound state — Scattering state — Scattering matrix

TRIUMF

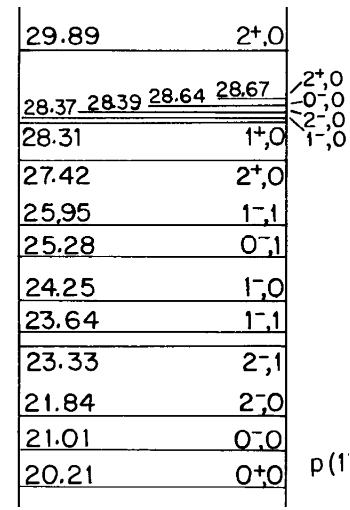


n-^{4}He scattering: NN vs. NN+NNN interactions



chiral NN+NNN(500)
chiral NN+NNN-induced
SRG λ=2 fm^{-1}
HO N_{max}=13, hΩ=20 MeV

^{4}He g.s. and 6 excited states

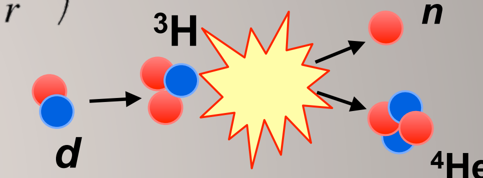


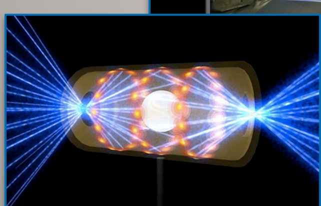
The largest splitting between the P-waves obtained with the chiral NN+NNN interaction

Talk by Guillaume Hupin, A5, Wednesday 15:50

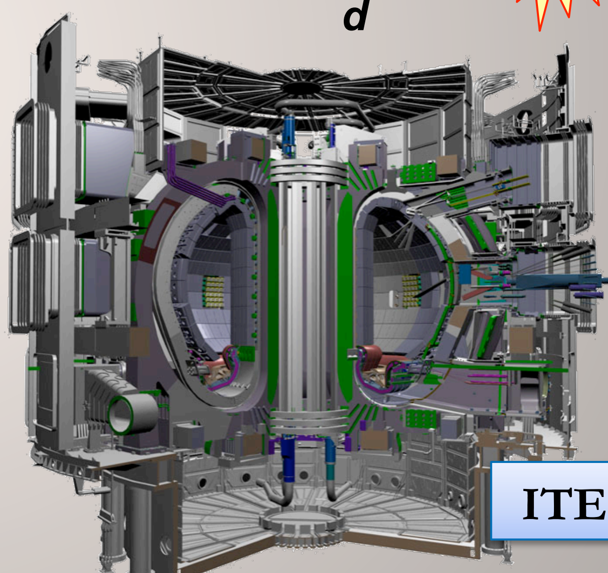
Ab initio calculation of the ^{3}H(*d*,*n*)^{4}He fusion

$$\int dr\, r^2 \begin{pmatrix} \left\langle {}_{n}^{r'}\alpha \right| \hat{A}_1 (H-E) \hat{A}_1 \left| \alpha\, {}_{n}^{r} \right\rangle & \left\langle {}_{n}^{r'}\alpha \right| \hat{A}_1 (H-E) \hat{A}_2 \left| {}^3\mathrm{H}\, {}_{d}^{r} \right\rangle \\ \left\langle {}_{d}^{r'}\, {}^3\mathrm{H} \right| \hat{A}_2 (H-E) \hat{A}_1 \left| \alpha\, {}_{n}^{r} \right\rangle & \left\langle {}_{d}^{r'}\, {}^3\mathrm{H} \right| \hat{A}_2 (H-E) \hat{A}_2 \left| {}^3\mathrm{H}\, {}_{d}^{r} \right\rangle \end{pmatrix} \begin{pmatrix} \frac{g_1(r)}{r} \\ \frac{g_2(r)}{r} \end{pmatrix} = 0$$





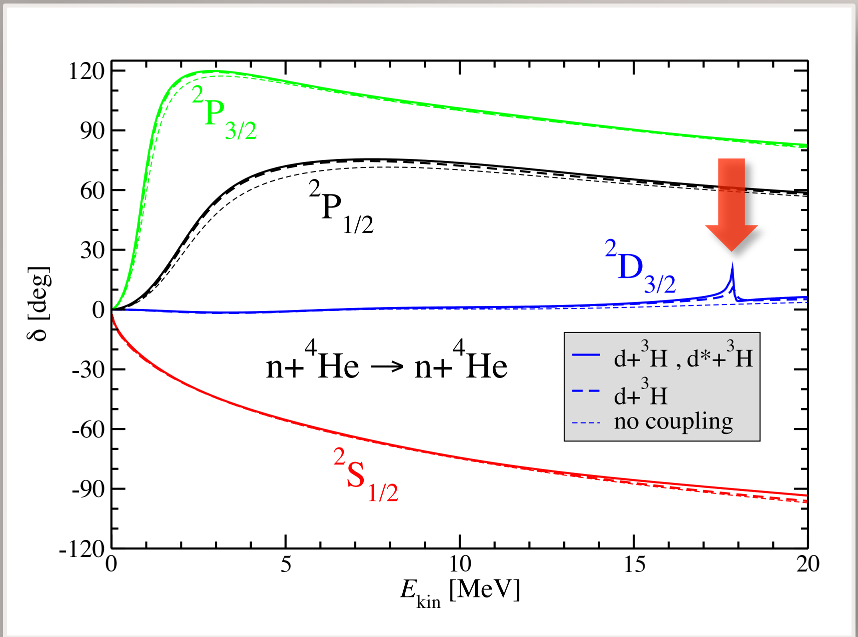
NIF

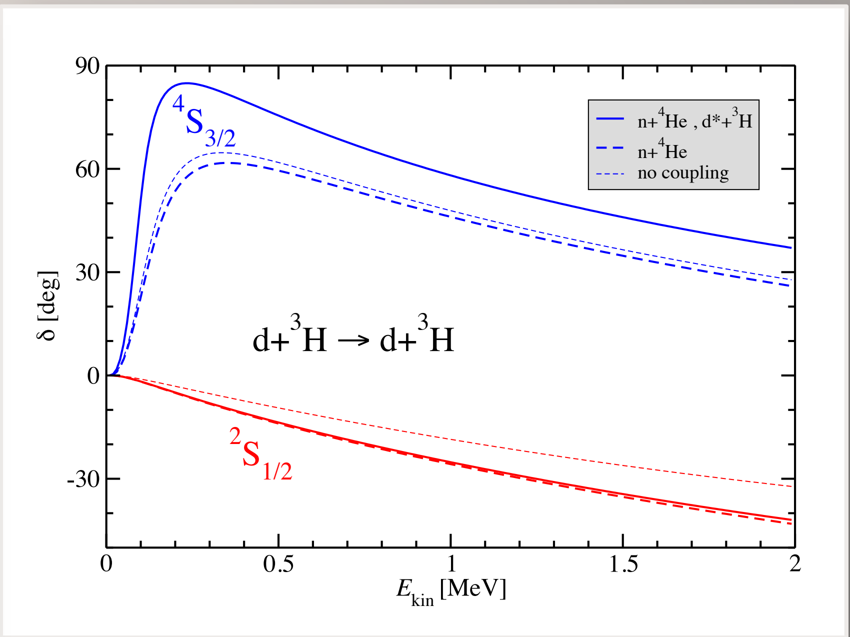


ITER

energy generation

d+^{3}H and n+^{4}He elastic scattering: phase shifts





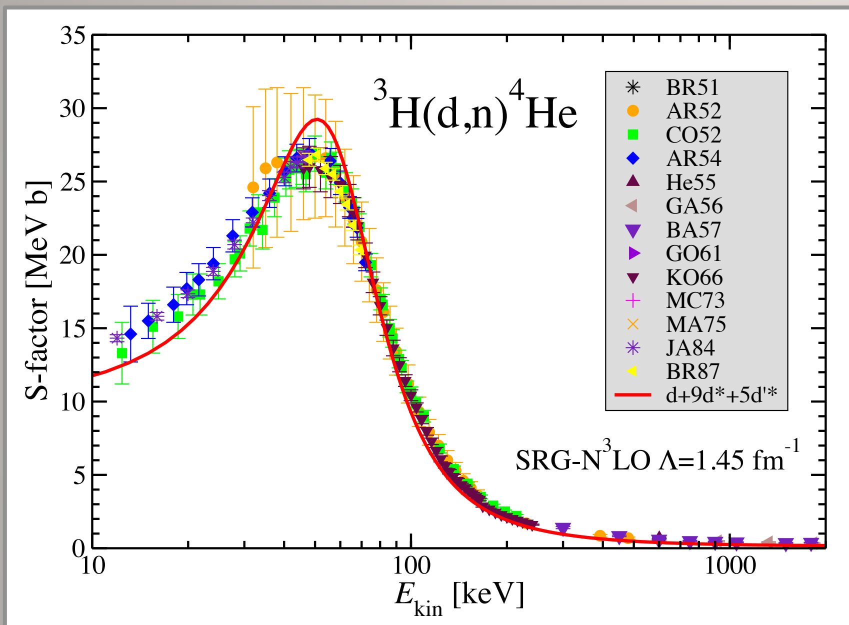
- *n*+^{4}He elastic phase shifts:
  - *d*+^{3}H channels produces slight increase of the *P* phase shifts
  - Appearance of resonance in the 3/2$^+$ *D*-wave, just above *d*-^{3}H threshold
- *d*+^{3}H elastic phase shifts:
  - Resonance in the $^4S_{3/2}$ channel
  - Repulsive behavior in the $^2S_{1/2}$ channel ➔ Pauli principle

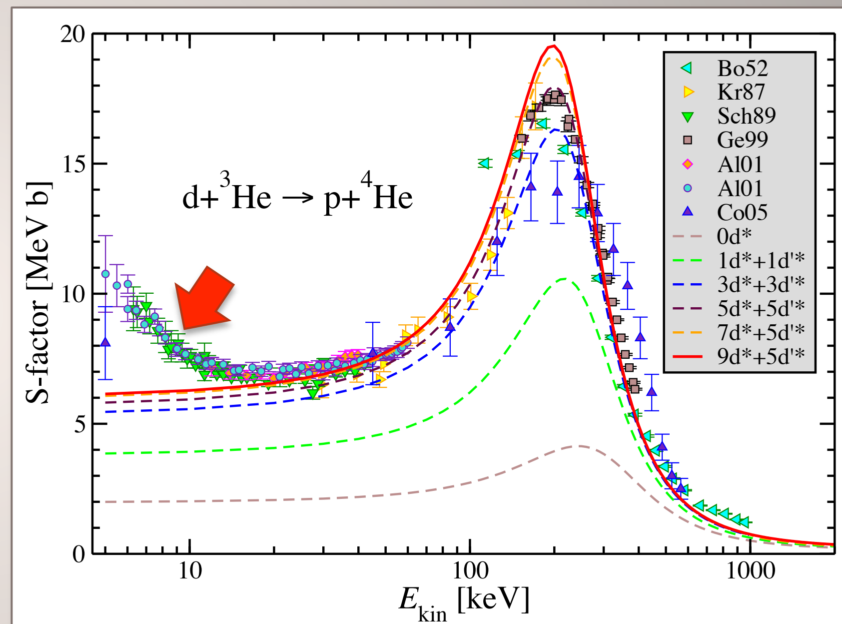
*d** deuteron pseudo state in $^3S_1$-$^3D_1$ channel: deuteron polarization, virtual breakup

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

$^3H(d,n)^4He$ & $^3He(d,p)^4He$ fusion

- NCSM/RGM with *SRG-N^{3}LO NN* potentials

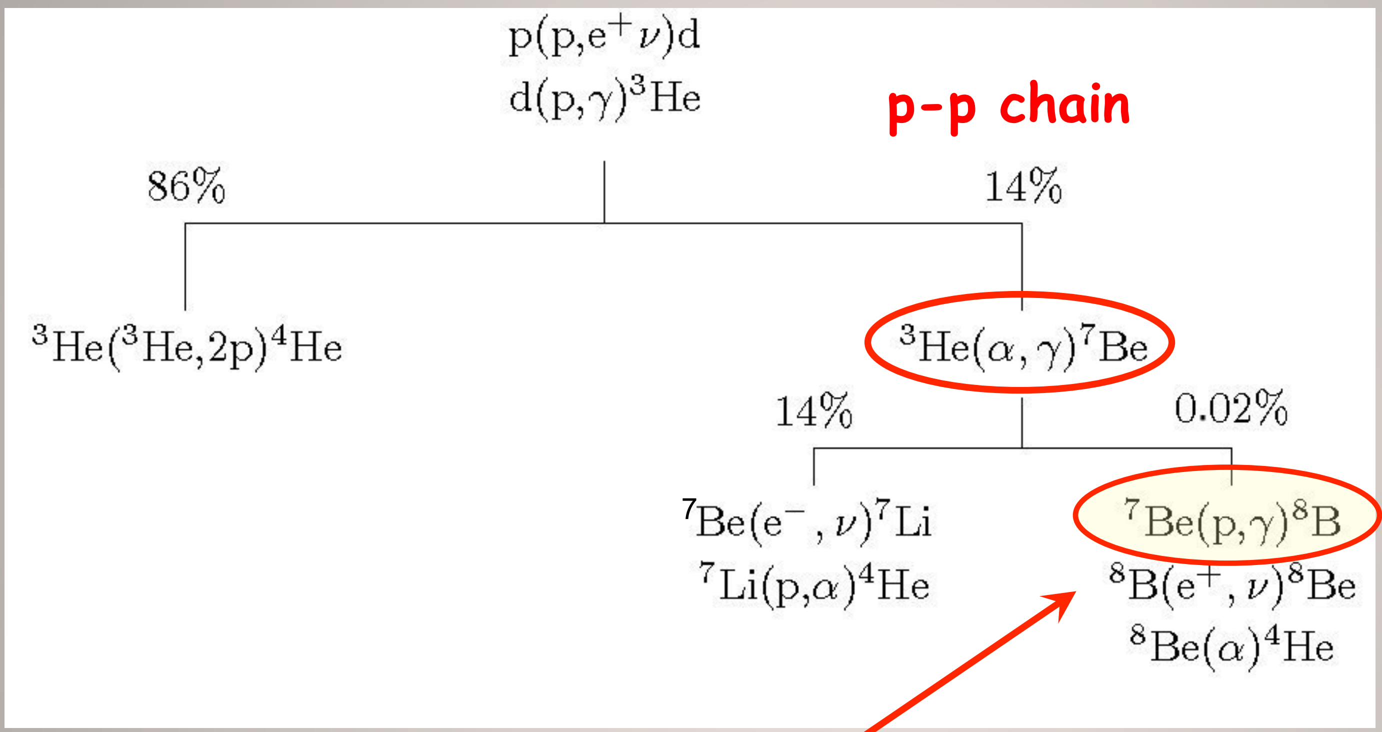




Potential to address unresolved fusion research related questions:
^{3}H(*d*,*n*)^{4}He fusion with polarized deuterium and/or tritium,
^{3}H(*d*,*n* γ)^{4}He bremsstrahlung,
Electron screening at very low energies …

P.N., S. Quaglioni,
PRL **108**, 042503 (2012)

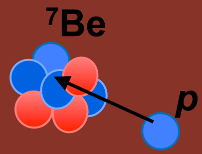
Solar *p-p* chain



Solar neutrinos

$E_\nu < 15$ MeV

$^{7}Be(p,\gamma)^{8}B$ radiative capture

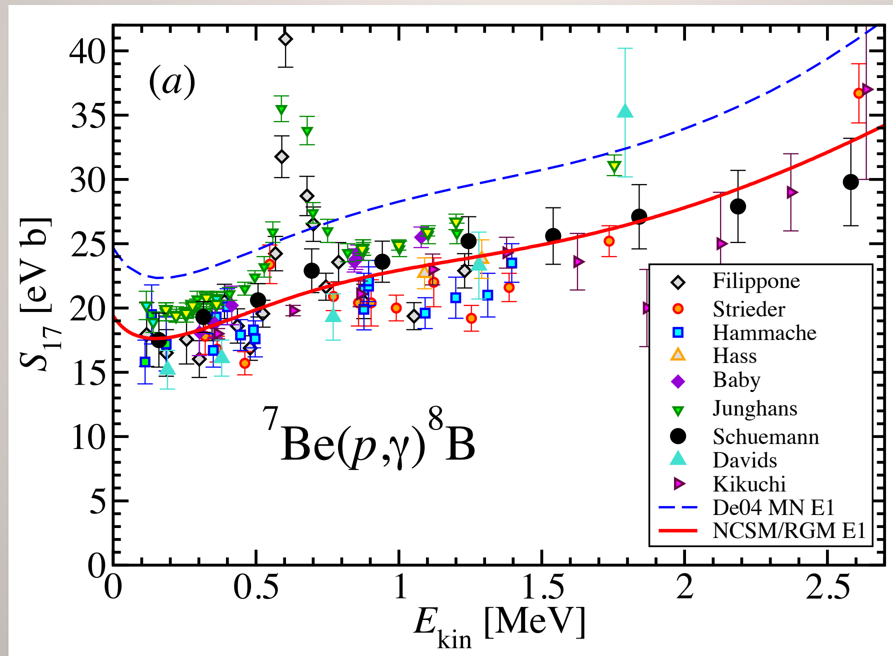


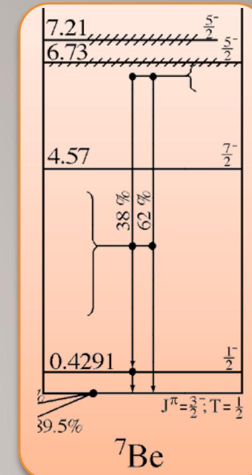
- NCSM/RGM calculation
  - ^{7}Be states $3/2^-$, $1/2^-$, $7/2^-$, $5/2^-_1$, $5/2^-_2$
  - Soft NN potential (chiral SRG-N^{3}LO with Λ = 1.86 fm^{-1})

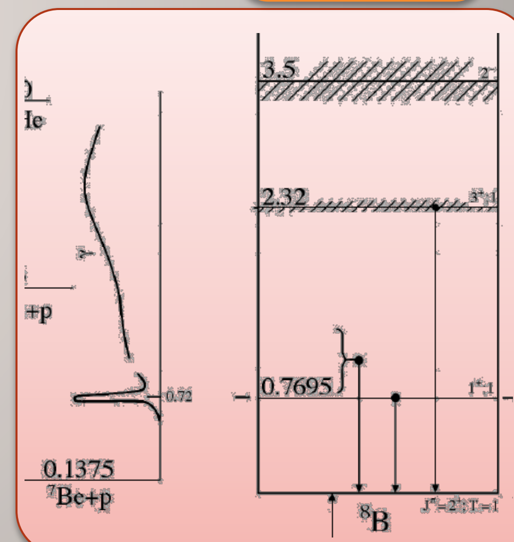
^{8}B 2^+ g.s. **bound** by 136 keV
(expt. 137 keV)

S(0) ~ 19.4(0.7) eV b

Data evaluation:
S(0)=20.8(2.1) eV b

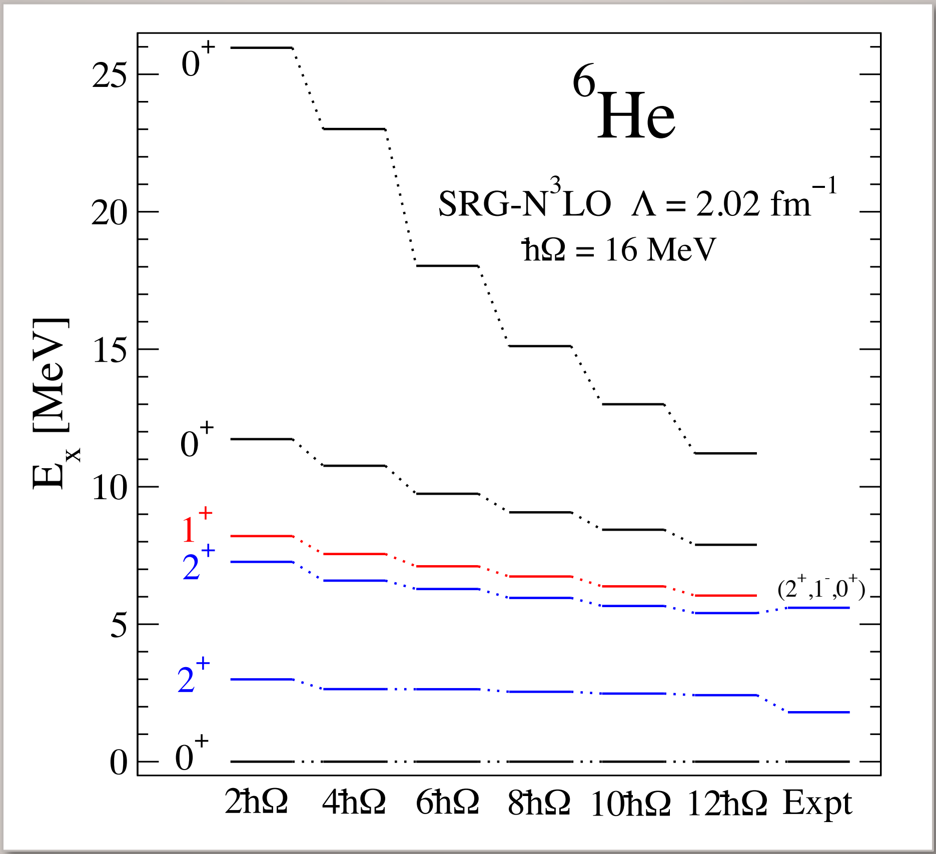






P.N., R. Roth, S. Quaglioni,
Physics Letters B 704 (2011) 379

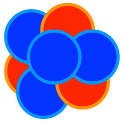
How about ^{7}He as n+^{6}He?



- All ^{6}He excited states above 2^+_1 broad resonances or states in continuum
- Convergence of the NCSM/RGM n+^{6}He calculation slow with number of ^{6}He states
  - Negative parity states also relevant
  - Technically not feasible to include more than ~ 5 states

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

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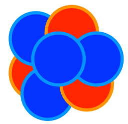

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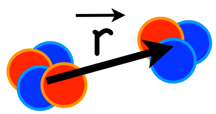
NCSM/RGM



$$|\Psi_A^{J^\pi T}\rangle = \sum_\nu \int d\vec{r} \chi_\nu(\vec{r}) \hat{A} \Phi_{\nu\vec{r}}^{J^\pi T(A-a,a)}$$

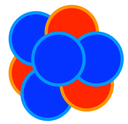
$$\mathcal{H}\chi = E\mathcal{N}\chi$$

$$\bar{\chi} = \mathcal{N}^{+\frac{1}{2}}\chi$$

$$\boxed{(\mathcal{N}^{-\frac{1}{2}}\mathcal{H}\mathcal{N}^{-\frac{1}{2}})\bar{\chi} = E\bar{\chi}}$$

New developments: NCSM with continuum

NCSM



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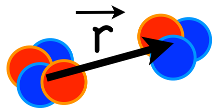

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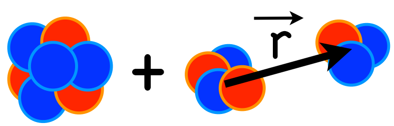
NCSMC

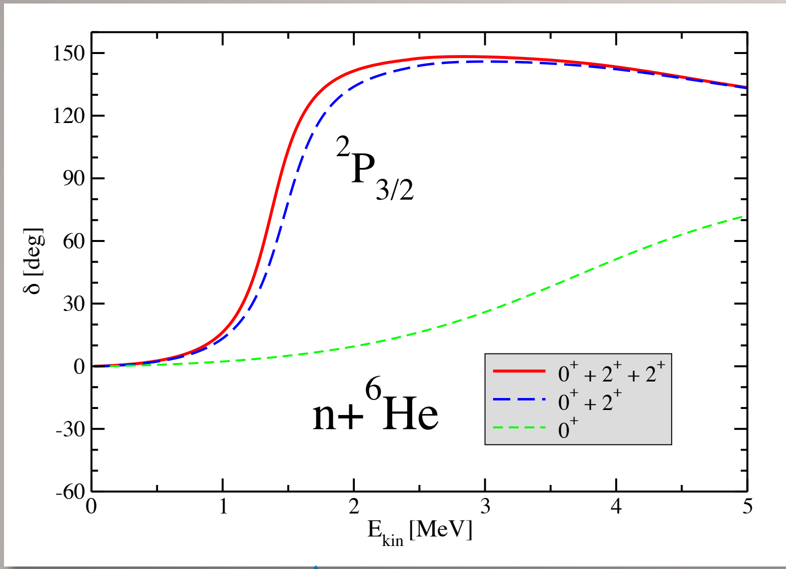


S. Baroni, P. N., and S. Quaglioni,
PRL **110**, 022505 (2013); PRC **87**, 034326 (2013).

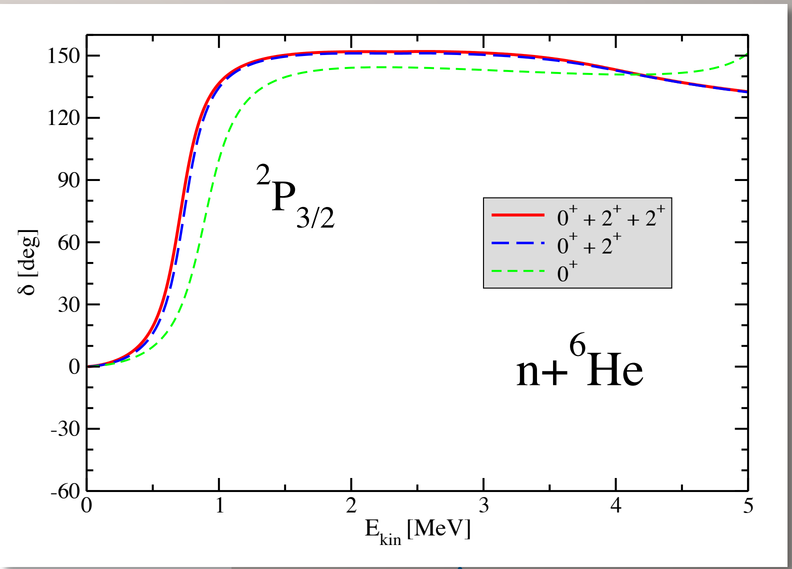
$$|\Psi_A^{J^\pi T}\rangle = \sum_\lambda c_\lambda |A\lambda J^\pi T\rangle + \sum_\nu \int d\vec{r} \left(\sum_{\nu'} \int d\vec{r}\,' \mathcal{N}_{\nu\nu'}^{-\frac{1}{2}}(\vec{r}, \vec{r}\,') \bar{\chi}_{\nu'}(\vec{r}\,') \right) \hat{A} \Phi_{\nu\vec{r}}^{J^\pi T(A-a,a)}$$

$$\begin{pmatrix} H_{NCSM} & \bar{h} \\ \bar{h} & \mathcal{N}^{-\frac{1}{2}}\mathcal{H}\mathcal{N}^{-\frac{1}{2}} \end{pmatrix} \begin{pmatrix} c \\ \bar{\chi} \end{pmatrix} = E \begin{pmatrix} 1 & \bar{g} \\ \bar{g} & 1 \end{pmatrix} \begin{pmatrix} c \\ \bar{\chi} \end{pmatrix}$$

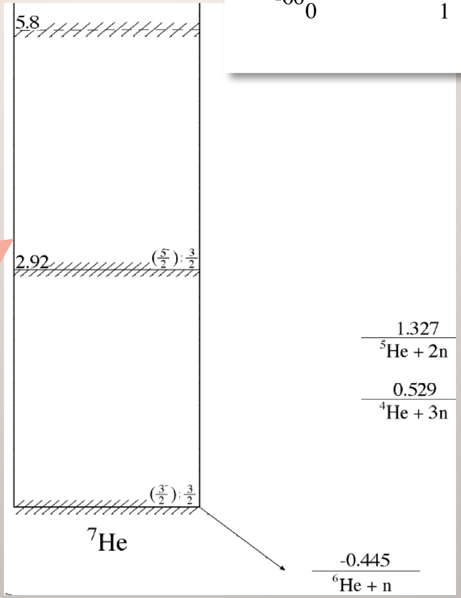
NCSM with continuum: ^{7}He $\leftrightarrow$ ^{6}He+n

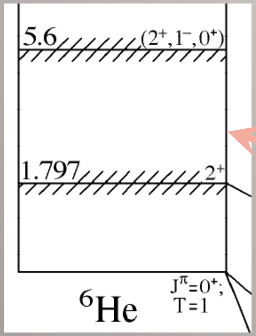


NCSM/RGM
with up to three ^{6}He states



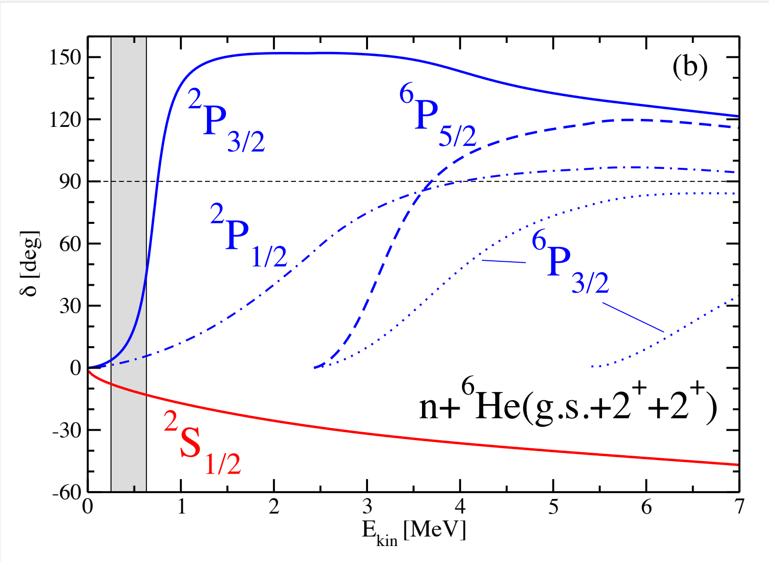
NCSMC
with up to three ^{6}He states
and four ^{7}He eigenstates
More **7-nucleon correlations**
Fewer target states needed



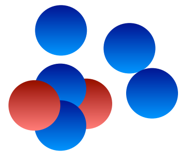


Expt.

NCSM with continuum: ^{7}He ↔ ^{6}He+*n*



^{7}He

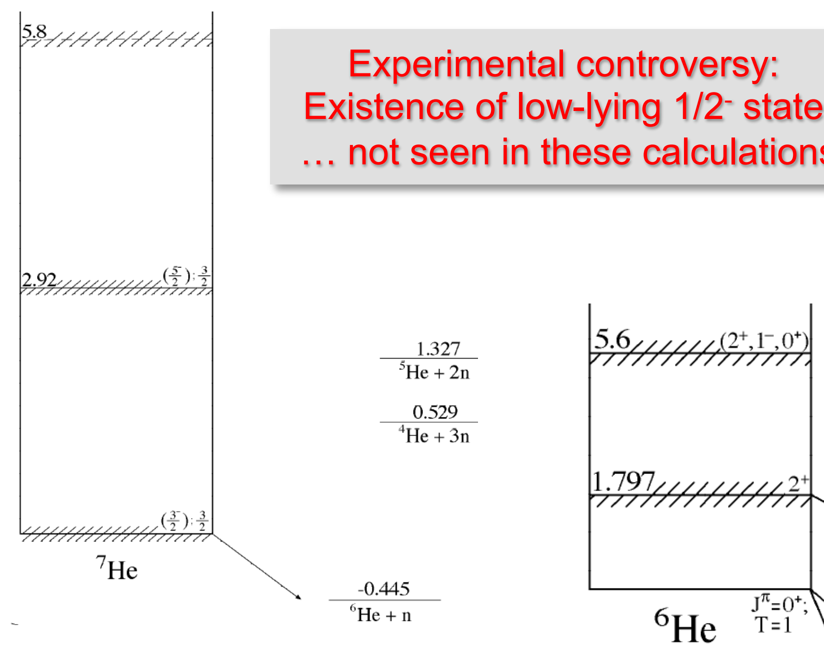


unbound

J^{π}	experiment E_R	Γ	Ref.	NCSMC E_R	Γ
$3/2^-$	0.430(3)	0.182(5)	[2]	0.71	0.30
$5/2^-$	3.35(10)	1.99(17)	[40]	3.13	1.07
$1/2^-$	3.03(10)	2	[11]	2.39	2.89
	3.53	10	[15]		
	1.0(1)	0.75(8)	[5]		

[11] A. H. Wuosmaa *et al.*, Phys. Rev. C **72**, 061301 (2005).

NCSMC
with three ^{6}He states
and ten ^{7}He eigenstates
More **7-nucleon correlations**
Fewer ^{6}He-core states needed

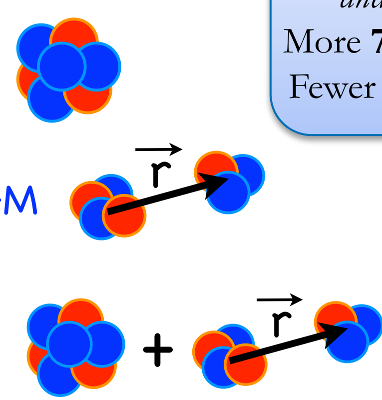


Experimental controversy:
Existence of low-lying $1/2^-$ state
… not seen in these calculations

NCSM

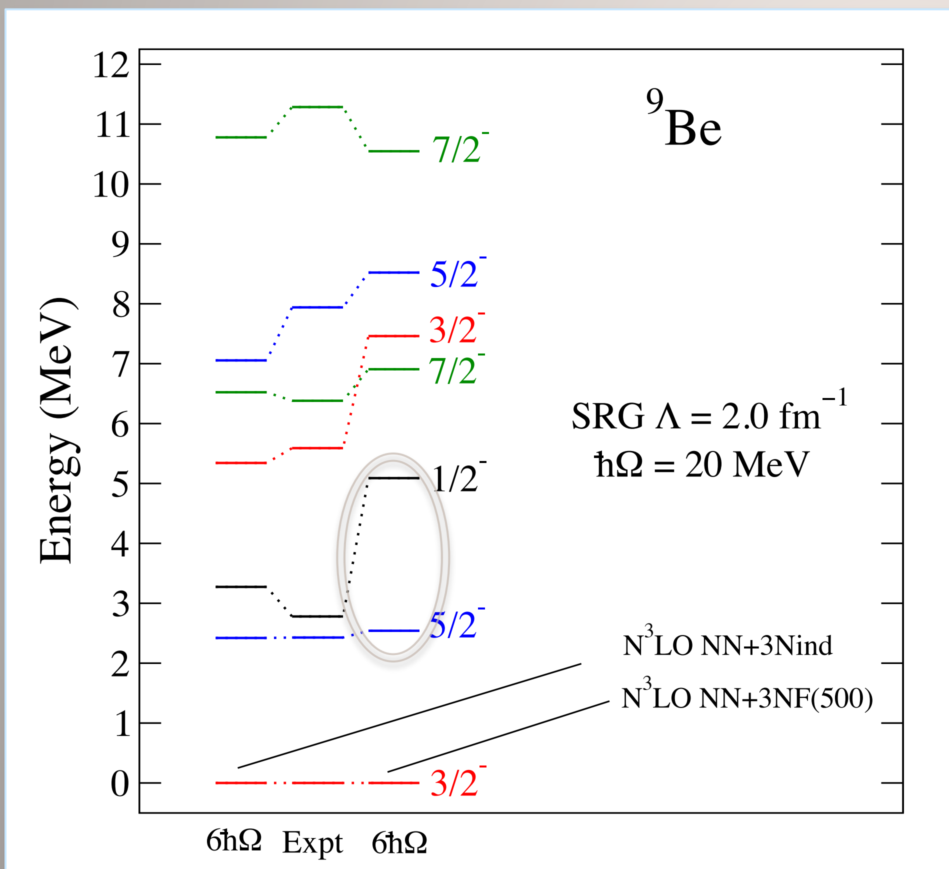
NCSM/RGM

NCSMC



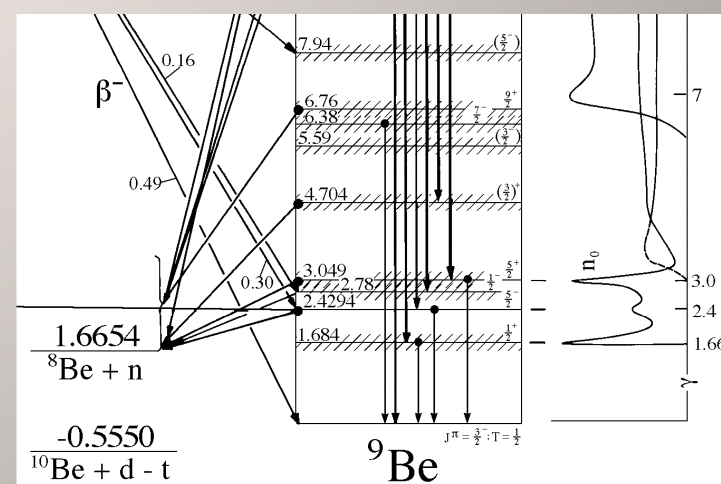
Structure of ^{9}Be

- The lightest nucleus where the 3N interaction appear to make the description of low lying states worse: Does this suggest our 3N interaction models are wrong?



1/2⁻ state moved to high energy by the 3N interaction

However, all excited states are resonances. What is the effect of the continuum?



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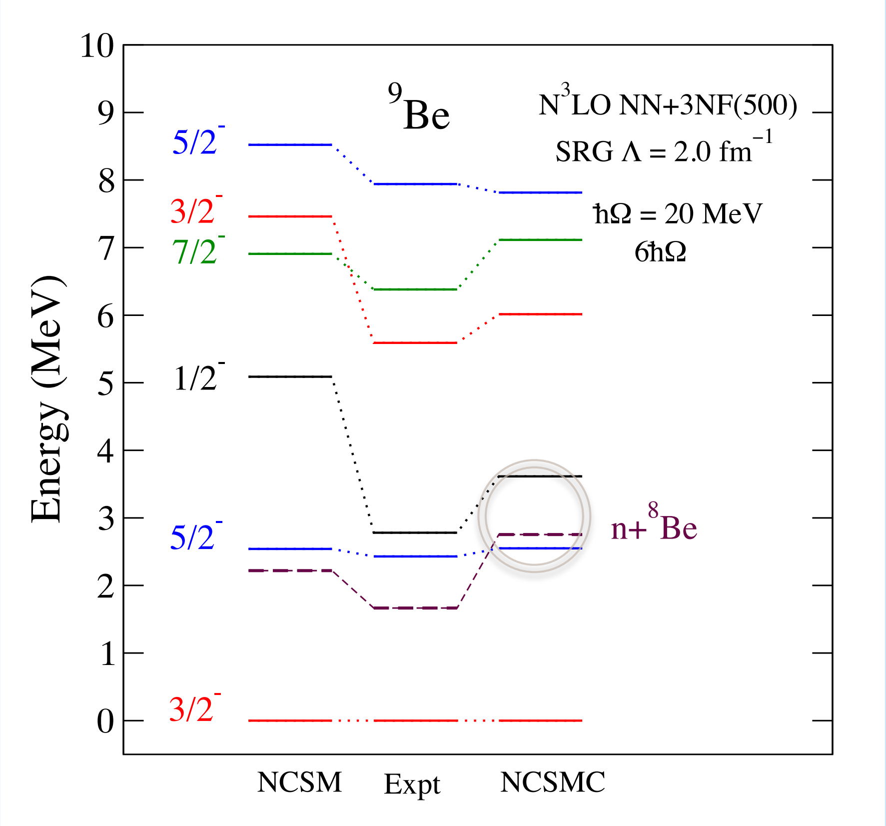


NCSMC with the 3N under way

Preliminary results in N_{max}=6 space:

5/2$^-$ a very narrow (or bound) *F*-wave – no shift

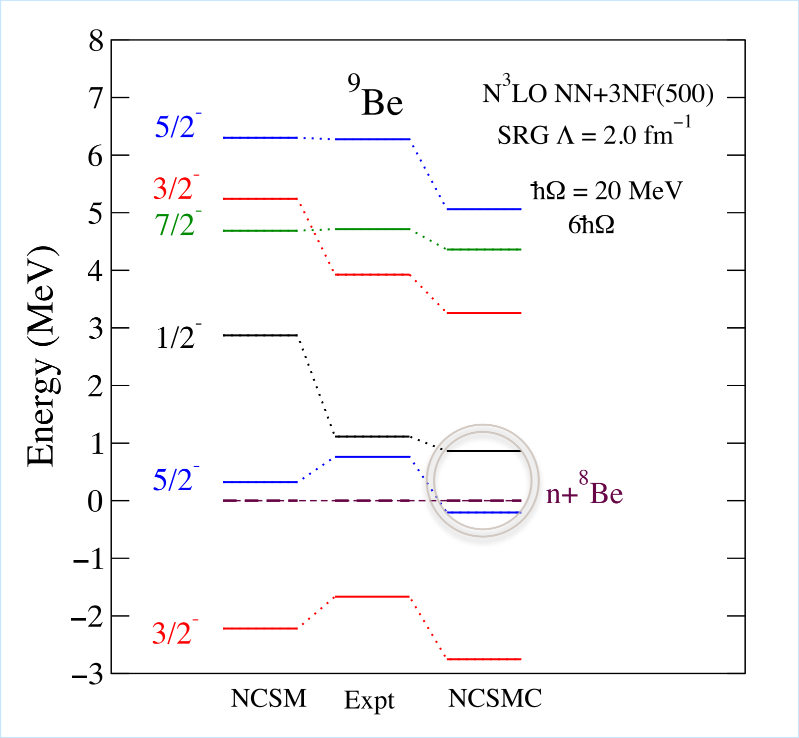
1/2$^-$ a broader *P*-wave – a large shift due to the continuum

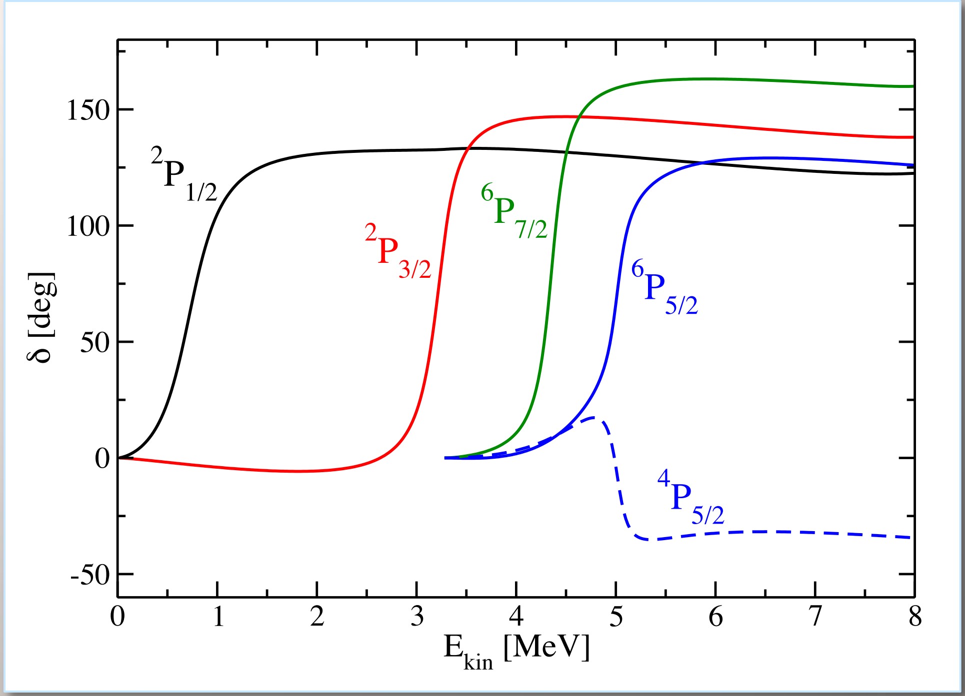
Structure of ^{9}Be

- The lightest nucleus where the 3N interaction appear to make the description of low lying states worse: Does this suggest our 3N interaction models are wrong?

No!

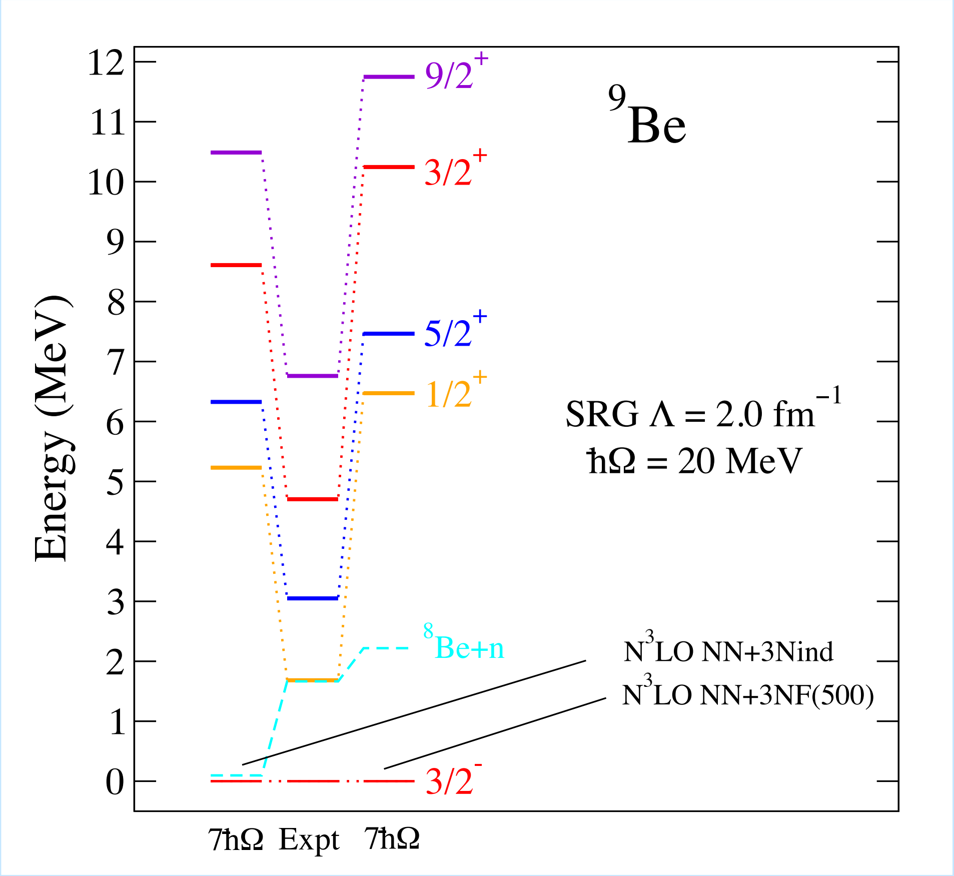
NCSMC
n-^{8}Be(0^+,2^+) + ^{9}Be





Structure of ^{9}Be

- The unnatural parity states are predicted too high in the NCSM calculations. Is this a HO basis size problem? Is this an interaction dependent problem?



Bad with any interaction

Large HO basis size (N_{max}) definitely helps.

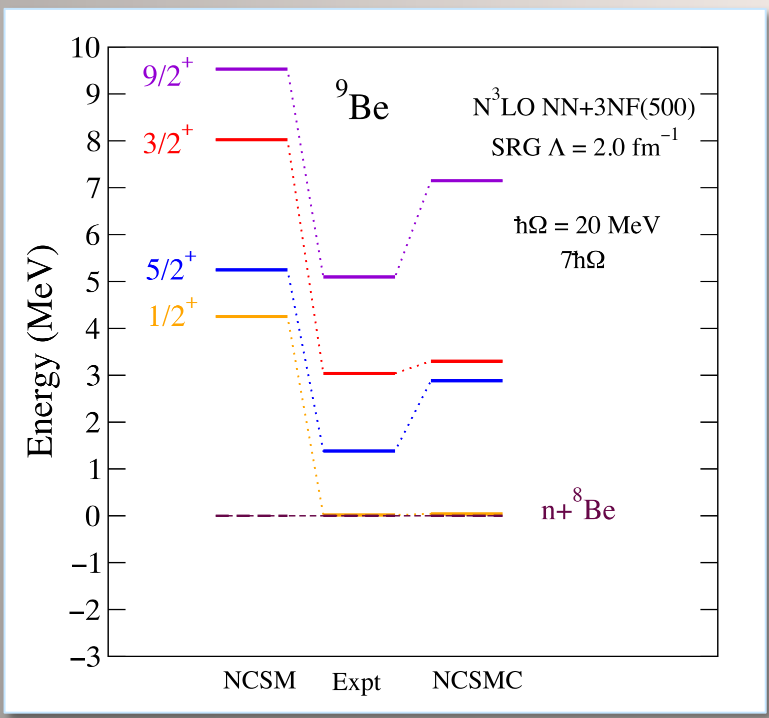
But…

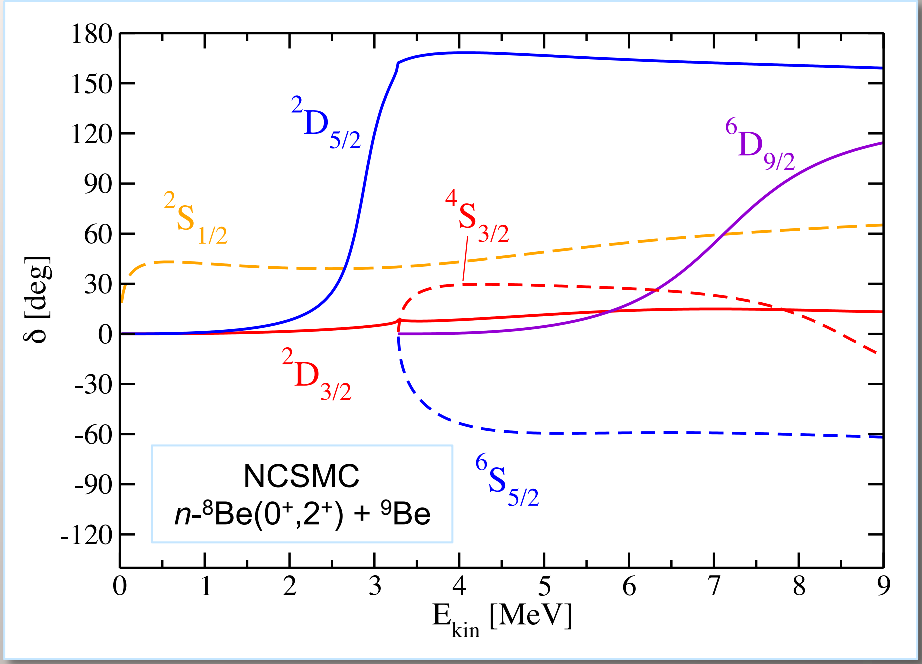
Structure of ^{9}Be

- The unnatural parity states are predicted too high in the NCSM calculations. Is this a HO basis size problem? Is this an interaction dependent problem?

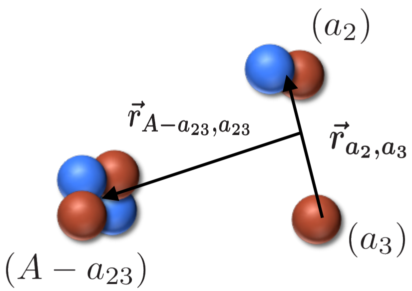
Need to switch to NCSMC!

Breakup thresholds impact *S*-waves
Continuum important for other waves as well





NCSM/RGM for three-body clusters



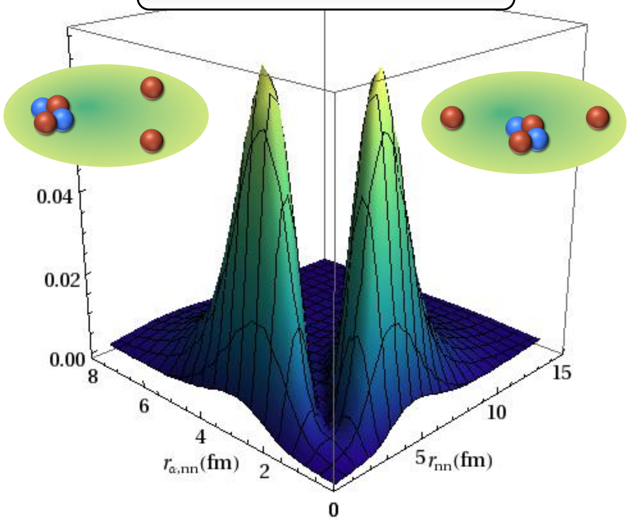
$$|\Phi^{J^\pi T}_{\nu r}\rangle \sim \Psi^{A-a_{23}}_{\alpha_1}\ \Psi^{a_2}_{\alpha_2}\ \Psi^{a_3}_{\alpha_3}$$

NCSM

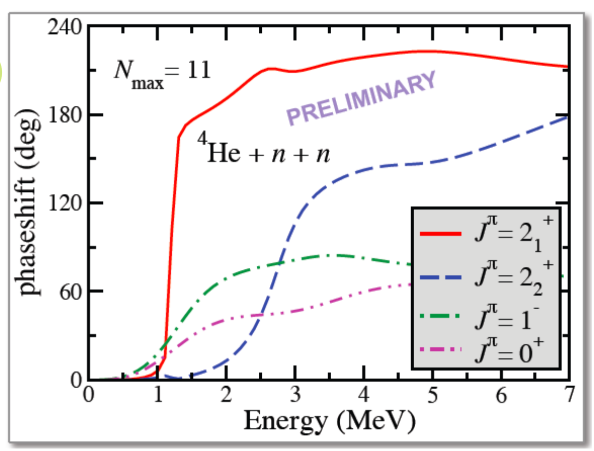
$$|\Psi^{J^\pi T}\rangle = \sum_\nu \int dx x^2 \int dy y^2 G_\nu^{J^\pi T}(x,y)\hat{A}_\nu |\Phi^{J^\pi T}_{\nu xy}\rangle$$

^{4}He(g.s.)+n+n

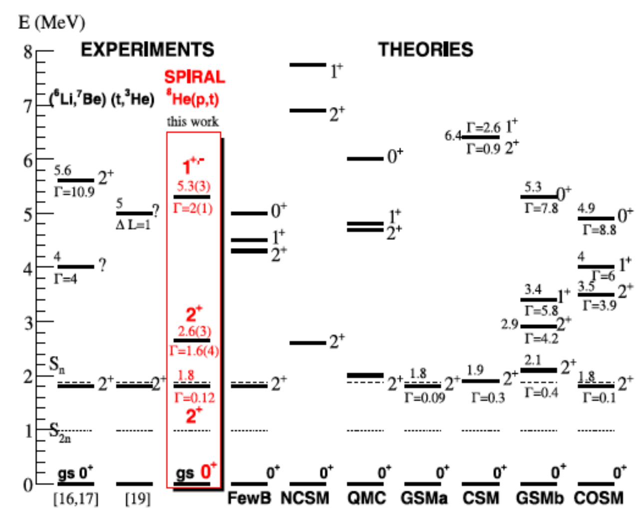
$$\ell_x = \ell_y = L = S_{nn} = 0$$



Phaseshifts (preliminary results)



Recent exp.: Phys. Lett. B 718 (2012) 441



Talk by Carolina Romero-Redondo, B3, Tuesday 15:50

TRIUMF

Conclusions and Outlook

- *Ab initio* calculations of nuclear structure and reactions is a dynamic field with significant 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:
  - Inclusion of three-nucleon interactions in reaction calculations for A>5 systems
  - Extension to composite projectiles (deuteron, ^{3}H, ^{3}He, ^{4}He)
  - Extension to three-body clusters (^{6}He ~ ^{4}He+n+n)
  - Composite-projectile reactions on targets heavier than ^{4}He

Talk by Guillaume Hupin, A5, Wednesday 15:50

Talk by Carolina Romero-Redondo, B3, Tuesday 15:50

NCSMC and NCSM/RGM collaborators

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Joachim Langhammer, Angelo Calci, Robert Roth (TU Darmstadt)

Carolina Romero-Redondo, Francesco Raimondi (TRIUMF)

Guillaume Hupin, Michael Kruse (LLNL)

Simone Baroni (ULB)