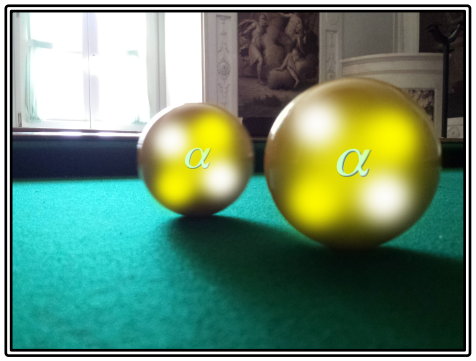
Ab initio approaches to nuclear reactions

Dean Lee
North Carolina State University
Nuclear Lattice EFT Collaboration

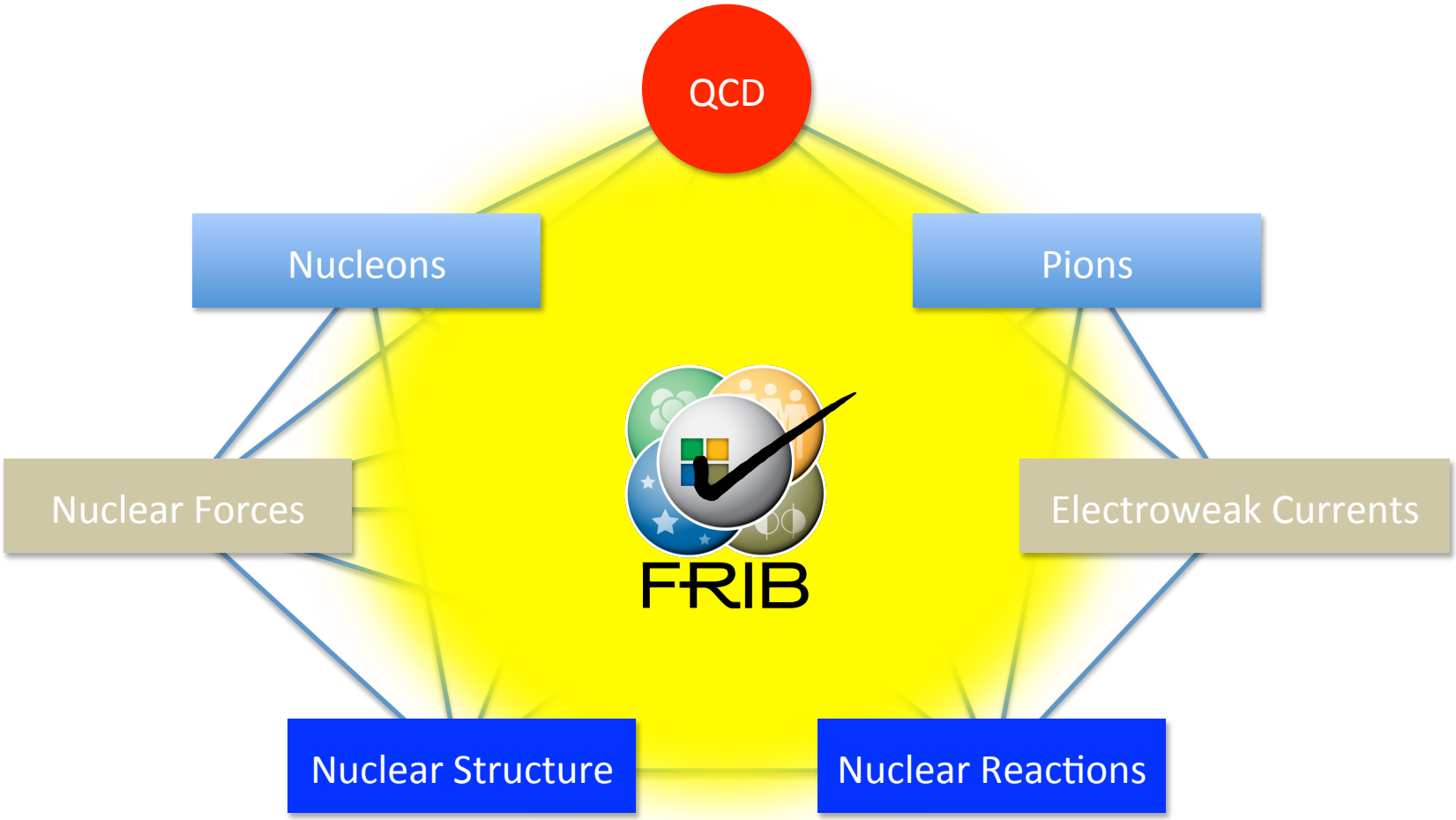


$$\Psi^{(A)} = \sum_{\lambda} c_{\lambda} \left| {}^{(A)} \right\rangle, \lambda \rangle + \sum_{\nu} \int d\vec{r}\ \gamma_{\nu}(\vec{r}\,)\ \hat{A}_{\nu} \left| \vec{r} \right\rangle_{(A-a)} \; {}_{(a)} \rangle, \nu \rangle$$

With thanks to Thomas Neff and Petr Navratil for providing slides

FRIB Theory Alliance Meeting
Michigan State University, April 1, 2016

A Golden Era for *Ab Initio* Nuclear Theory



See Amy Nicholson's talk this afternoon about this lattice QCD calculation

PRL 115, 132001 (2015) PHYSICAL REVIEW LETTERS week ending 25 SEPTEMBER 2015

Ab initio Calculation of the $np \to d\gamma$ Radiative Capture Process

Silas R. Beane,[1] Emmanuel Chang,[2] William Detmold,[3] Kostas Orginos,[4,5] Assumpta Parreño,[6] Martin J. Savage,[2] and Brian C. Tiburzi[7,8,9]

(NPLQCD Collaboration)

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[7]*Department of Physics, The City College of New York, New York, New York 10031, USA*
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(Received 25 June 2015; revised manuscript received 14 August 2015; published 24 September 2015)

Lattice QCD calculations of two-nucleon systems are used to isolate the short-distance two-body electromagnetic contributions to the radiative capture process $np \to d\gamma$, and the photo-disintegration processes $\gamma^{(*)}d \to np$. In nuclear potential models, such contributions are described by phenomenological meson-exchange currents, while in the present work, they are determined directly from the quark and gluon interactions of QCD. Calculations of neutron-proton energy levels in multiple background magnetic fields are performed at two values of the quark masses, corresponding to pion masses of $m_\pi \sim 450$ and 806 MeV, and are combined with pionless nuclear effective field theory to determine the amplitudes for these low-energy inelastic processes. At $m_\pi \sim 806$ MeV, using only lattice QCD inputs, a cross section $\sigma^{806\ \mathrm{MeV}} \sim 17$ mb is found at an incident neutron speed of $v = 2,200$ m/s. Extrapolating the short-distance contribution to the physical pion mass and combining the result with phenomenological scattering information and one-body couplings, a cross section of $\sigma^{\mathrm{lqcd}}(np \to d\gamma) = 334.9(^{+5.2}_{-5.4})$ mb is obtained at the same incident neutron speed, consistent with the experimental value of $\sigma^{\mathrm{expt}}(np \to d\gamma) = 334.2(0.5)$ mb.

DOI: 10.1103/PhysRevLett.115.132001 PACS numbers: 12.38.Gc, 11.15.Ha, 13.40.Gp

^{3}He(α,γ)^{7}Be and ^{3}H(α,γ)^{7}Li Radiative Capture

Microscopic description of structure and reactions in Fermionic Molecular Dynamics

PRL **106,** 042502 (2011) PHYSICAL REVIEW LETTERS week ending 28 JANUARY 2011

Microscopic Calculation of the ^{3}He$(\alpha, \gamma)^7$Be and ^{3}H$(\alpha, \gamma)^7$Li Capture Cross Sections Using Realistic Interactions

Thomas Neff*

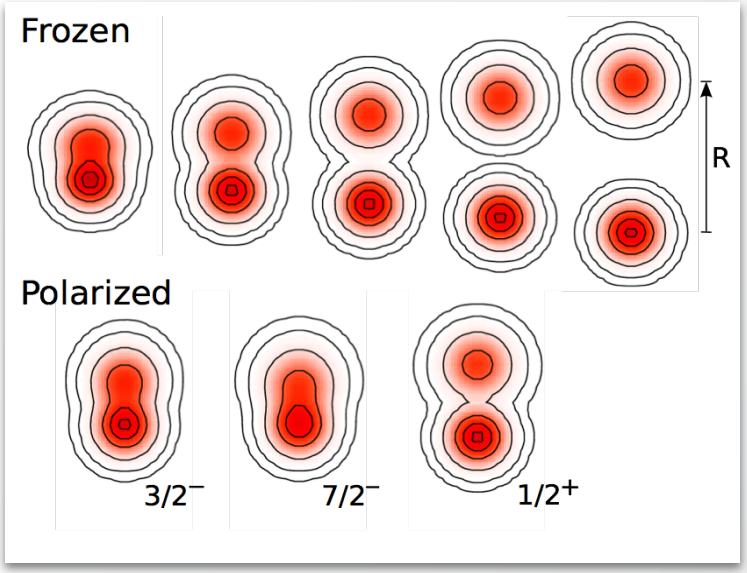
GSI Helmholtzzentrum für Schwerionenforschung GmbH, Planckstraße 1, 64291 Darmstadt, Germany

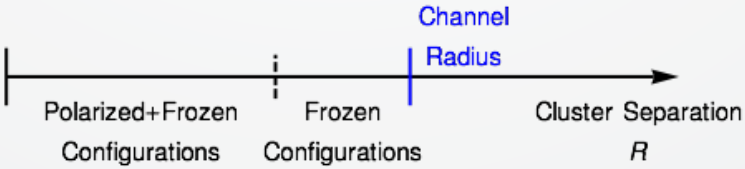
(Received 12 November 2010; published 25 January 2011)

Fermionic Molecular Dynamics

- FMD wave functions use **Gaussian wave packets** as single-particle basis states
- Many-body basis states are Slater determinants projected on parity, angular momentum and total linear momentum
- FMD basis contains both harmonic oscillator and Brink-type cluster wave functions as special cases
- a realistic low-momentum interaction is obtained from the Argonne v_{18} interaction by the Unitary Correlation Operator Method in two-body approximation
- **Polarized** configurations are obtained by **variation after projection** for all spins and parities

- **Frozen** configurations are generated from ^{4}He and ^{3}He ground states
- at the channel radius many-body wave functions are matched to Whittaker and Coulomb solutions for point-like clusters with the ***R*-matrix** method





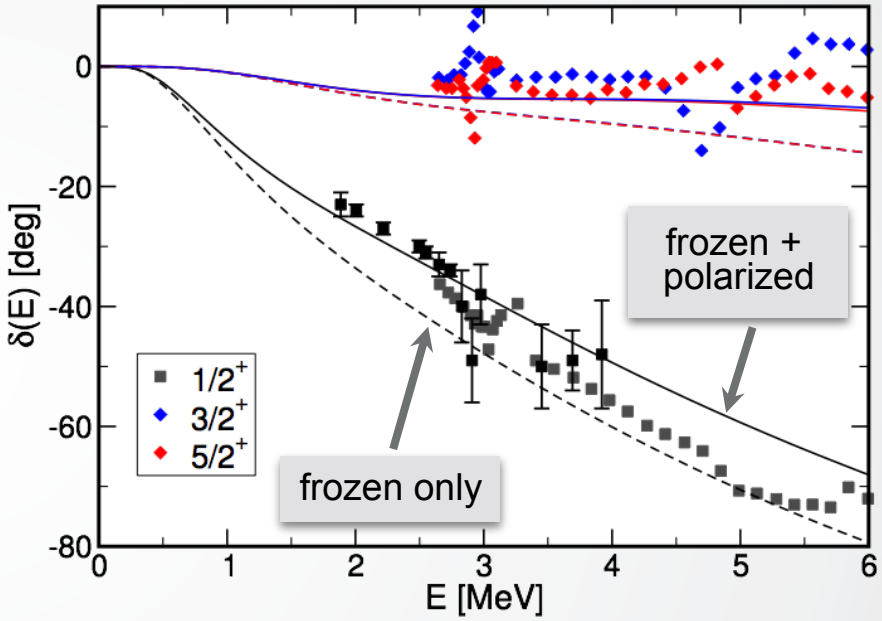
Bound and Scattering States

Bound States

		FMD	Experiment
^{7}Be	$E_{3/2^-}$ [MeV]	-1.49	-1.59
	$E_{1/2^-}$ [MeV]	-1.31	-1.15
	r_{ch} [fm]	2.67	2.647(17)
	Q [e fm^2]	-6.83	-
^{7}Li	$E_{3/2^-}$ [MeV]	-2.39	-2.467
	$E_{1/2^-}$ [MeV]	-2.17	-1.989
	r_{ch} [fm]	2.46	2.444(43)
	Q [e fm^2]	-3.91	-4.00(3)

- centroid energy of bound states well reproduced, splitting between $3/2^-$ and $1/2^-$ states too small
- charge radii and quadrupole moment test the tails of bound state wave functions

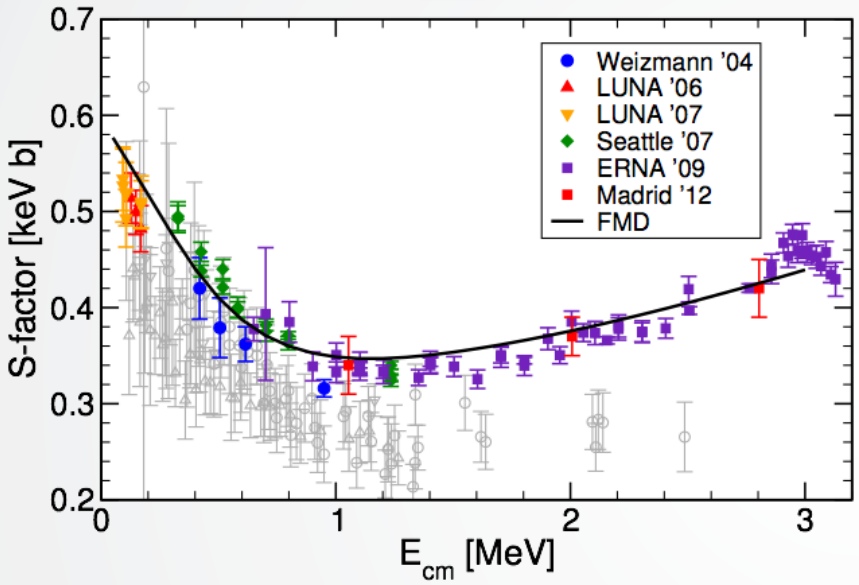
Scattering States



- *s- and d-wave capture dominate at small energies*
- *polarized configurations are important for describing the phase shifts*

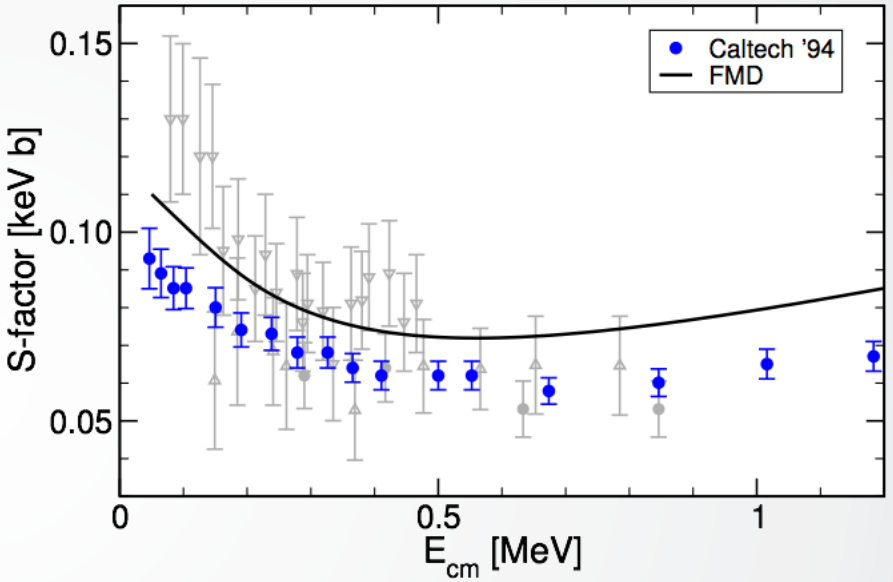
Capture Cross Section

$^3He(\alpha,\gamma)^7Be$



- good agreement with new high quality $^3He(\alpha,\gamma)^7Be$ data regarding both energy dependence and normalization

$^3H(\alpha,\gamma)^7Li$



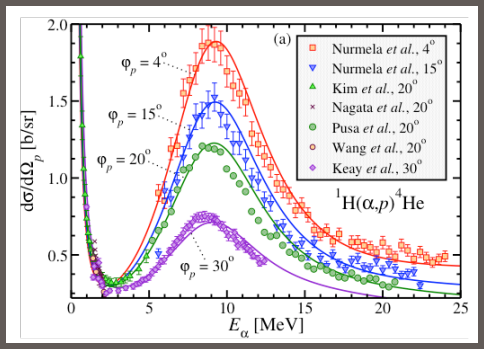
- calculations reproduce energy dependence but not normalization of $^3H(\alpha,\gamma)^7Li$ data by Brune *et al.*

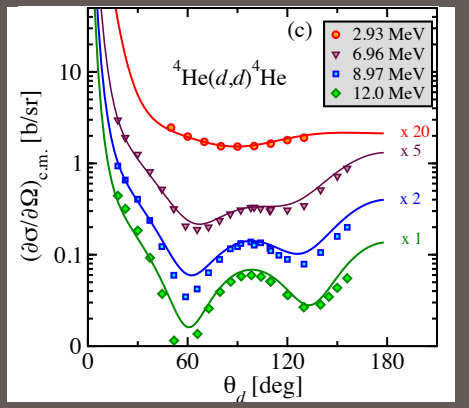
TRIUMF

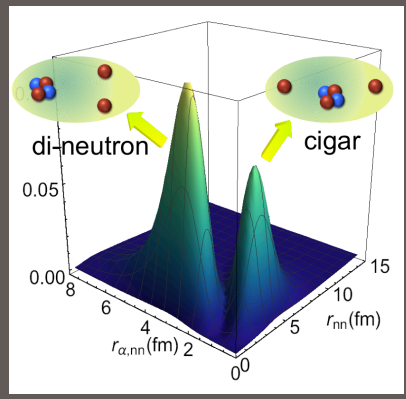
Canada's national laboratory for particle and nuclear physics
Laboratoire national canadien pour la recherche en physique nucléaire
et en physique des particules

Unified approach to nuclear structure and reactions within the No-Core Shell Model with Continum (NCSMC)

Sofia Quaglioni, Carolina Romero-Redondo (LLNL)
Petr Navratil, Jeremy Dohet-Eraly, Angelo Calci (TRIUMF)
Guillaume Hupin (CEA/DAM)

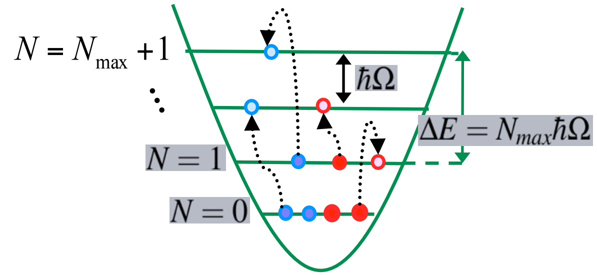




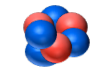


Unified approach to bound & continuum states; to nuclear structure & reactions

- *Ab initio* no-core shell model
  - Short- and medium range correlations
  - Bound-states, narrow resonances



Harmonic oscillator basis



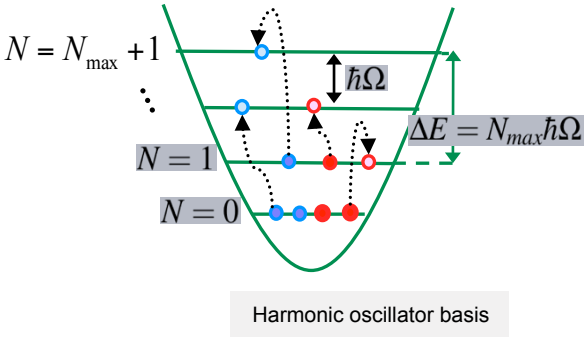
NCSM

$$\Psi^{(A)} = \sum_{\lambda} c_{\lambda} \left| (A), \lambda \right\rangle$$

Unknowns

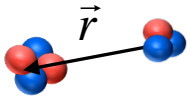
Unified approach to bound & continuum states; to nuclear structure & reactions

- *Ab initio* no-core shell model
  - Short- and medium range correlations
  - Bound-states, narrow resonances



NCSM

- …with resonating group method
  - Bound & scattering states, reactions
  - Cluster dynamics, long-range correlations



NCSM/RGM

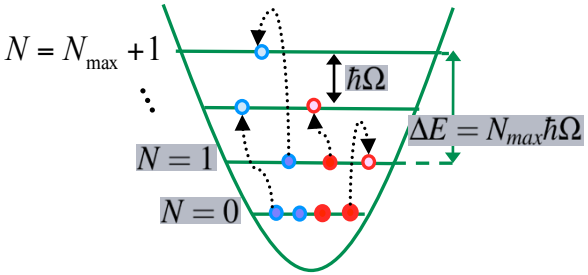
$$\Psi^{(A)} = \sum_{\nu} \int d\vec{r}\ \gamma_{\nu}(\vec{r})\ \hat{A}_{\nu} \left| \overbrace{\vec{r}\ \ (a)}^{(A-a)}\ , \nu \right\rangle$$

NCSM/RGM channel states

Unknowns

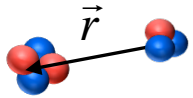
Unified approach to bound & continuum states; to nuclear structure & reactions

- *Ab initio* no-core shell model
  - Short- and medium range correlations
  - Bound-states, narrow resonances



NCSM

- …with resonating group method
  - Bound & scattering states, reactions
  - Cluster dynamics, long-range correlations



NCSM/RGM

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

- Most efficient: *ab initio* no-core shell model with continuum

NCSMC

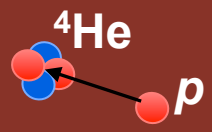
NCSM eigenstates

NCSM/RGM channel states

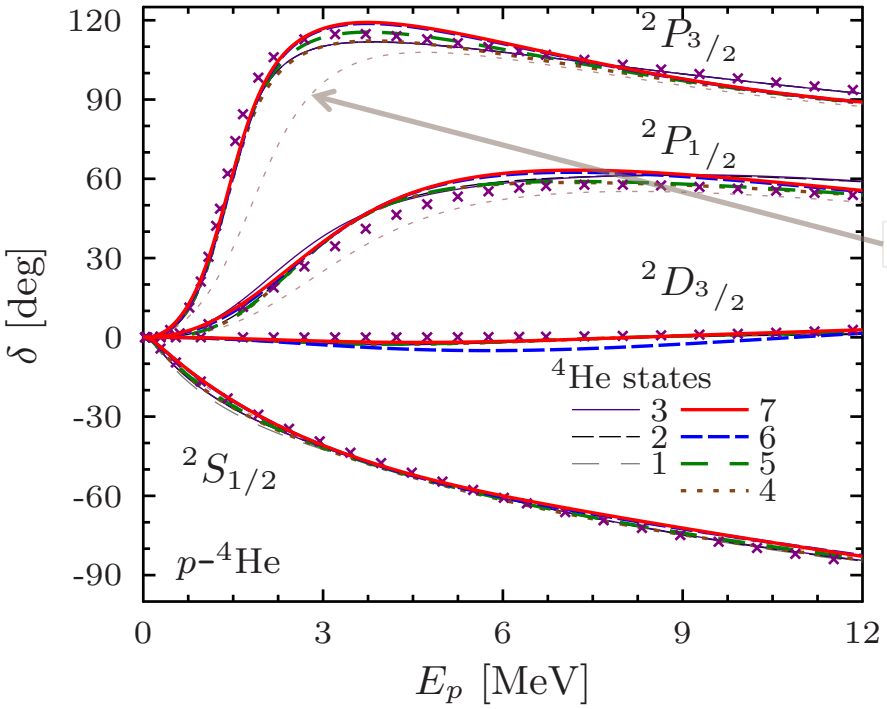
$$\Psi^{(A)} = \sum_{\lambda} c_{\lambda} \left| (A), \lambda \right\rangle + \sum_{\nu} \int d\vec{r}\ \gamma_{\nu}(\vec{r})\ \hat{A}_{\nu} \left| (A-a), (a), \vec{r}, \nu \right\rangle$$

Unknowns

p-^{4}He scattering within NCSMC



p-^{4}He scattering phase-shifts for NN+3N potential: Convergence



Short- and medium range correlation from NCSM eigenstates essential for convergence

Predictive power in the 3/2$^-$ resonance region: Applications to material science

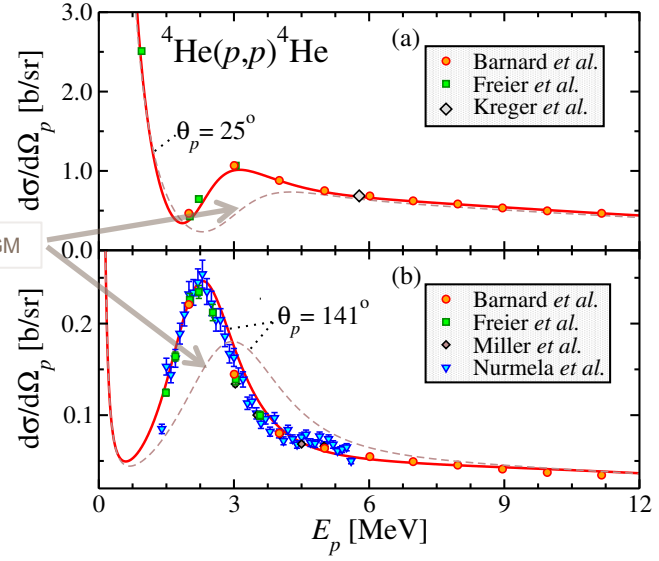
PHYSICAL REVIEW C **90**, 061601(R) (2014)

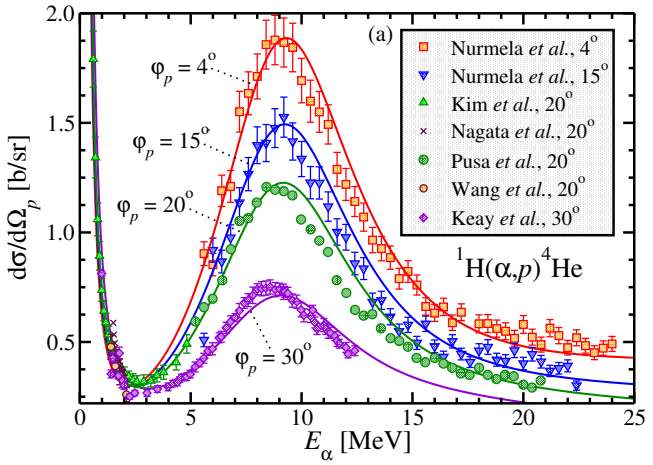
Predictive theory for elastic scattering and recoil of protons from ^{4}He

Guillaume Hupin,[1,*] Sofia Quaglioni,[1,†] and Petr Navrátil[2,‡]

Differential p-^{4}He cross section with NN+3N potentials

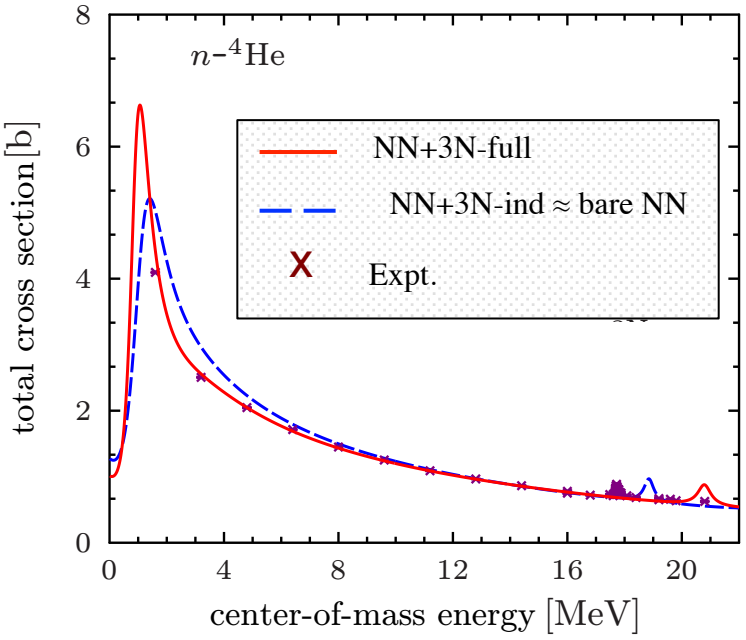
NCSM/RGM





Importance of 3N interaction for scattering and structure

Total n-^{4}He cross section with NN and NN+3N potentials

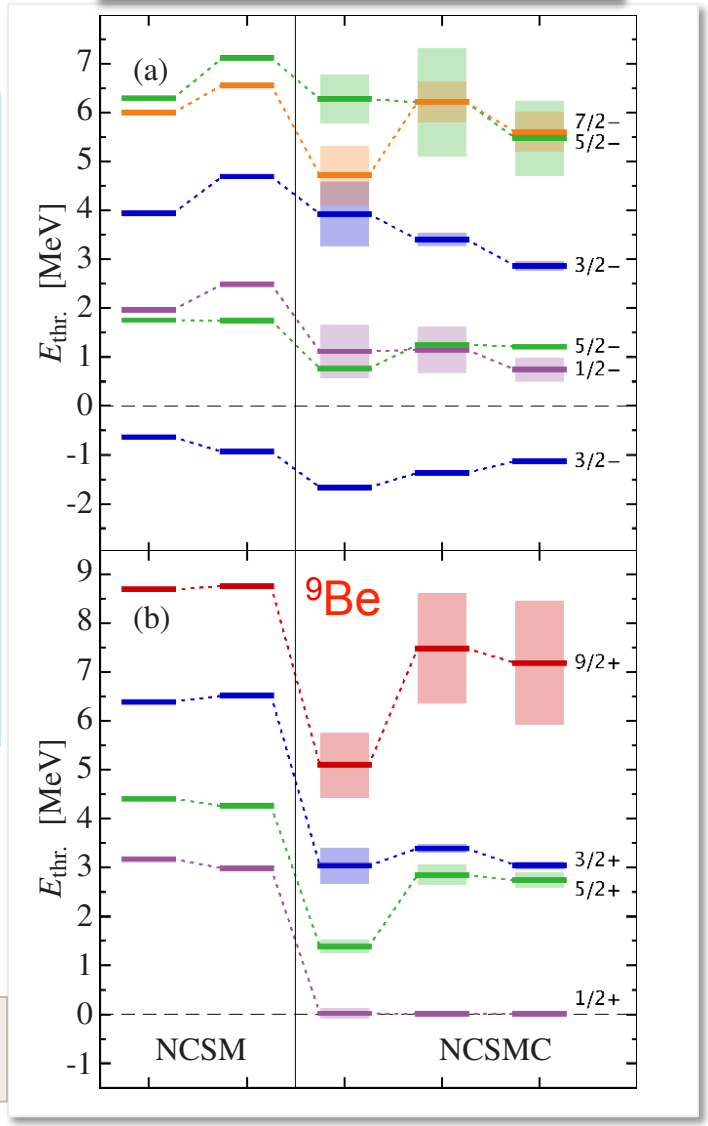


^{9}Be
is a stable
nucleus
… but all its
excited states
unbound

3N interaction
&
continuum
improve
agreement
with
experiment

3N force enhances $1/2^- \leftrightarrow 3/2^-$ splitting:
Essential at low energies!

NN NN+3N Expt. NN+3N NN



IOP Publishing | Royal Swedish Academy of Sciences | Physica Scripta
Phys. Scr. 00 (2016) 000000 (37pp)

Invited Comment

Unified *ab initio* approaches to nuclear structure and reactions

Petr Navrátil[1], Sofia Quaglioni[2], Guillaume Hupin[3,4], Carolina Romero-Redondo[2] and Angelo Calci[1]

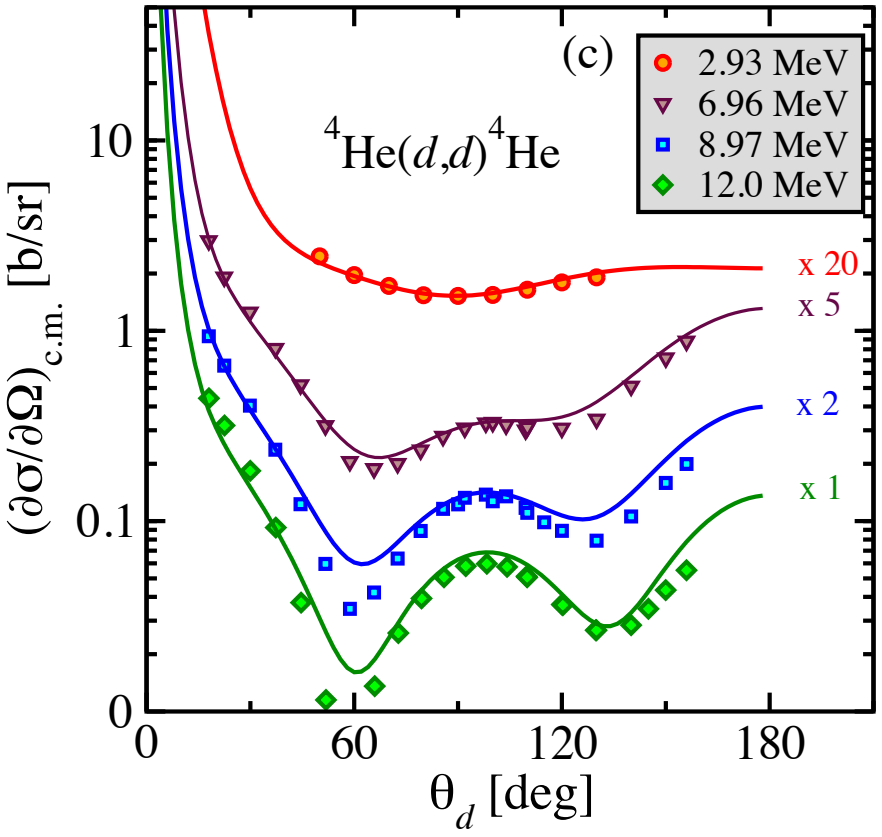
PHYSICAL REVIEW C **91**, 021301(R) (2015)

Continuum and three-nucleon force effects on ^{9}Be energy levels

Joachim Langhammer,[1,*] Petr Navrátil,[2,†] Sofia Quaglioni,[3] Guillaume Hupin,[3,‡] Angelo Calci,[1,2] and Robert Roth[1,§]

Structure & reactions with composite projectiles within NCSMC

Unified description of d+^{4}He and ^{6}Li with chiral NN+3N forces

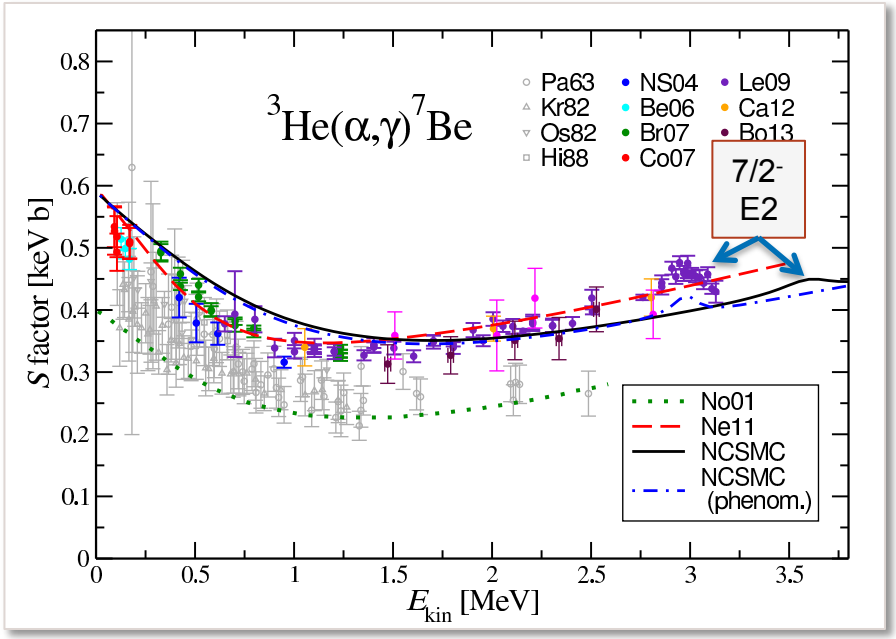


PRL 114, 212502 (2015) PHYSICAL REVIEW LETTERS week ending 29 MAY 2015

Unified Description of ^{6}Li Structure and Deuterium-^{4}He Dynamics with Chiral Two- and Three-Nucleon Forces

Guillaume Hupin,[1,*] Sofia Quaglioni,[1,†] and Petr Navrátil[2,‡]

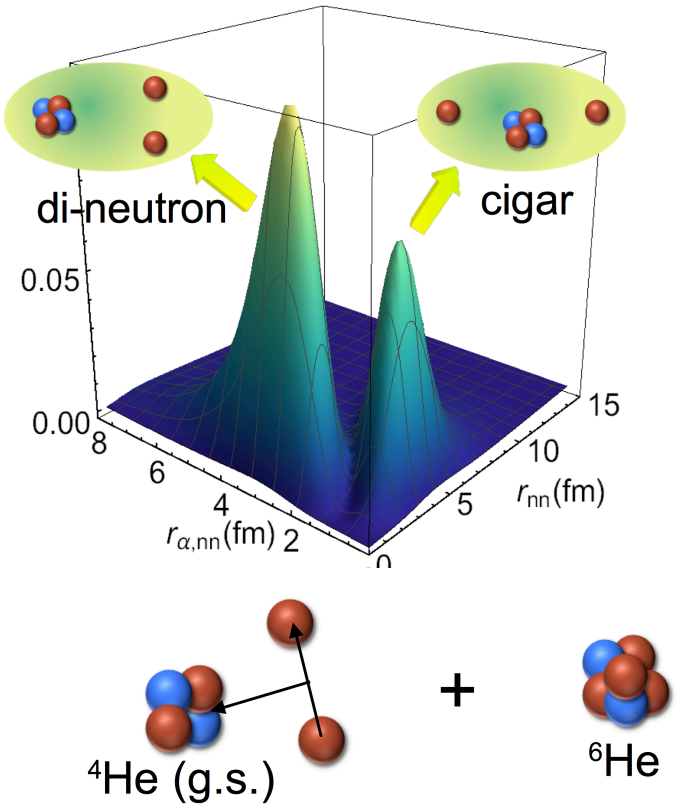
^{3}He(α,γ)^{7}Be radiative capture with NN force



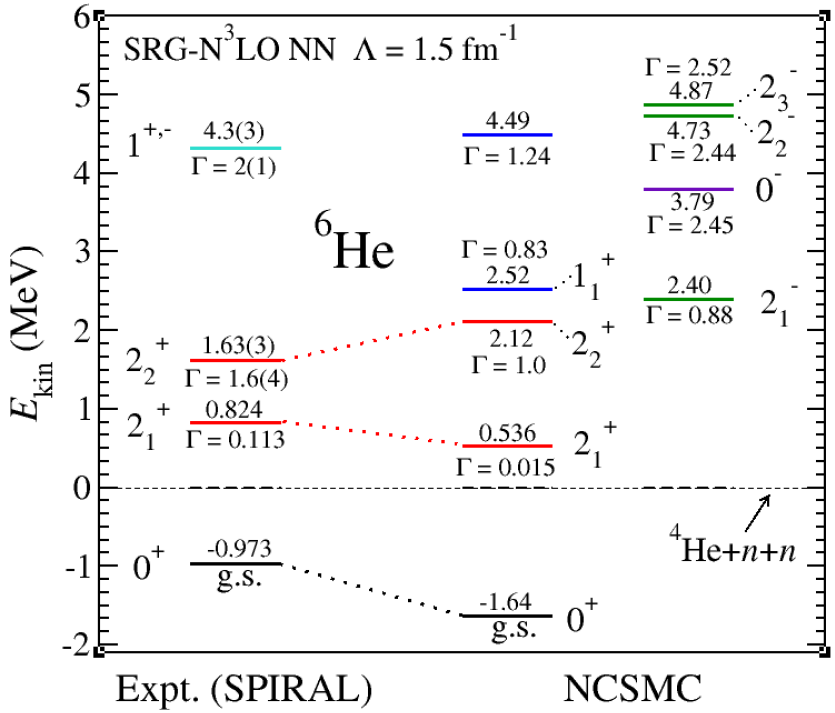
J. Dohet-Eraly, P. Navratil, S. Quaglioni, W. Horiuchi, G. Hupin, F. Raimondi, arXiv:1510.07717 [nucl-th]

NCSMC for three-body clusters: ^{6}He ~ ^{4}He+n+n

The probability distribution of the ^{6}He g.s.: The di-neutron and cigar configurations



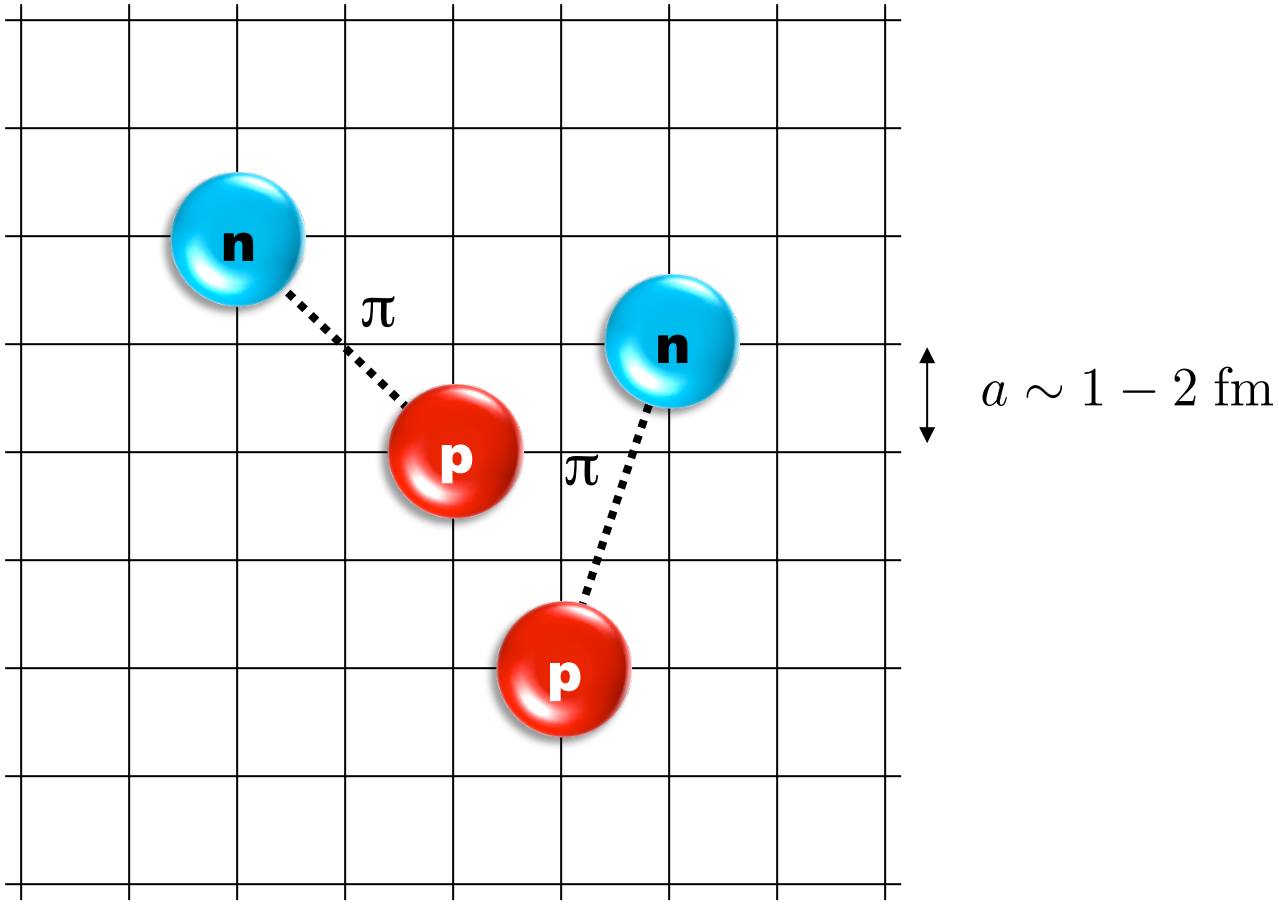
NCSMC calculations with NN interaction predict lots of low-lying resonances. Experimental picture incomplete



Height of peaks impacted by ^{4}He core excitations achieved via ^{6}He NCSM eigenstate

C. Romero-Redondo, S. Quaglioni, P. Navrátil, G. Hupin, arXiv: 1509.00878

Lattice chiral effective field theory



Review: D.L, Prog. Part. Nucl. Phys. 63 117-154 (2009)

Challenges

How to reduce computational scaling with number of nucleons in participating nuclei?

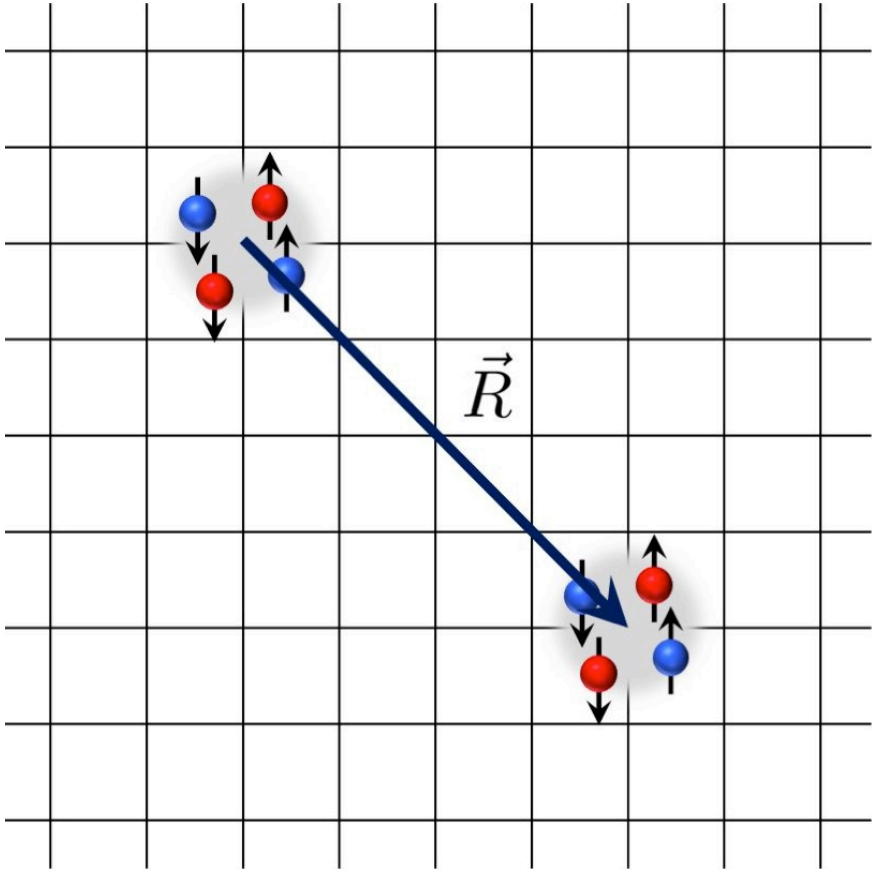
Adiabatic projection method

Strategy is to divide the problem into two parts. In the first part, we use Euclidean time projection and lattice Monte Carlo to derive an *ab initio* low-energy cluster Hamiltonian, called the adiabatic Hamiltonian (adiabatic transfer matrix for nonzero temporal lattice spacing).

In the second part, we use the adiabatic Hamiltonian to compute scattering phase shifts or reaction amplitudes.

Start with localized cluster states for all possible separation vectors $\vec{R}$

$$|\vec{R}\rangle = \sum_{\vec{r}} |\vec{r}+\vec{R}\rangle_1 \otimes |\vec{r}\rangle_2$$



Use projection Monte Carlo to propagate cluster wavefunctions in Euclidean time to form dressed cluster states

$$|\vec{R}\rangle_\tau = \exp(-H\tau)|\vec{R}\rangle$$

Evaluate matrix elements of the full microscopic Hamiltonian with respect to the dressed cluster states,

$$[H_\tau]_{\vec{R},\vec{R}'} = {}_\tau\langle\vec{R}|H|\vec{R}'\rangle_\tau$$

Since the dressed cluster states are in general not orthogonal, we construct a norm matrix given by the inner product

$$[N_\tau]_{\vec{R},\vec{R}'} = {}_\tau\langle\vec{R}|\vec{R}'\rangle_\tau$$

The adiabatic Hamiltonian is defined by the matrix product

$$[H^a_\tau]_{\vec{R},\vec{R}'} = \left[N_\tau^{-1/2} H_\tau N_\tau^{-1/2}\right]_{\vec{R},\vec{R}'}$$

Distortion and polarization of the nuclear wave functions are automatically produced by the Euclidean time projection.

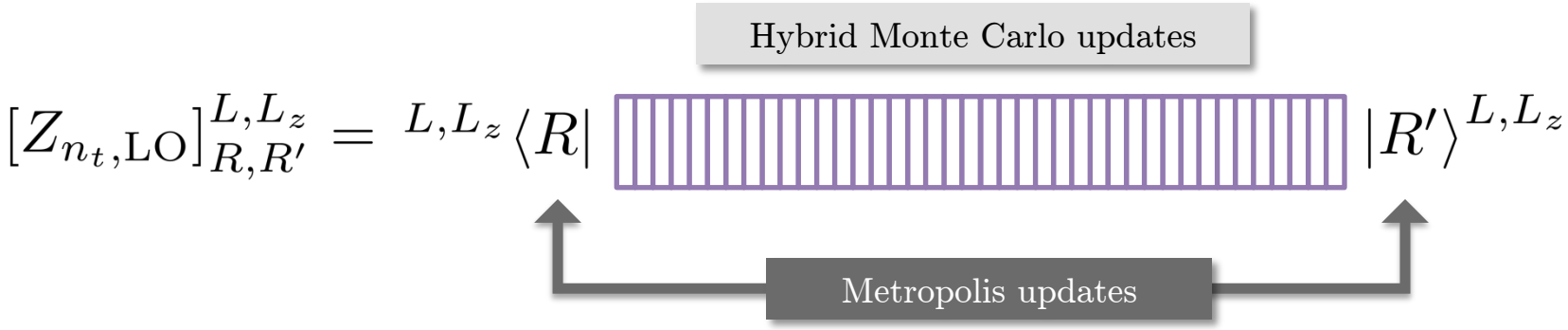
As we increase the projection time, the adiabatic Hamiltonian exactly reproduces the low-energy spectrum of the full microscopic Hamiltonian. We can read off the scattering phase shifts for the asymptotic long-distance properties of the scattering wave functions.

Rokash, Pine, Elhatisari, D.L., Epelbaum, Krebs, PRC 106, 054612, 2015
Elhatisari, D.L., PRC 90, 064001, 2014

We use projections onto spherical harmonics defined on sets of lattice points with the same distance from the origin.

$$|R\rangle^{L,L_z} = \sum_{\vec{R}'} Y_{L,L_z}(\hat{R}')\delta_{R,|\vec{R}'|}|\vec{R}'\rangle$$

New algorithm developed for auxiliary field updates and initial/final state updates



$$^4\mathrm{He} + {}^4\mathrm{He} \rightarrow {}^4\mathrm{He} + {}^4\mathrm{He}$$

We now present *ab initio* results for alpha-alpha scattering up to NNLO with lattice spacing 1.97 fm.

Using the adiabatic projection method, we performed lattice simulations for the S-wave and D-wave channels.

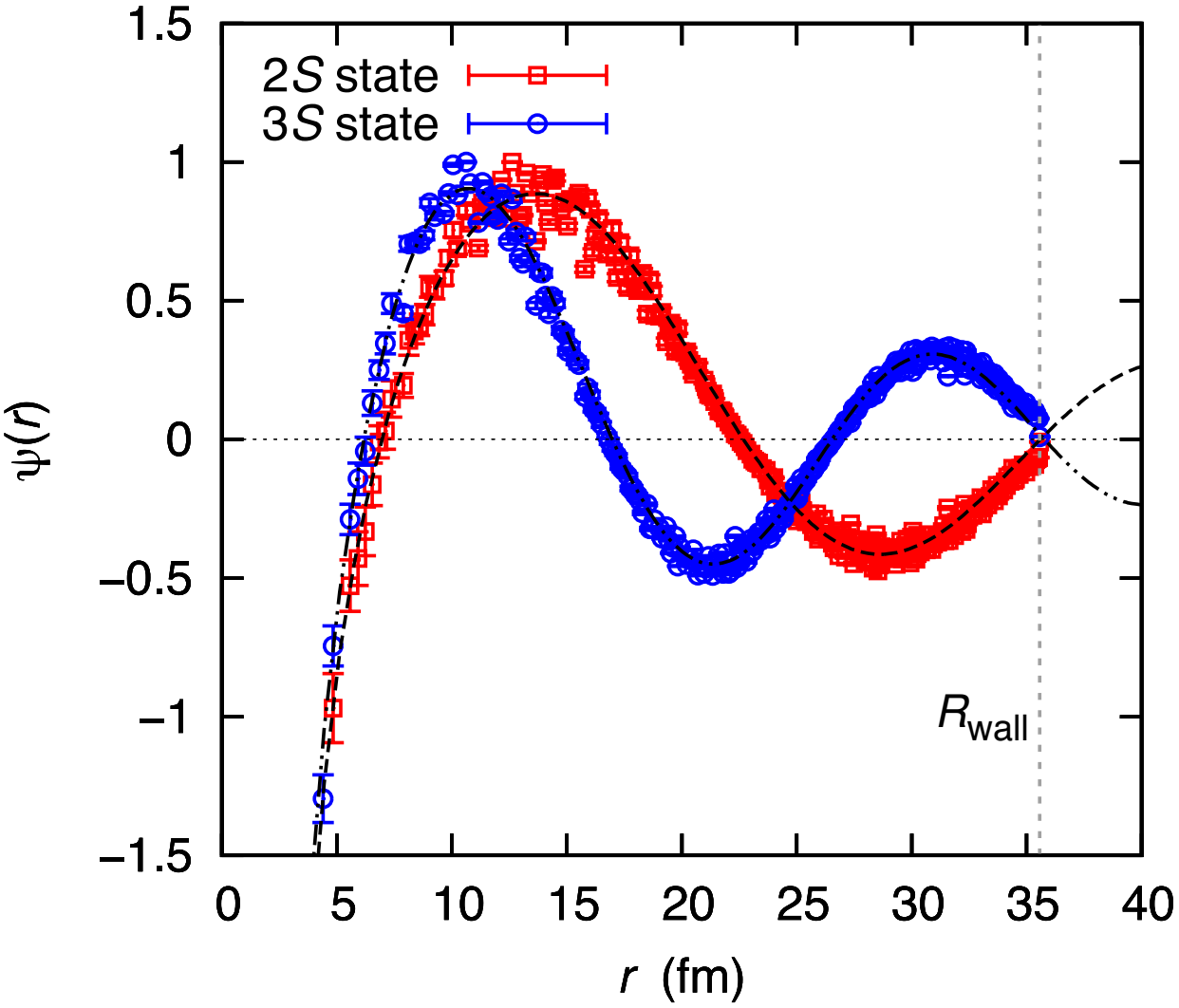
LETTER

doi:10.1038/nature16067

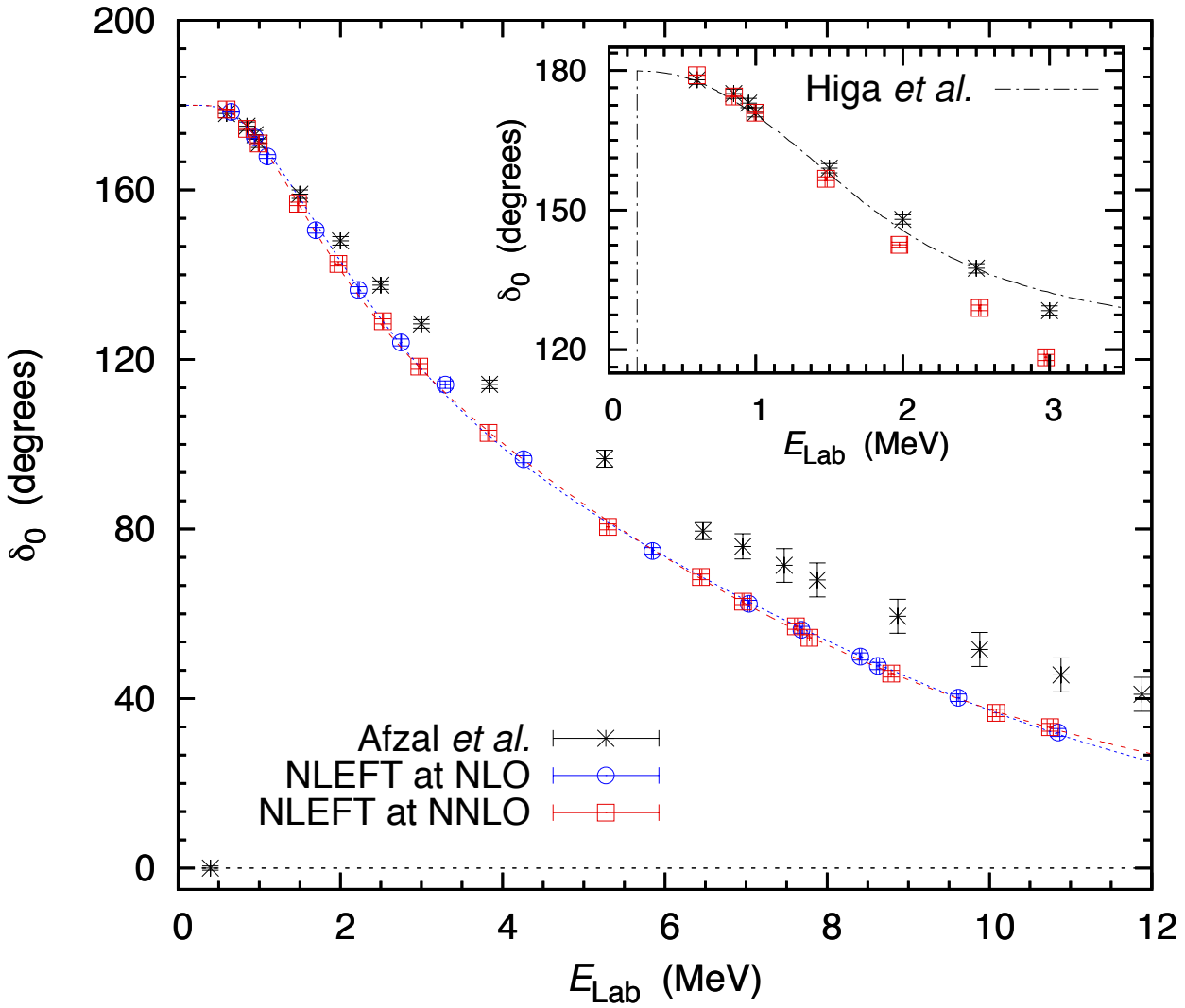
Nature 528, 111 (2015)

Ab initio alpha–alpha scattering

Serdar Elhatisari[1], Dean Lee[2], Gautam Rupak[3], Evgeny Epelbaum[4], Hermann Krebs[4], Timo A. Lähde[5], Thomas Luu[1,5] & Ulf-G. Meißner[1,5,6]


2S state
3S state
1.5
1
0.5
0
−0.5
−1
−1.5
ψ(r)
0
5
10
15
20
25
30
35
40
r (fm)
R_wall

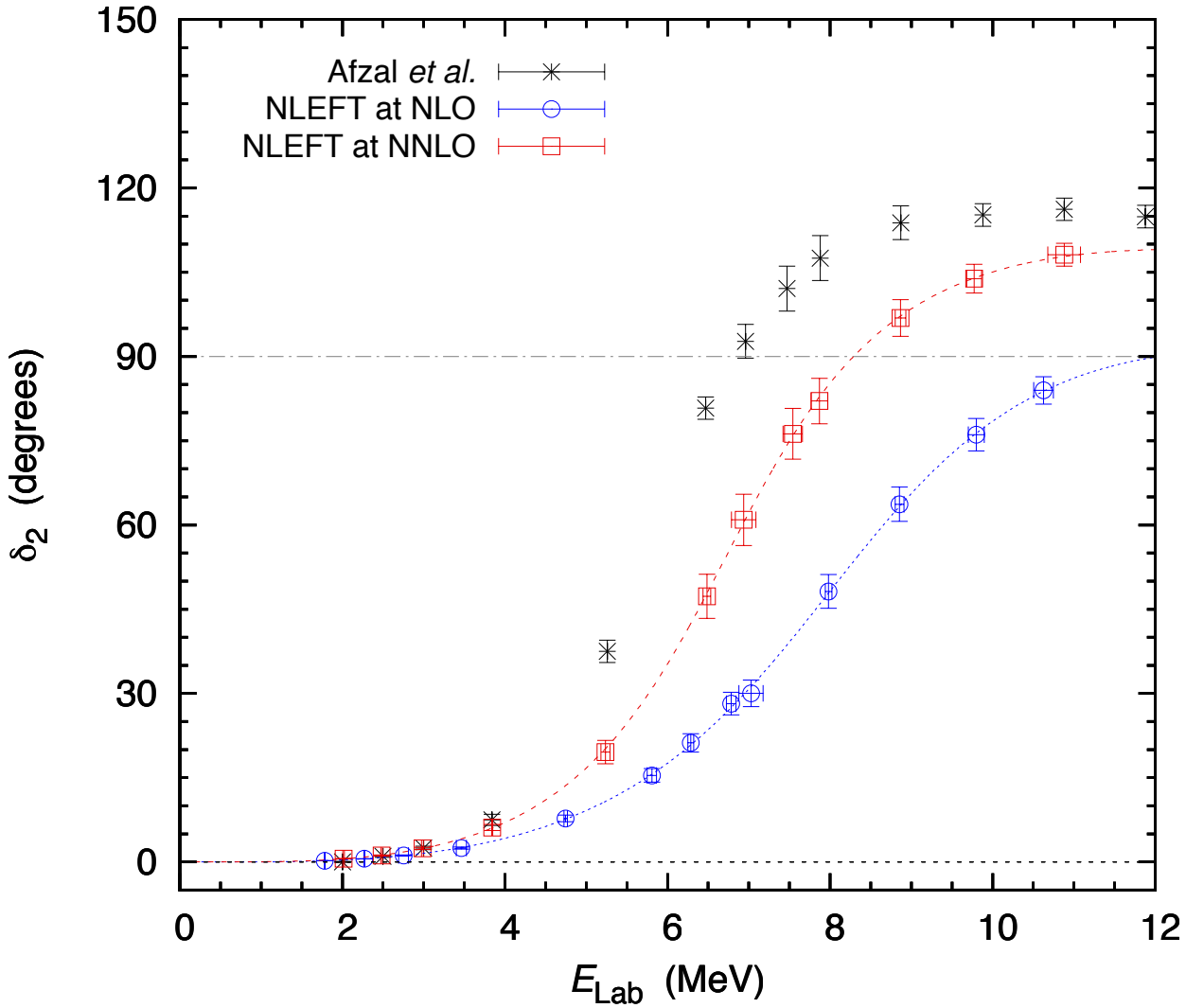
S-wave scattering



Afzal, Ahmad, Ali, RMP 41 247 (1969)

Higa, Hammer, van Kolck, NPA 809 171(2008)

D-wave scattering



We have also found that alpha-alpha scattering is quite sensitive to the locality/non-locality of the nucleon-nucleon interaction.

See preceding talk by Gaute Hagen

Elhatisari, Li, Rokash, Alarcon, Du, Klein, Lu, Meißner, Epelbaum, Krebs, Lähde, D.L., Rupak, arXiv:1602.04539

For an A_1-body + A_2-body scattering or reaction process the computational scaling is typically $\sim (A_1 + A_2)^2$.

For mass and charge transfer processes, we do the same steps but consider coupled channel scattering. For capture reactions, we include one-photon matrix elements and compute overlaps between bound states and scattering states.

Rupak, D.L., PRL 111 032502 (2013)

Stay tuned for coming developments in the near future