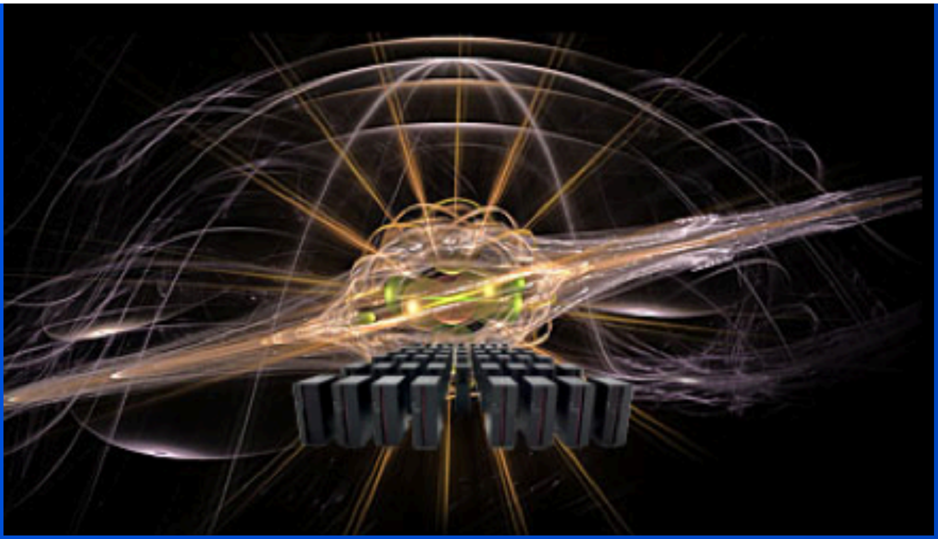


Nuclear Structure from Short to Medium Distances

James P. Vary
Iowa State University

Nuclear Structure and Dynamics
February 13-22, 2013

NUCLEI
Nuclear Computational Low-Energy Initiative

U.S. DEPARTMENT OF ENERGY
INCITE
LEADERSHIP COMPUTING

National Science Foundation
WHERE DISCOVERIES BEGIN

Ab initio nuclear physics - fundamental questions

- What controls nuclear saturation?
- How the nuclear shell model emerges from the underlying theory?
- What are the properties of nuclei with extreme neutron/proton ratios?
- Can we predict useful cross sections that cannot be measured?
- Can nuclei provide precision tests of the fundamental laws of nature?
- Under what conditions do we need QCD to describe nuclear structure?

U.S. DEPARTMENT OF ENERGY | Office of Science

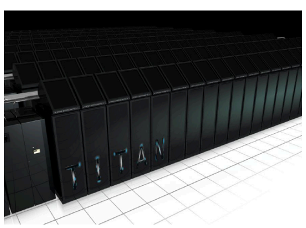
National Science Foundation — WHERE DISCOVERIES BEGIN

SciDAC — Scientific Discovery through Advanced Computing

INCITE — Advancing America's Science and Industrial Competitiveness

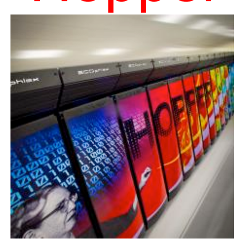
NUCLEI — Nuclear Computational Low-Energy Initiative

TITAN

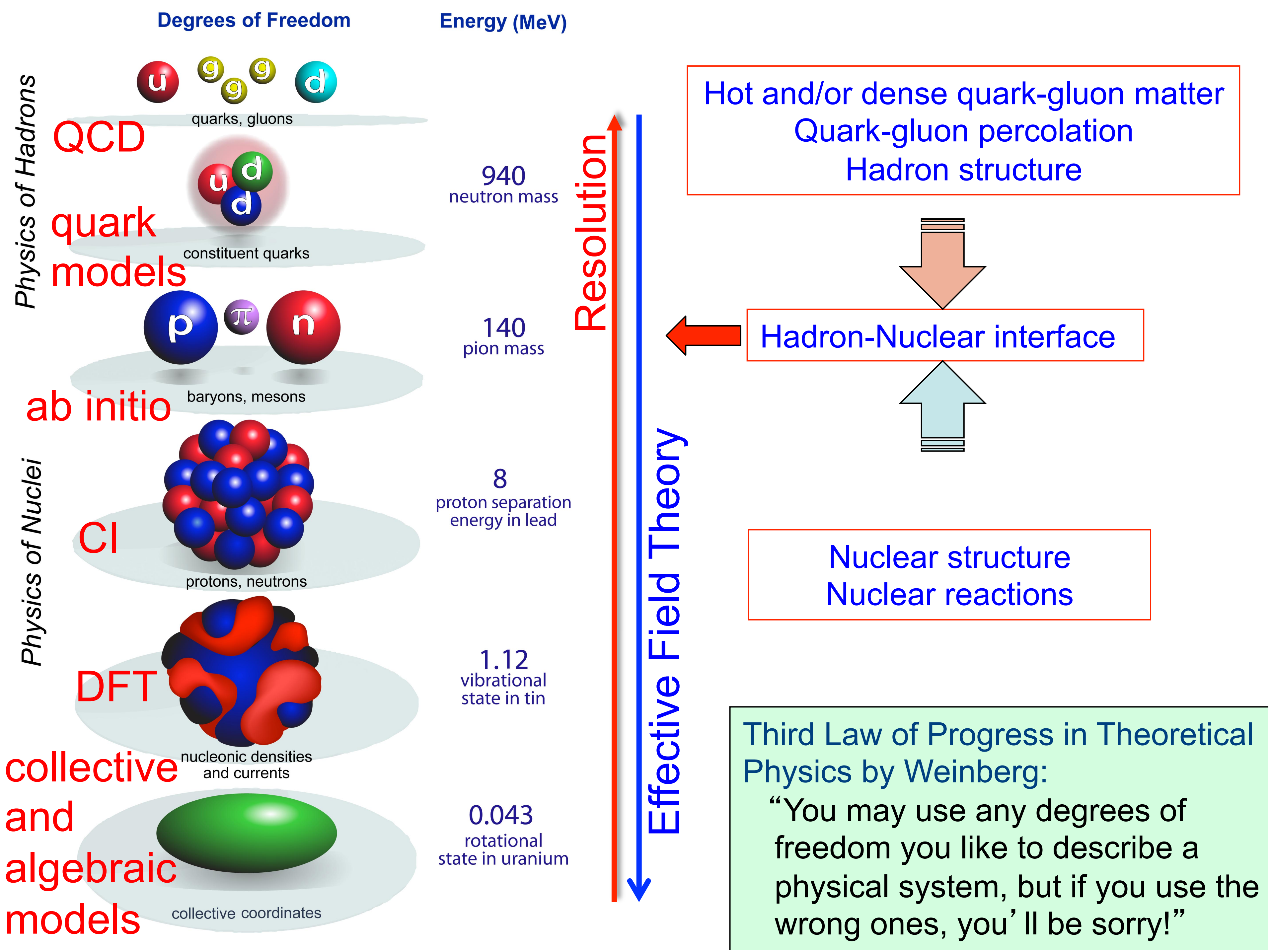


MIRA

Hopper



\+
K-super.
Blue Waters
\+ . . .



Degrees of Freedom
Energy (MeV)
Physics of Hadrons
QCD
quarks, gluons
quark models
constituent quarks
940
neutron mass
ab initio
baryons, mesons
140
pion mass
Physics of Nuclei
CI
protons, neutrons
8
proton separation energy in lead
DFT
nucleonic densities and currents
1.12
vibrational state in tin
collective and algebraic models
collective coordinates
0.043
rotational state in uranium
Resolution
Effective Field Theory
Hot and/or dense quark-gluon matter
Quark-gluon percolation
Hadron structure
Hadron-Nuclear interface
Nuclear structure
Nuclear reactions
Third Law of Progress in Theoretical Physics by Weinberg:
"You may use any degrees of freedom you like to describe a physical system, but if you use the wrong ones, you'll be sorry!"

All interactions are "effective" until the ultimate theory unifying all forces in nature is attained.

Thus, even the Standard Model, incorporating QCD,
is an effective theory valid below the Planck scale
$\lambda < 10^{19}$ GeV/c

The "bare" NN interaction, usually with derived quantities,
is thus an effective interaction valid up to some scale, typically
the scale of the known NN phase shifts and Deuteron gs properties
$\lambda \sim 600$ MeV/c (3.0 fm^{-1})

Effective NN interactions can be further renormalized to lower scales
and this can enhance convergence of the many-body applications
$\lambda \sim 300$ MeV/c (1.5 fm^{-1})

"Consistent" NNN and higher-body forces, as well as electroweak
currents, are those valid to the same scale as their corresponding
NN partner, and obtained in the same renormalization scheme.

ab initio renormalization schemes

SRG: Similarity Renormalization Group
OLS: Okubo-Lee-Suzuki
Vlowk: V with low k scale limit
UCOM: Unitary Correlation Operator Method
and there are more!

Realistic NN & NNN interactions
High quality fits to 2- & 3- body data

Need
Consistent
EW operators

Meson-exchange (Argonne, Illinois, . . .)

NN: AV18, CD-Bonn, Nijmegen, . . .

NNN: Tucson-Melbourne, UIX, IL7, . . .

Need
Improved NNN

Chiral EFT (Idaho, Bochum, . . .)

NN: N3LO

NNN: N2LO

4N: predicted & needed for consistent N3LO

Need
Fully derived/coded
N3LO

Inverse Scattering (Russia, USA, . . .)

NN: JISP16

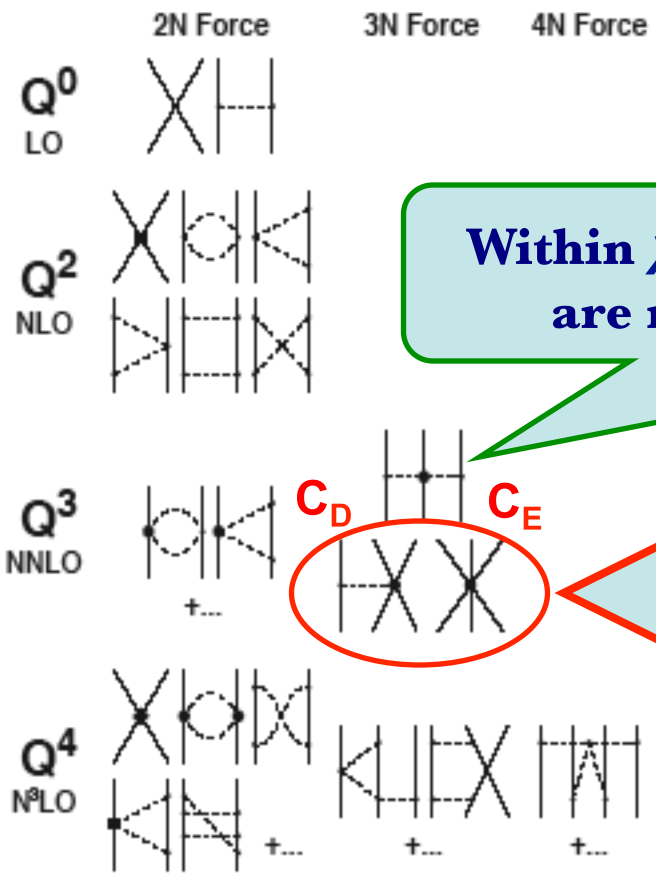
Need
JISP40
Consistent NNN

Effective Intra-Nucleon Interactions
(Chiral Perturbation Theory)

Chiral perturbation theory (χPT) allows for controlled power series expansion

Expansion parameter : $\left(\frac{Q}{\Lambda_\chi}\right)^{\upsilon}$, $Q-$momentum transfer,

$\chi-$symmetry breaking scale: $\Lambda_\chi \approx 1$ GeV $\approx \frac{2\pi}{r} \Rightarrow r \approx 1$ fm



R. Machleidt, D. R. Entem, nucl-th/0503025

Within χPT 2π-NNN Low Energy Constants (LEC) are related to the NN-interaction LECs $\{c_i\}$.

Terms suggested within the
Chiral Perturbation Theory

Regularization is essential, which is obvious within the Harmonic Oscillator wave function basis.

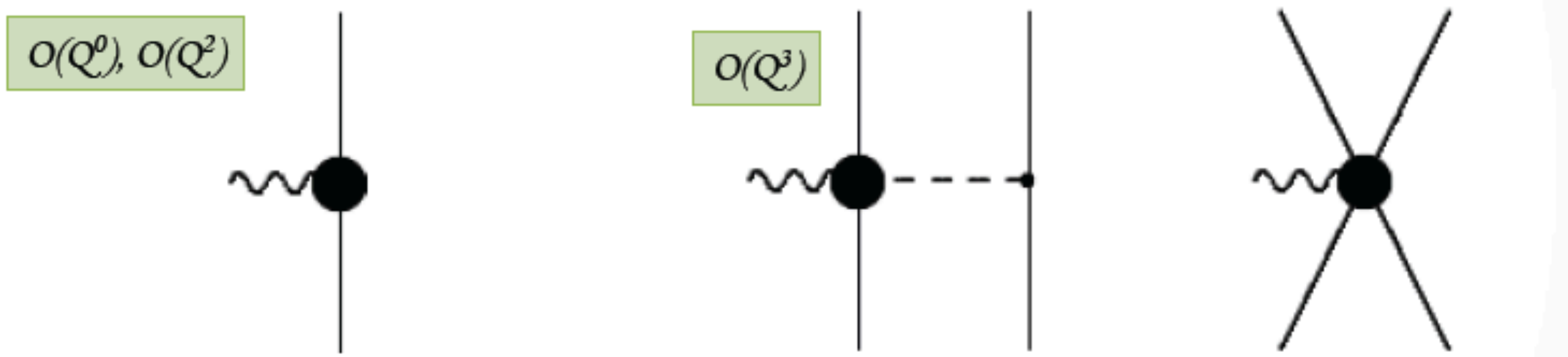
Coupling to External Probes in Chiral EFT

- Nuclear Current Operators

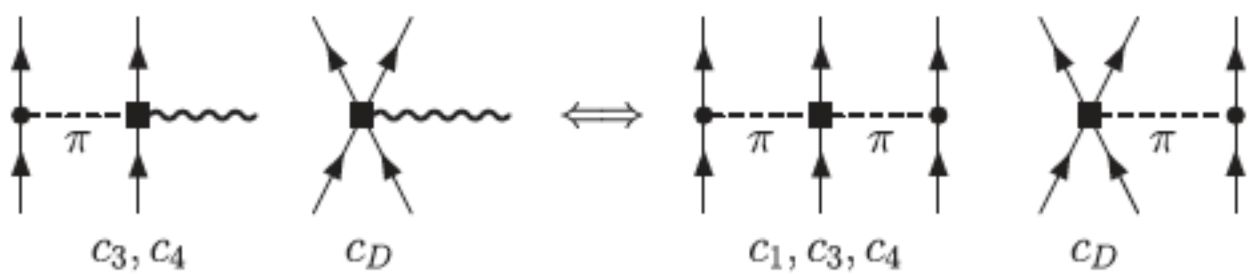
Single nucleon current

1 pion exchange

Contact term



Two-Body Currents (N^2LO)



The Nuclear Many-Body Problem

The many-body Schroedinger equation for bound states consists of $2^A \binom{A}{Z}$ coupled second-order differential equations in 3A coordinates using strong (NN & NNN) and electromagnetic interactions.

Successful *ab initio* quantum many-body approaches (A > 6)

Stochastic approach in coordinate space
Greens Function Monte Carlo (**GFMC**)

Hamiltonian matrix in basis function space
No Core Shell Model (**NCSM**)
No Core Full Configuration (**NCFC**)

Cluster hierarchy in basis function space
Coupled Cluster (**CC**)

Lattice + EFT approach (New)

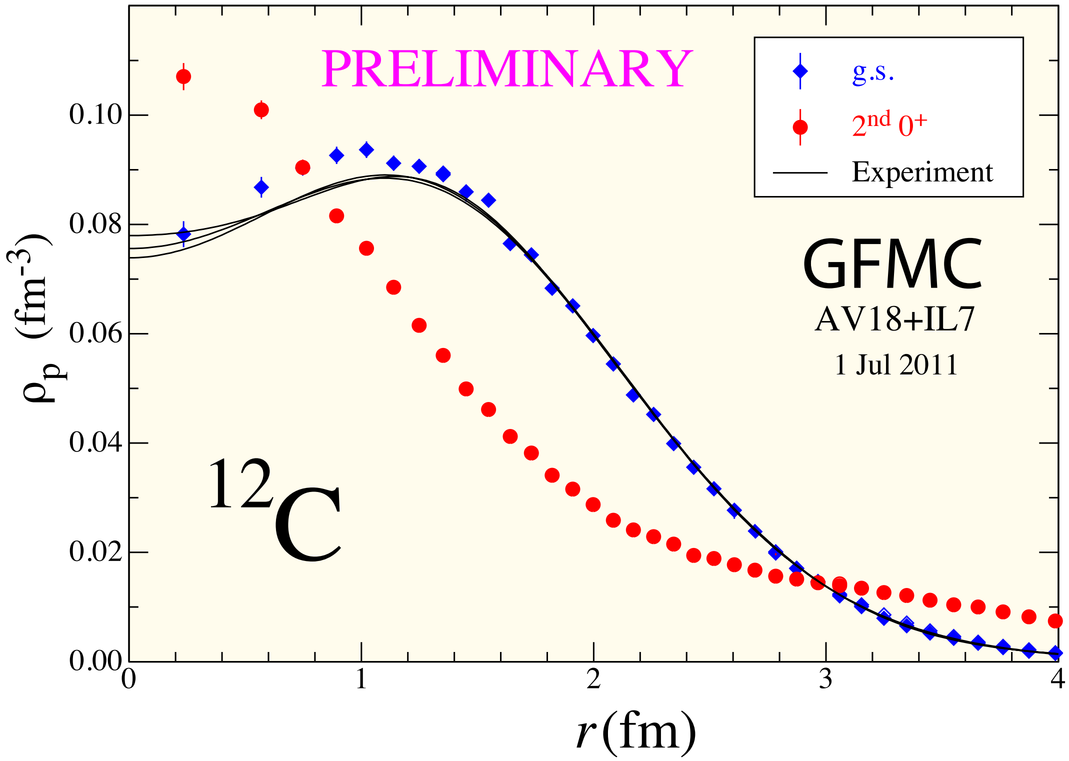
Coming - Gorkov Green's Function, . . .

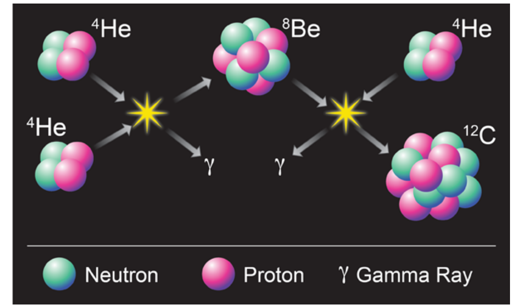
Comments

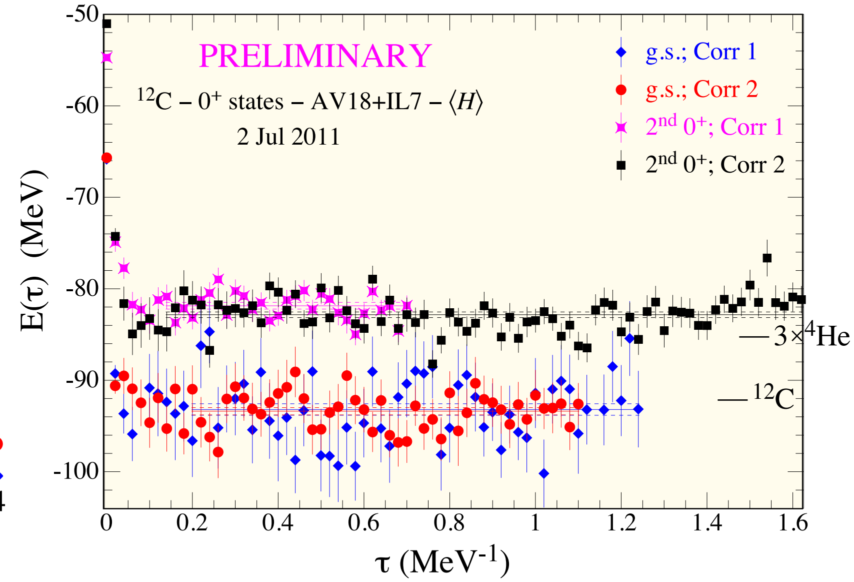
All work to preserve and exploit symmetries
Extensions of each to scattering/reactions are well-underway
They have different advantages and limitations

Examples: Ab Initio

^{12}C in GFMC: Pieper et al.







The ADLB (Asynchronous Dynamic Load-Balancing) version of GFMC was used to make calculations of ^{12}C with a complete Hamiltonian (two- and three-nucleon potential AV18+IL7) on 32,000 processors of the Argonne BGP. These are believed to be the best converged ab initio calculations of ^{12}C ever made. The computed binding energy is 93.5(6) MeV compared to the experimental value of 92.16 MeV and the point rms radius is 2.35 fm vs 2.33 from experiment.

Lattice spacing 1.97 fm

Epelbaum et al., Phys. Rev. Lett. 106, 192501 (2011)

TABLE II. Lattice results for the low-lying excited states of ^{12}C. For comparison the experimentally observed energies are shown. All energies are in units of MeV.

	0_2^+	$2_1^+, J_z = 0$	$2_1^+, J_z = 2$
LO $[O(Q^0)]$	−94(2)	−92(2)	−89(2)
NLO $[O(Q^2)]$	−82(3)	−87(3)	−85(3)
IB + EM $[O(Q^2)]$	−74(3)	−80(3)	−78(3)
NNLO $[O(Q^3)]$	−85(3)	−88(3)	−90(4)
Experiment	−84.51	−87.72	

Quantum Monte Carlo calculations of electromagnetic moments and transitions in $A \leq 9$ nuclei with meson-exchange currents derived from chiral effective field theory

S. Pastore[1,*] Steven C. Pieper[1,†] R. Schiavilla[2,3,‡] and R. B. Wiringa[1,§]

arXiv: 1212.3375

AV18 + IL7 for Hamiltonian
Meson exch & Chiral EFT
for 1-body and 2-body currents

Shown here are the results "TOT" that include Chiral EFT 1-body and 2-body currents.

Produces near perfect agreement with experiment!

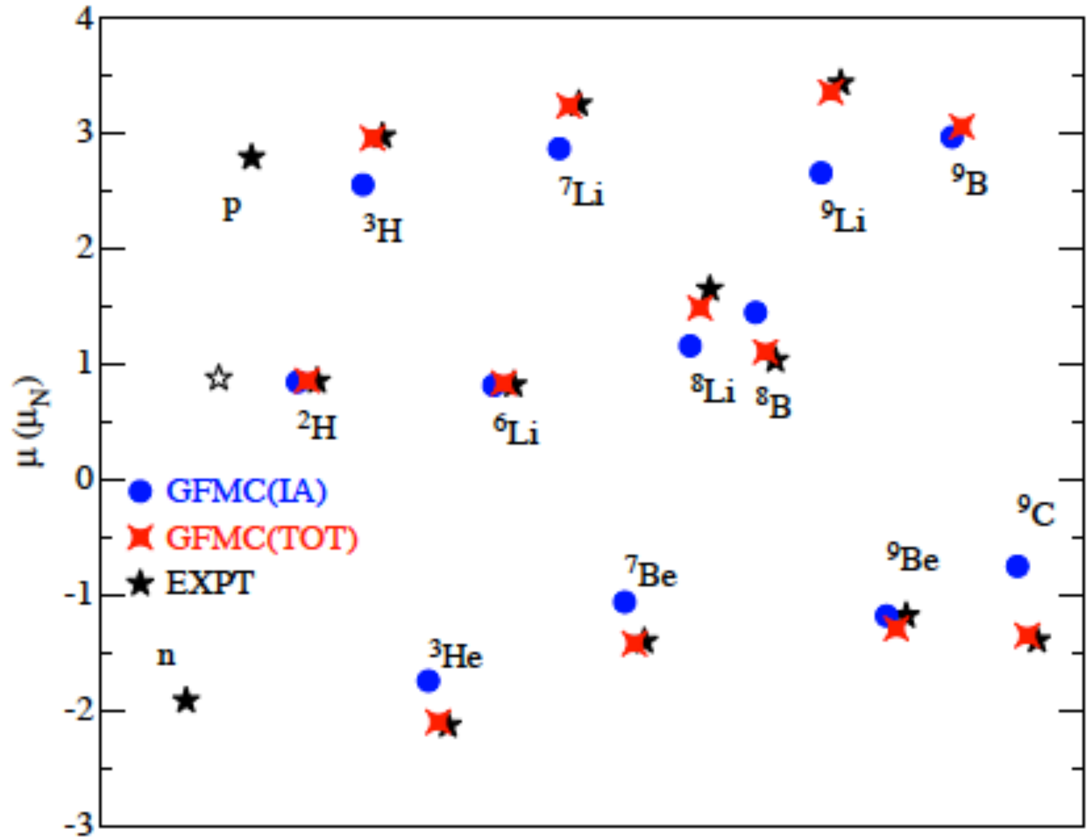
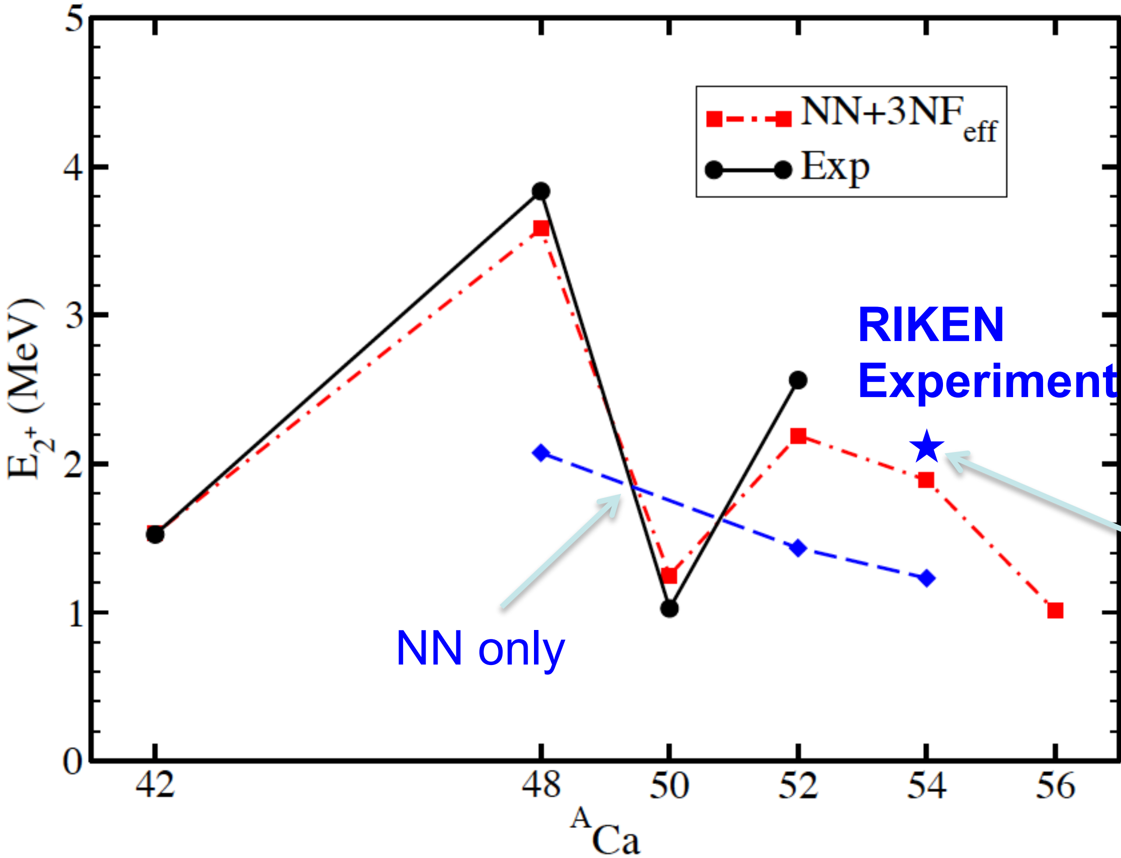


FIG. 4: (Color online) Magnetic moments in nuclear magnetons for $A \leq 9$ nuclei. Black stars indicate the experimental values [35, 36], while blue dots (red diamonds) represent GFMC calculations which include the IA one-body EM current (total χEFT current up to N3LO). Predictions are for nuclei with $A > 3$.

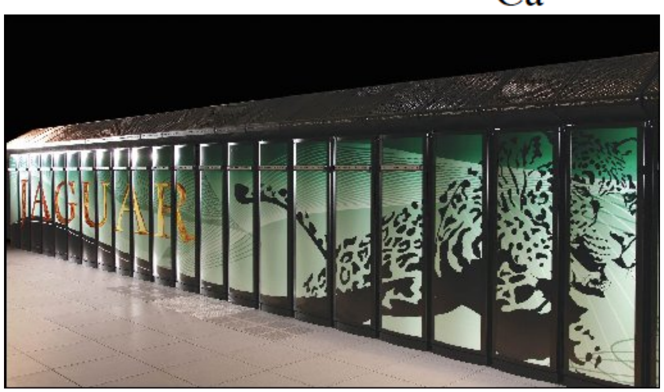
Is ^{54}Ca a magic nucleus? (Is N=34 a magic number?)



Main Features:

1. Good agreement between theory and experiment.
2. Shell closure in ^{48}Ca due to effects of 3NFs
3. Predict weak (sub-)shell closure in ^{54}Ca.

Measurement at RIKEN (Japan) agrees with theoretical prediction.



Coupled-cluster calculations were performed on Jaguar

G. Hagen, M. Hjorth-Jensen, G. R. Jansen, R. Machleidt, T. Papenbrock, Phys. Rev. Lett. **109**, 032502 (2012).

No Core Shell Model
A large sparse matrix eigenvalue problem

$$H = T_{rel} + V_{NN} + V_{3N} + \bullet\bullet\bullet$$

$$H|\Psi_i\rangle = E_i|\Psi_i\rangle$$

$$|\Psi_i\rangle = \sum_{n=0}^{\infty} A_n^i |\Phi_n\rangle$$

$$\text{Diagonalize } \{\langle\Phi_m|H|\Phi_n\rangle\}$$

- Adopt realistic NN (and NNN) interaction(s) & renormalize as needed - retain induced many-body interactions: Chiral EFT interactions and JISP16
- Adopt the 3-D Harmonic Oscillator (HO) for the single-nucleon basis states, α, β,…
- Evaluate the nuclear Hamiltonian, H, in basis space of HO (Slater) determinants (manages the bookkeeping of anti-symmetrization)
- Diagonalize this sparse many-body H in its "m-scheme" basis where [α =(n,l,j,$m_{j,}\tau_z$)]

$$|\Phi_n\rangle = [a_\alpha^+ \bullet\bullet\bullet a_\varsigma^+]_n|0\rangle$$

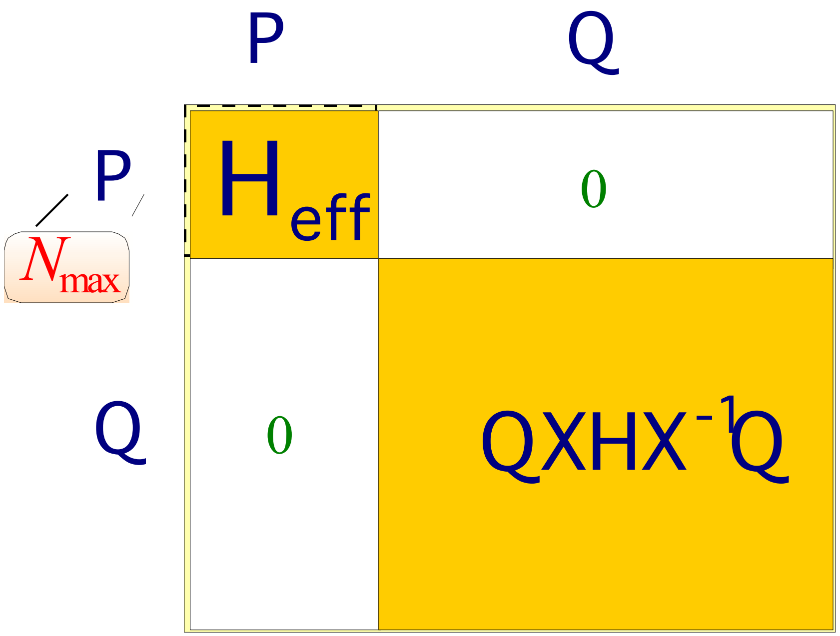
$$n = 1,2,\ldots,10^{10} \text{ or more!}$$

- Evaluate observables and compare with experiment

Comments

- Straightforward but computationally demanding => new algorithms/computers
- Requires convergence assessments and extrapolation tools
- Achievable for nuclei up to A=20 (40) today with largest computers available

Effective Hamiltonian in the NCSM
Okubo-Lee-Suzuki renormalization scheme



$$H: \quad E_1, E_2, E_3, \ldots E_{d_P}, \ldots E_\infty$$

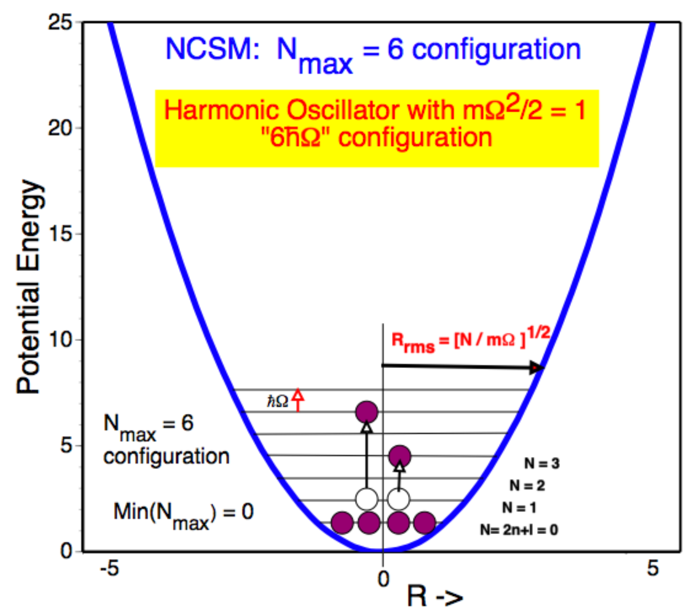
$$H_{eff}: \quad E_1, E_2, E_3, \ldots E_{d_P}$$

model space dimension

$$QXHX^{-1}P = 0$$

$$H_{eff} = PXHX^{-1}P$$

- n-body cluster approximation, $2 \le n \le A$
- $H^{(n)}_{eff}$ n-body operator
- Two ways of convergence:
  - For $P \to 1$ $H^{(n)}_{eff} \to H$
  - For $n \to A$ and fixed P: $H^{(n)}_{eff} \to H_{eff}$



Adapted from Petr Navratil's slide

Controlling the center-of-mass (cm) motion in order to preserve Galilean invariance

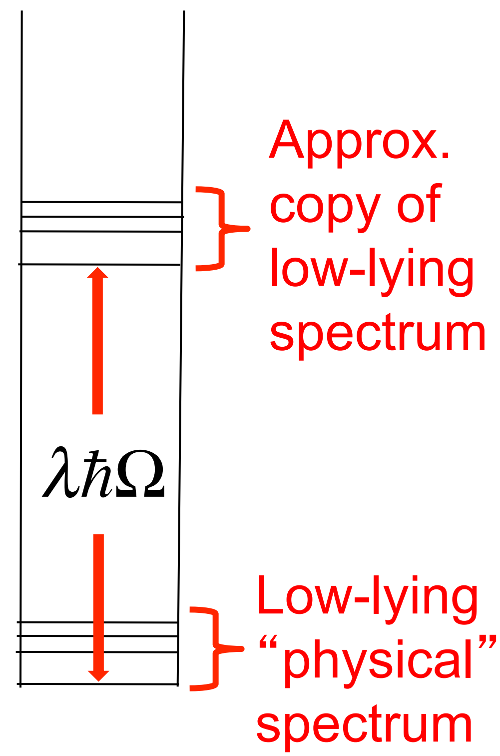
Add a Lagrange multiplier term acting on the cm alone so as not to interfere with the internal motion dynamics

$$H_{eff}\left(N_{\max},\hbar\Omega\right) \equiv P[T_{rel}+V^{a}\left(N_{\max},\hbar\Omega\right)]P$$

$$H = H_{eff}\left(N_{\max},\hbar\Omega\right) + \lambda H_{cm}$$

$$H_{cm} = \frac{P^2}{2M_A} + \frac{1}{2}M_A\Omega^2 R^2$$

$$\lambda \sim 10 \quad \text{suffices}$$



Along with the N_{max} truncation in the HO basis, the Lagrange multiplier term guarantees that all low-lying solutions have eigenfunctions that factorize into a 0s HO wavefunction for the cm times a translationaly invariant wavefunction.

PRL 99, 042501 (2007) PHYSICAL REVIEW LETTERS week ending 27 JULY 2007

Structure of $A = 10$–13 Nuclei with Two- Plus Three-Nucleon Interactions from Chiral Effective Field Theory

P. Navrátil,[1] V. G. Gueorguiev,[1,*] J. P. Vary,[1,2] W. E. Ormand,[1] and A. Nogga[3]

Strong correlation between c_D and c_E for exp'l properties of A = 3 & 4

=> Retain this correlation in applications to other systems

Range favored by various analyses & values are "natural"

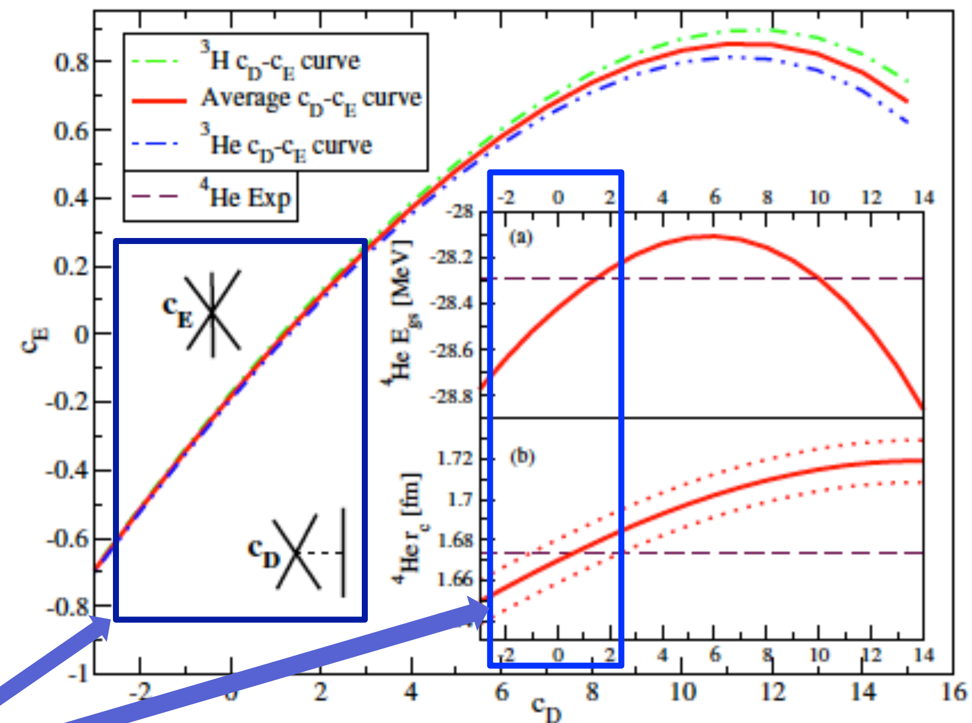
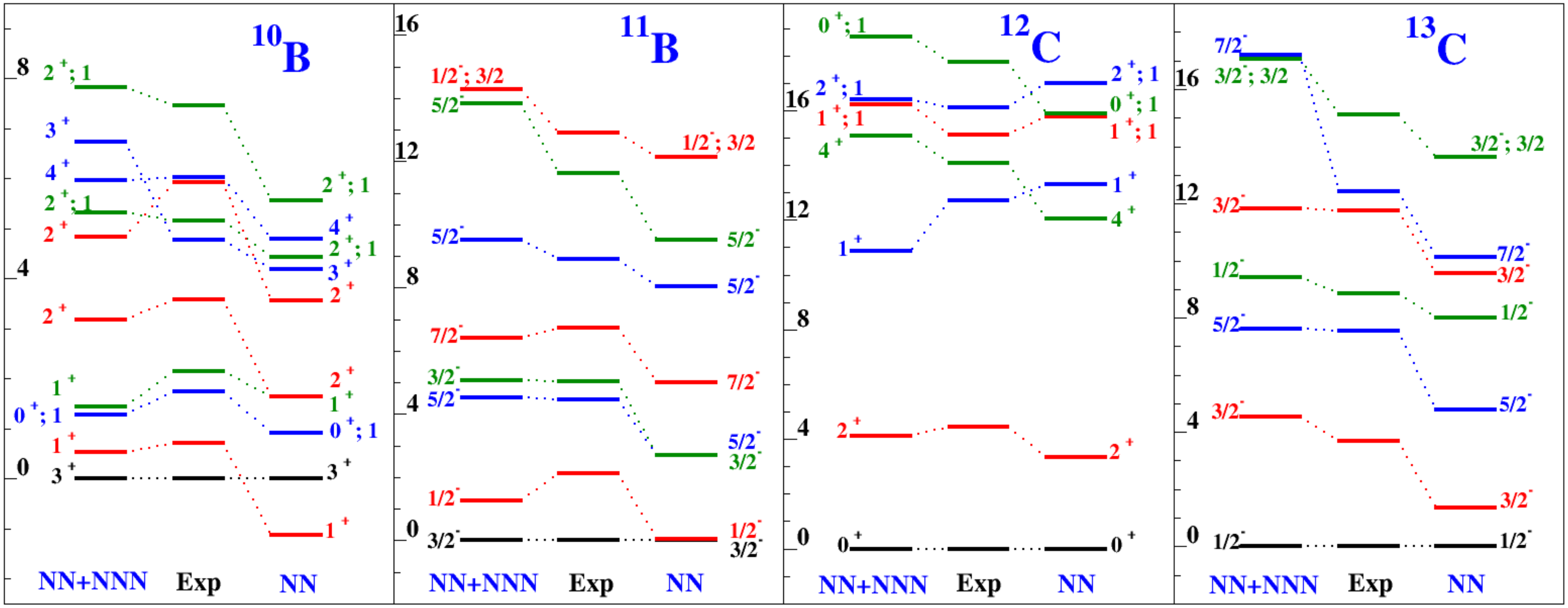


FIG. 1 (color online). Relations between c_D and c_E for which the binding energy of ^{3}H (8.482 MeV) and ^{3}He (7.718 MeV) are reproduced. (a) ^{4}He ground-state energy along the averaged curve. (b) ^{4}He charge radius r_c along the averaged curve. Dotted lines represent the r_c uncertainty due to the uncertainties in the proton charge radius.

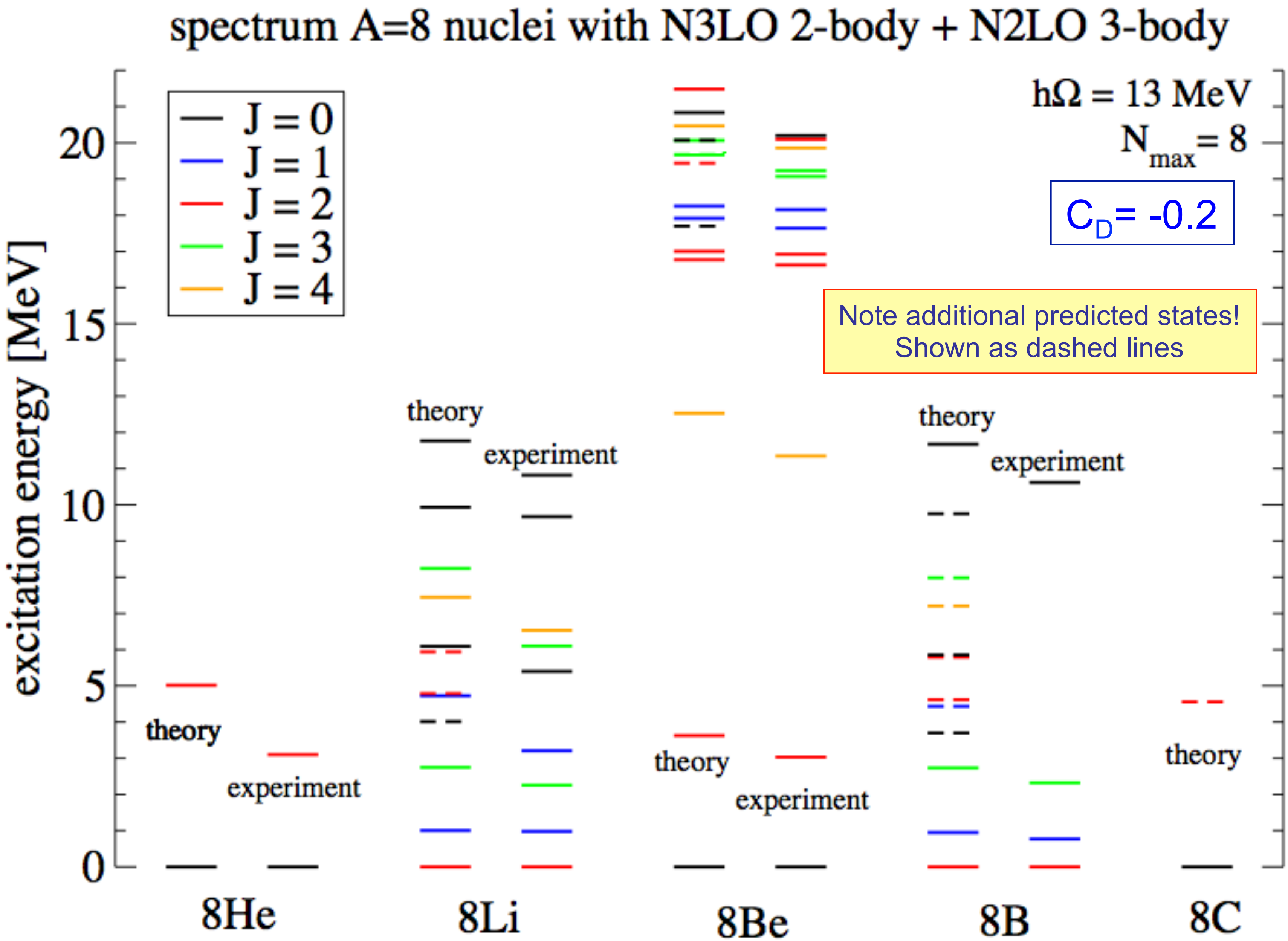
ab initio NCSM with χ_{EFT} Interactions

NNN interactions produce correct ^{10}B ground state spin and overall spectral improvements



c_D = -1

P. Navratil, V.G. Gueorguiev, J. P. Vary, W. E. Ormand and A. Nogga, Phys Rev Lett 99, 042501(2007); ArXiV: nucl-th 0701038.



P. Maris, J. P. Vary and P. Navratil, Phys. Rev. C87, 014327 (2013); arXiv 1205.5686

NCSM/NCFC - Assessing Convergence/Uncertainties

- Independence of basis space parameters ($N_{max}, \hbar\Omega$)
- Each observable must be investigated separately
- Standard approach for gs energy (next slide)
- Newest approach – IR and UV limits examined

Current status

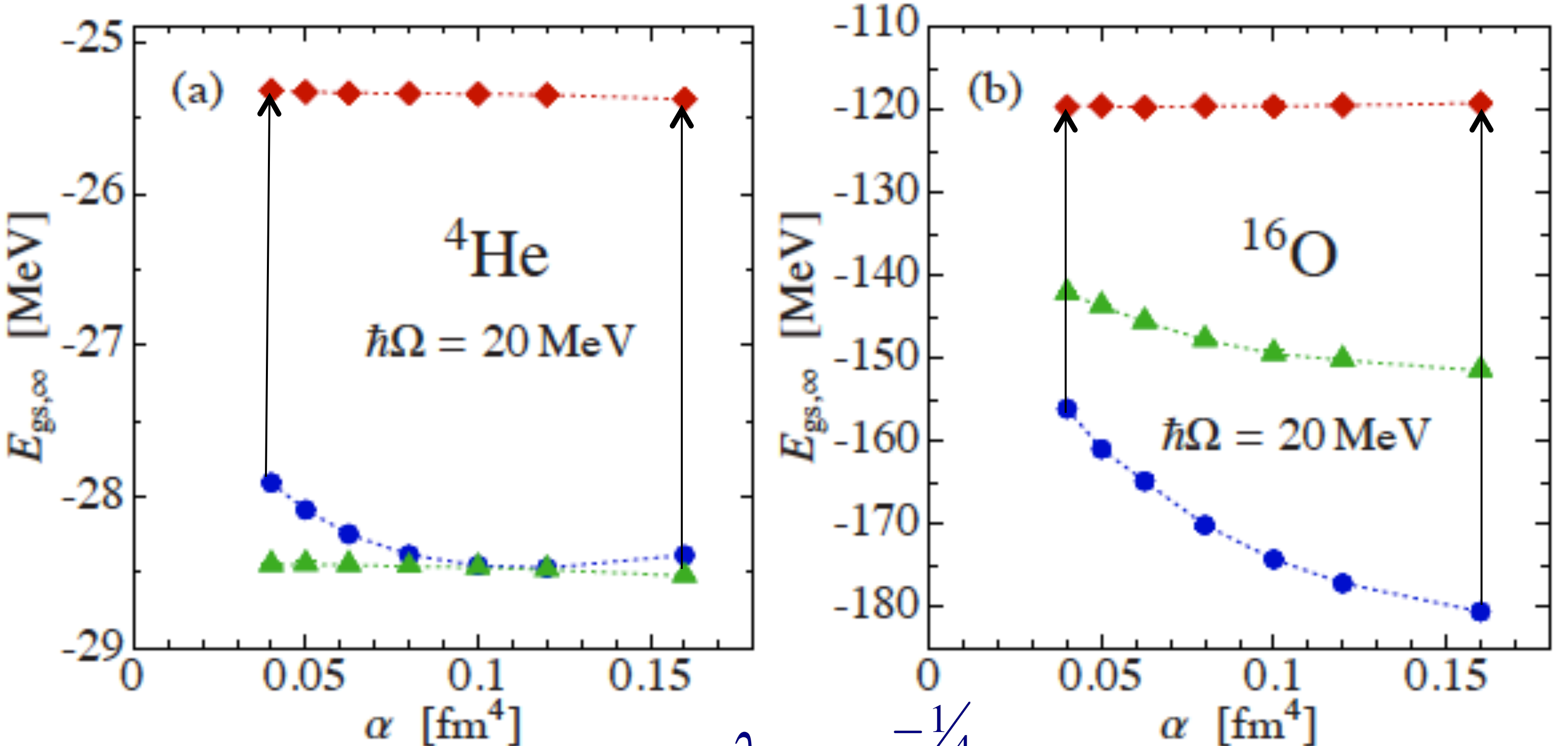
- Excitation spectra appear reasonably converged
- Exceptions are the cluster states and halo states
- Gamow-Teller transitions - well-converged
- M1 moments & B(M1)'s - reasonably converged
- Long-range ops (rms, Q, B(E2)) - poorly converged

Assessing role of induced 4N interactions
Where do we expect NN+3N-full + 4N-induced?

Similarity-Transformed Chiral NN+3N Interactions for the Ab Initio Description of ^{12}C and ^{16}O

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

Phys. Rev. Lett.107:072501,2011



$$\lambda = \alpha^{-1/4}$$

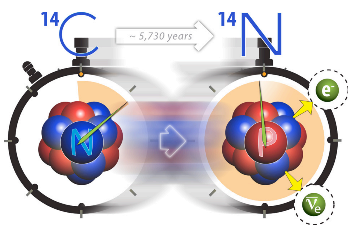
FIG. 3: (color online) N_{max}-extrapolated ground-state energies of ^{4}He and ^{16}O as function of the flow parameter α for the NN-only (●), the NN+3N-induced (◆), and the NN+3N-full Hamiltonian (▲).

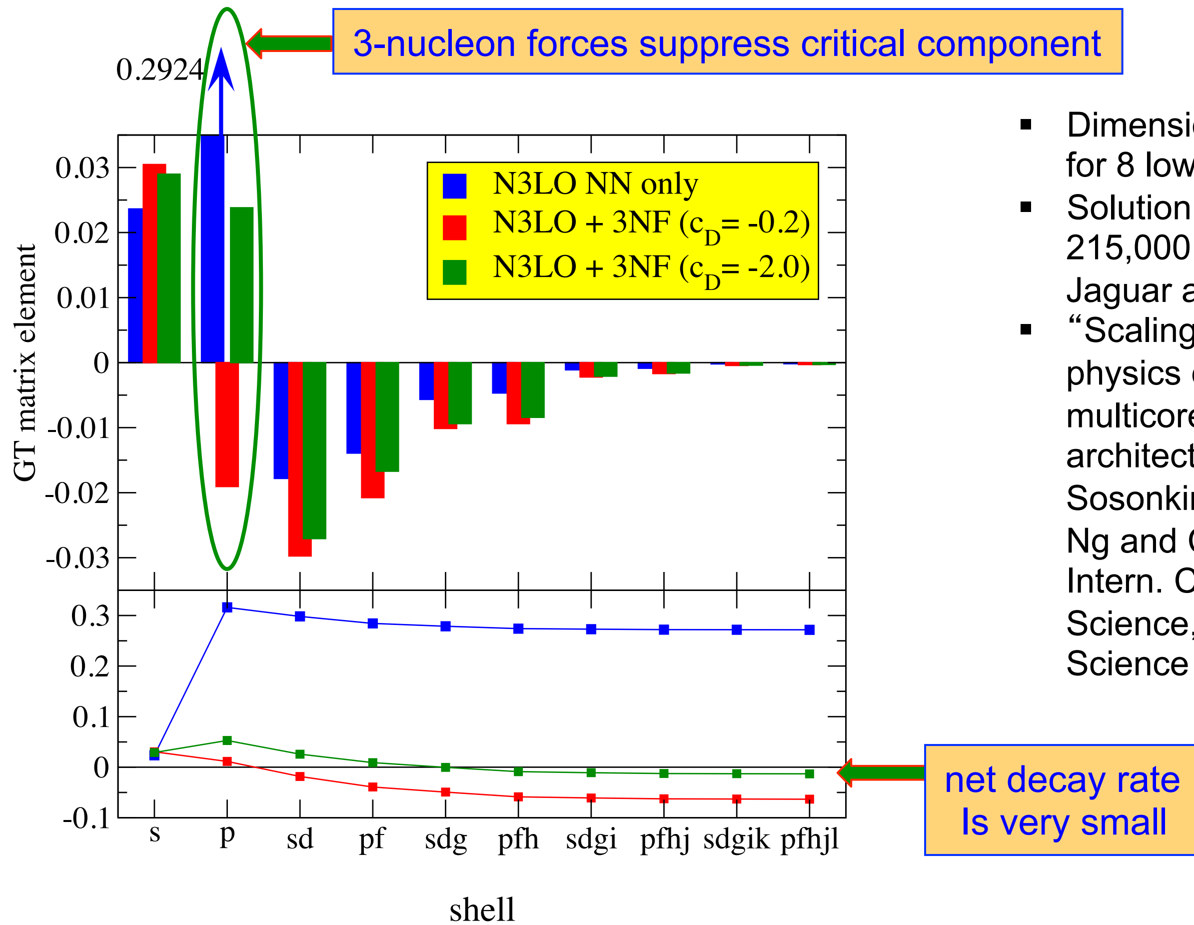
PRL 106, 202502 (2011) PHYSICAL REVIEW LETTERS week ending 20 MAY 2011

Origin of the Anomalous Long Lifetime of ^{14}C

P. Maris,[1] J.P. Vary,[1] P. Navrátil,[2,3] W.E. Ormand,[3,4] H. Nam,[5] and D. J. Dean[5]

- Solves the puzzle of the long but useful lifetime of ^{14}C
- Establishes a major role for strong 3-nucleon forces in nuclei
- Strengthens foundation for guiding DOE-supported experiments





- Dimension of matrix solved for 8 lowest states ~ 1x10^9
- Solution takes ~ 6 hours on 215,000 cores on Cray XT5 Jaguar at ORNL
- "Scaling of *ab initio* nuclear physics calculations on multicore computer architectures," P. Maris, M. Sosonkina, J. P. Vary, E. G. Ng and C. Yang, 2010 Intern. Conf. on Computer Science, Procedia Computer Science 1, 97 (2010)

Detailed results and estimated corrections due to chiral 2-body currents

TABLE I. Decomposition of p-shell contributions to M_{GT} in the LS scheme for the beta decay of ^{14}C without and with 3NF. The 3NF is included at two values of c_D where $c_D \simeq -0.2$ is preferred by the ^{3}H lifetime and $c_D \simeq -2.0$ is preferred by the ^{14}C lifetime. The calculations are performed in the $N_{max} = 8$ basis space with $\hbar\Omega = 14$ MeV.

(m_l, m_s)	NN only	NN + 3NF $c_D = -0.2$	NN + 3NF $c_D = -2.0$
$(1, +\frac{1}{2})$	0.015	0.009	0.009
$(1, -\frac{1}{2})$	−0.176	−0.296	−0.280
$(0, +\frac{1}{2})$	0.307	0.277	0.283
$(0, -\frac{1}{2})$	0.307	0.277	0.283
$(-1, +\frac{1}{2})$	−0.176	−0.296	−0.280
$(-1, -\frac{1}{2})$	0.015	0.009	0.009
Subtotal	0.292	−0.019	0.024
Total sum	0.275	−0.063	−0.013

Tritium half-life

c_D =	-0.20	-2.0
Thy/Exp. =	1.00	0.80

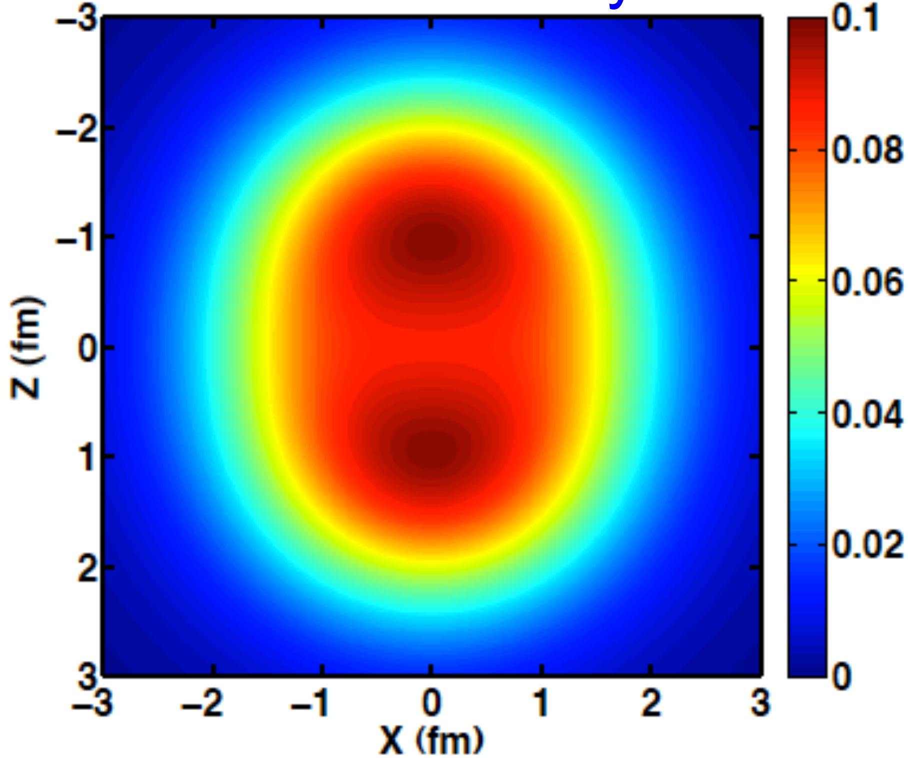
2-body current quenching (est'd)* x 0.75 => -0.047 x 0.93 => -0.012

Preliminary

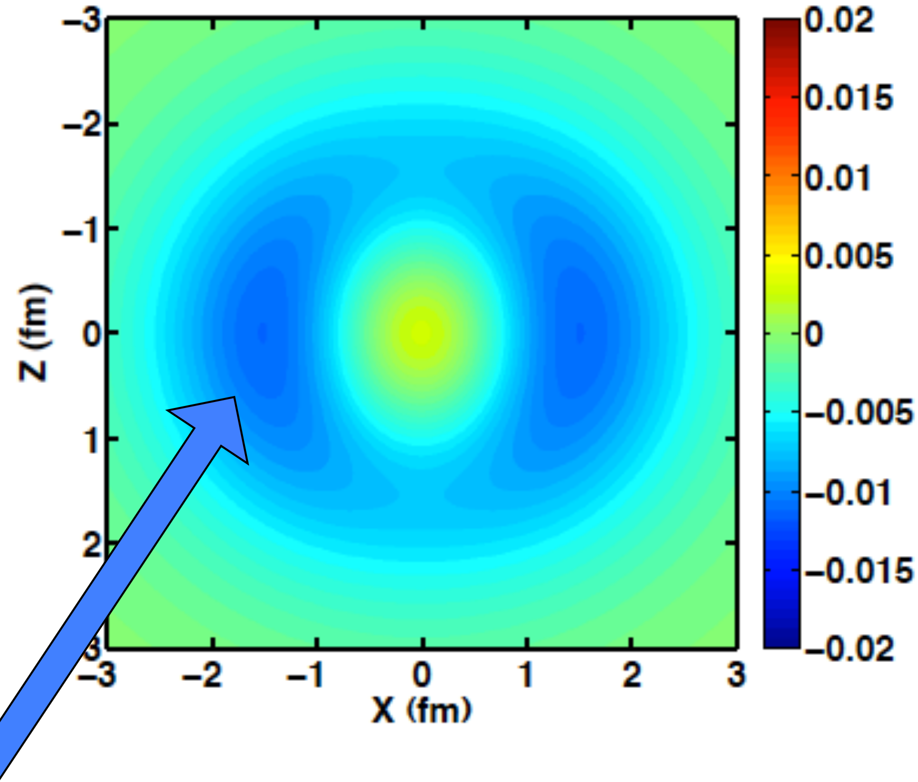
*J. Menéndez, D. Gazit and A. Schwenk, **Phys.Rev.Lett. 107 (2011) 062501**
(estimated using their effective density-dependent 1-body operator)

9Be Translationally invariant gs density
Full 3D densities = rotate around the vertical axis

Total density



Neutron – Proton density



Shows that one neutron provides a “ring” cloud around two alpha clusters binding them together

C. Cockrell, J.P. Vary, P. Maris, Phys. Rev. C 86, 034325 (2012); arXiv:1201.0724
C. Cockrell, PhD, Iowa State University

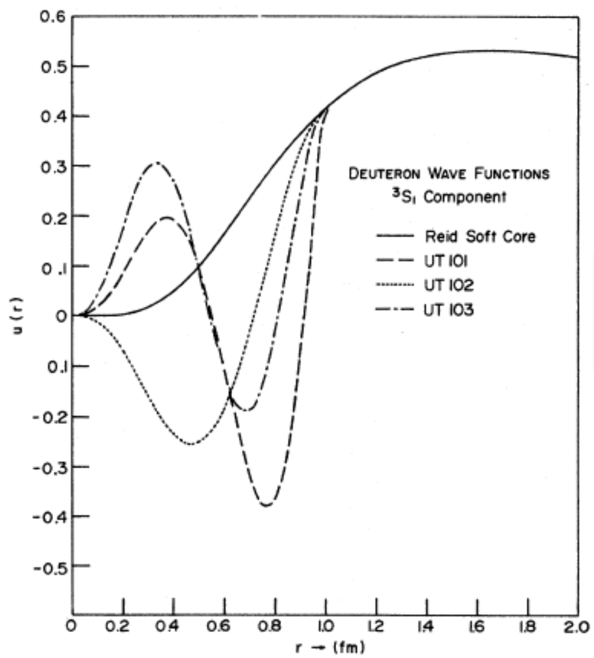


FIG. 4. $^3S_1$ component of the deuteron wave functions. The case (b) or fixed-range transformation wave functions are compared with the Reid soft-core wave function.

Same transformation on d-wave

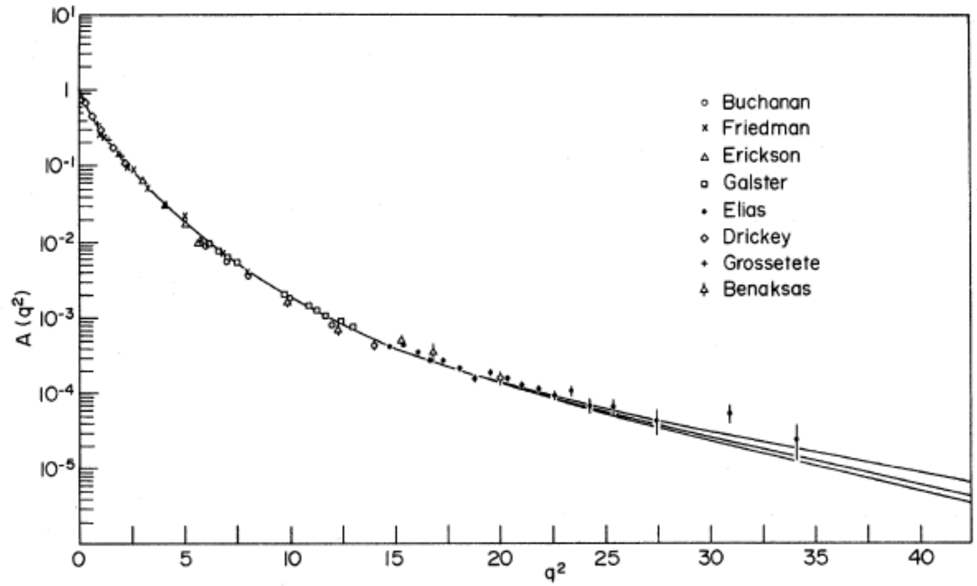


FIG. 6. Elastic scattering form factor $A(q^2)$ for the Reid soft-core and case (b) wave functions versus q^2 in fm^{-2}. All agree with the data. Reference 7 is the key to the experimental points.

Phase equivalent short range (< 1 fm) transformations introduced that leave measured Deuteron properties (static, form factors) unchanged within experimental constraints.

J.P. Vary, Phys. Rev. C7, 521(1973)

Role of “Fermi motion” in the “EMC-region” and the uncertainty in that role arising from undetermined SRCs

J.P. Vary, Phys. Rev. C7, 521(1973)

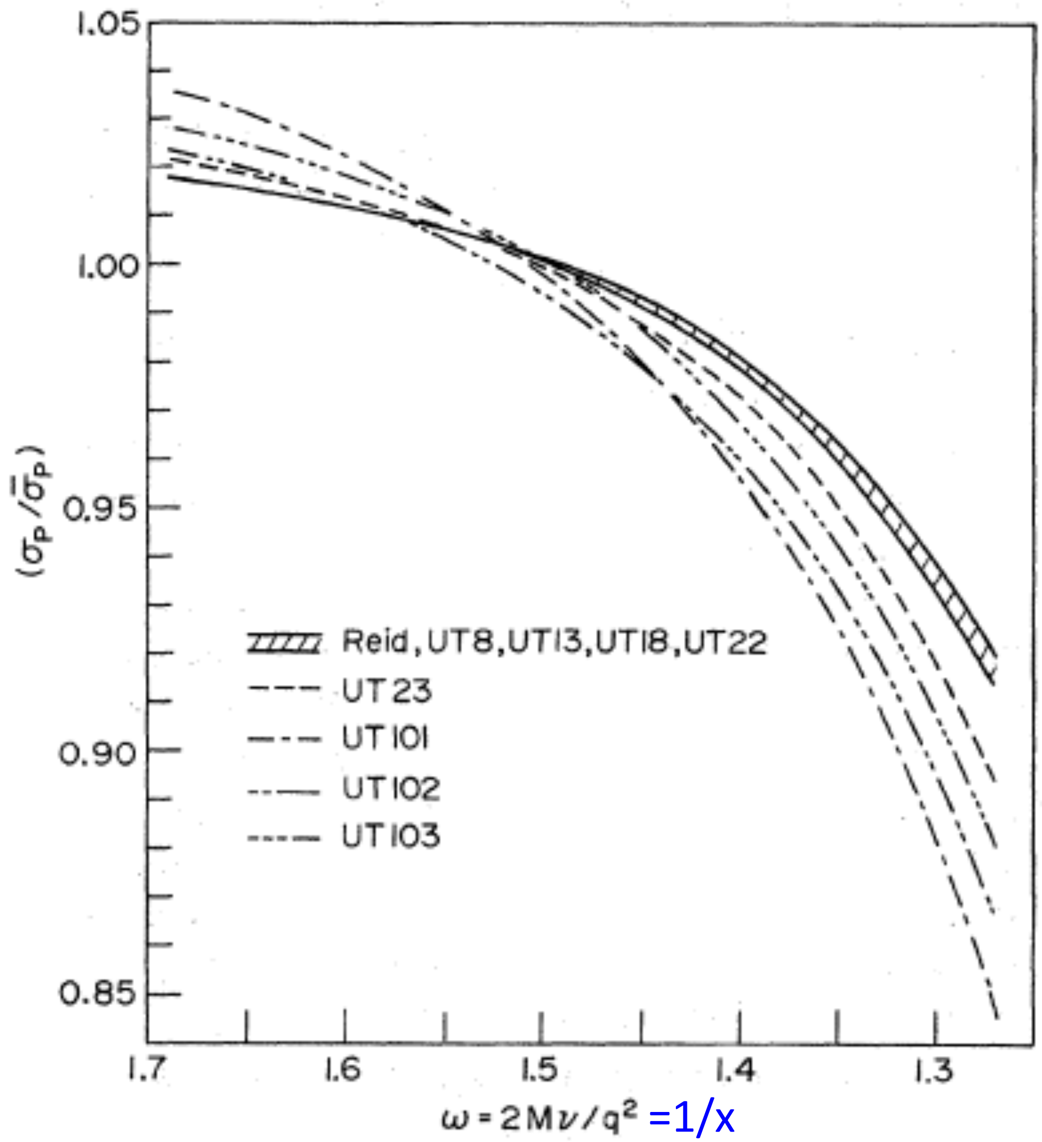


FIG. 7. Ratio of unsmeared to smeared proton cross section for different deuteron wave functions. These results are obtained using a beam energy of 17.0 GeV and a lab scattering angle of 18°.

Uncertainties in the nucleon momentum distribution in the Deuteron arising from undetermined SRCs

J.P. Vary, Phys. Rev. C7, 521(1973)

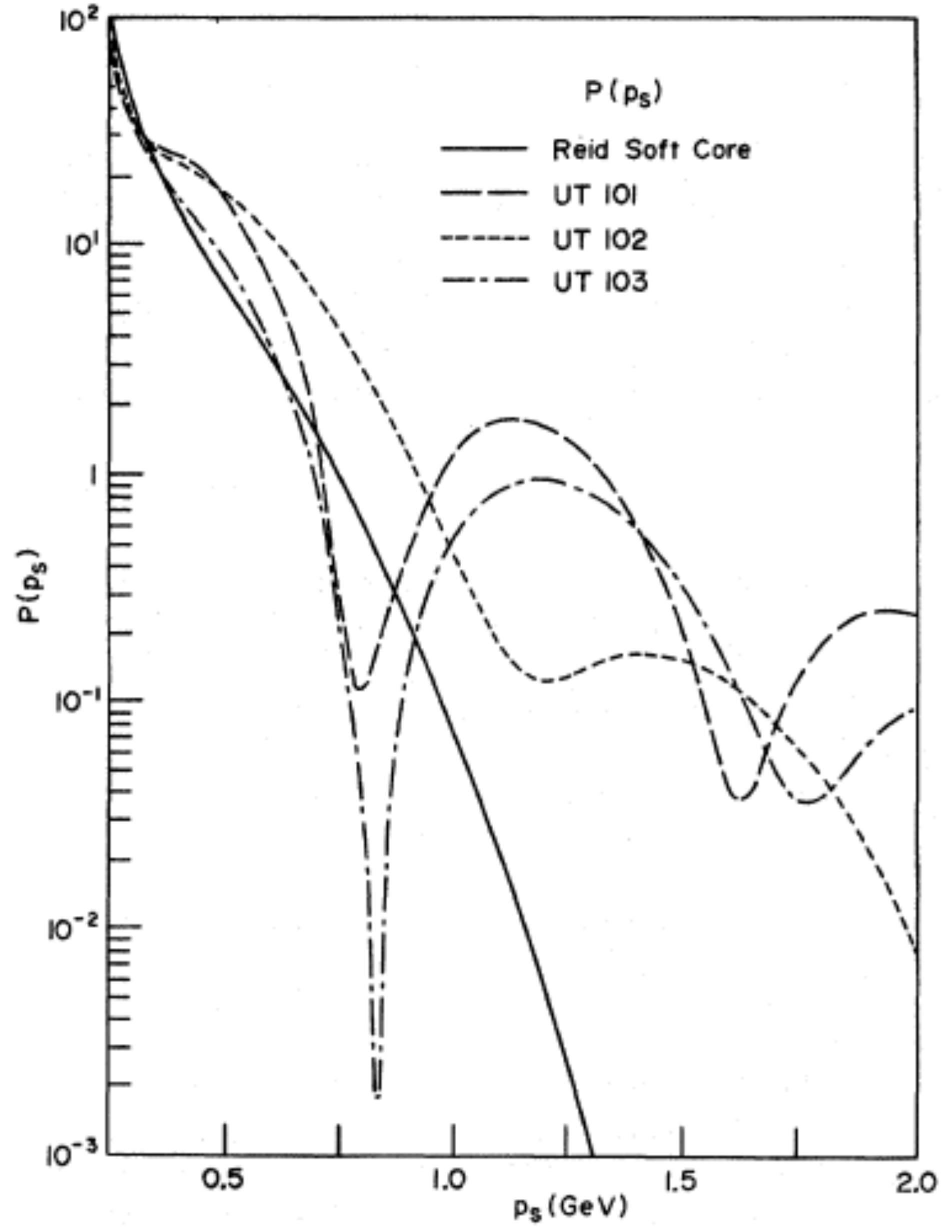


FIG. 12. Momentum-space probability distribution [Eq. (24)] of a nucleon in the deuteron. The distributions are given for the Reid soft core and the case (b) wave functions for the range $0.25 \le p_s \le 2.0$ GeV.

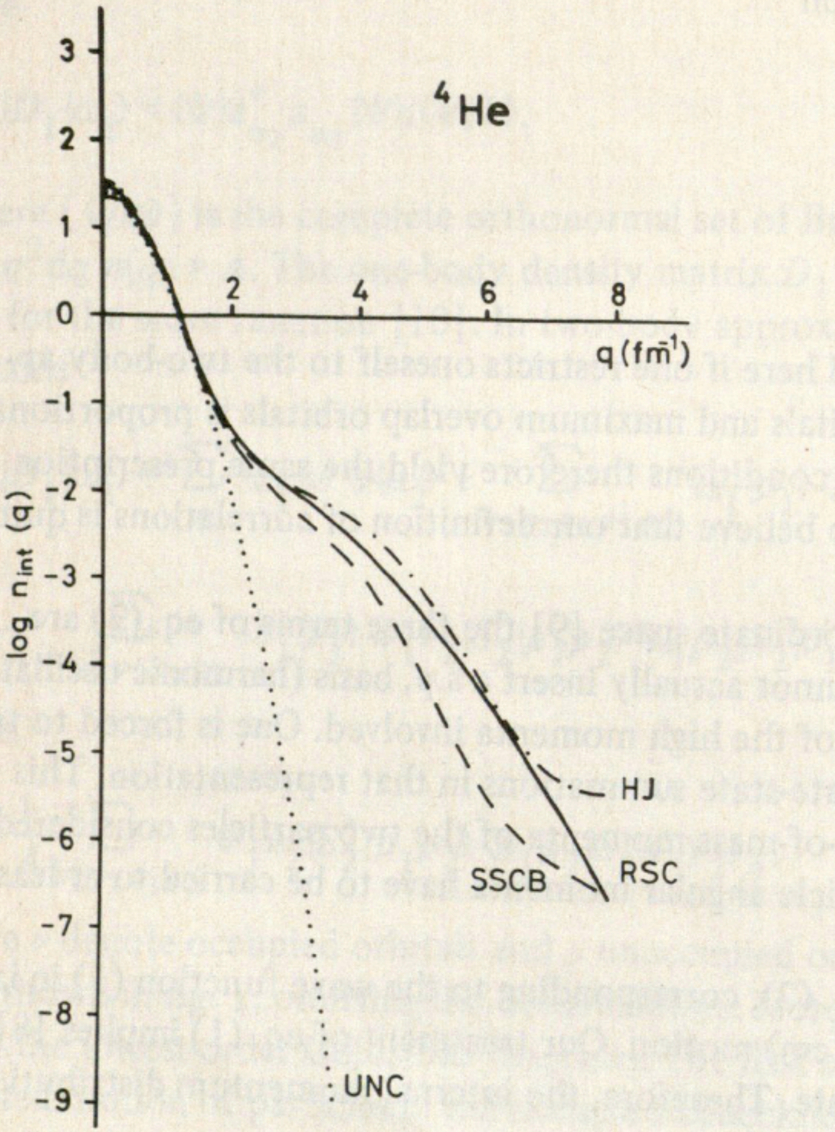


Fig. 2. Momentum distributions for ^{4}He, HJ: Hamada–Johnston potential, RSC: Reid soft core potential, SSCB: de Tourreil–Sprung super soft core potential B, UNC: uncorrelated, for the RSC potential. The other uncorrelated distributions do not differ appreciably for $q > 2$ fm^{-1}.

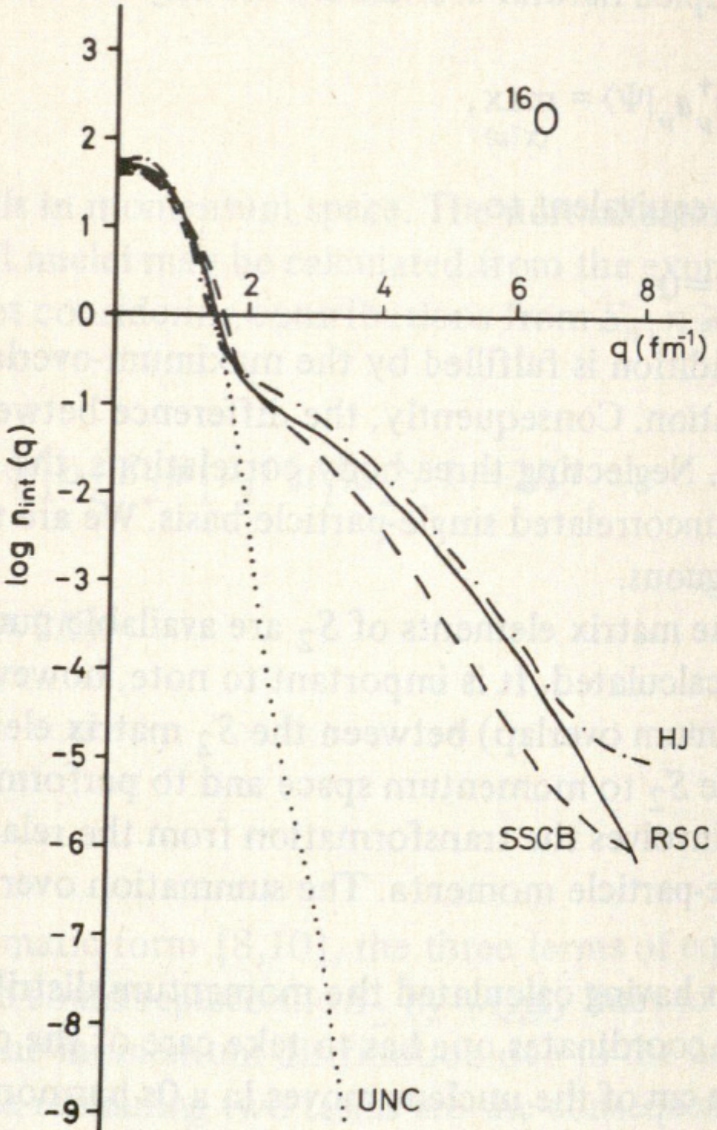
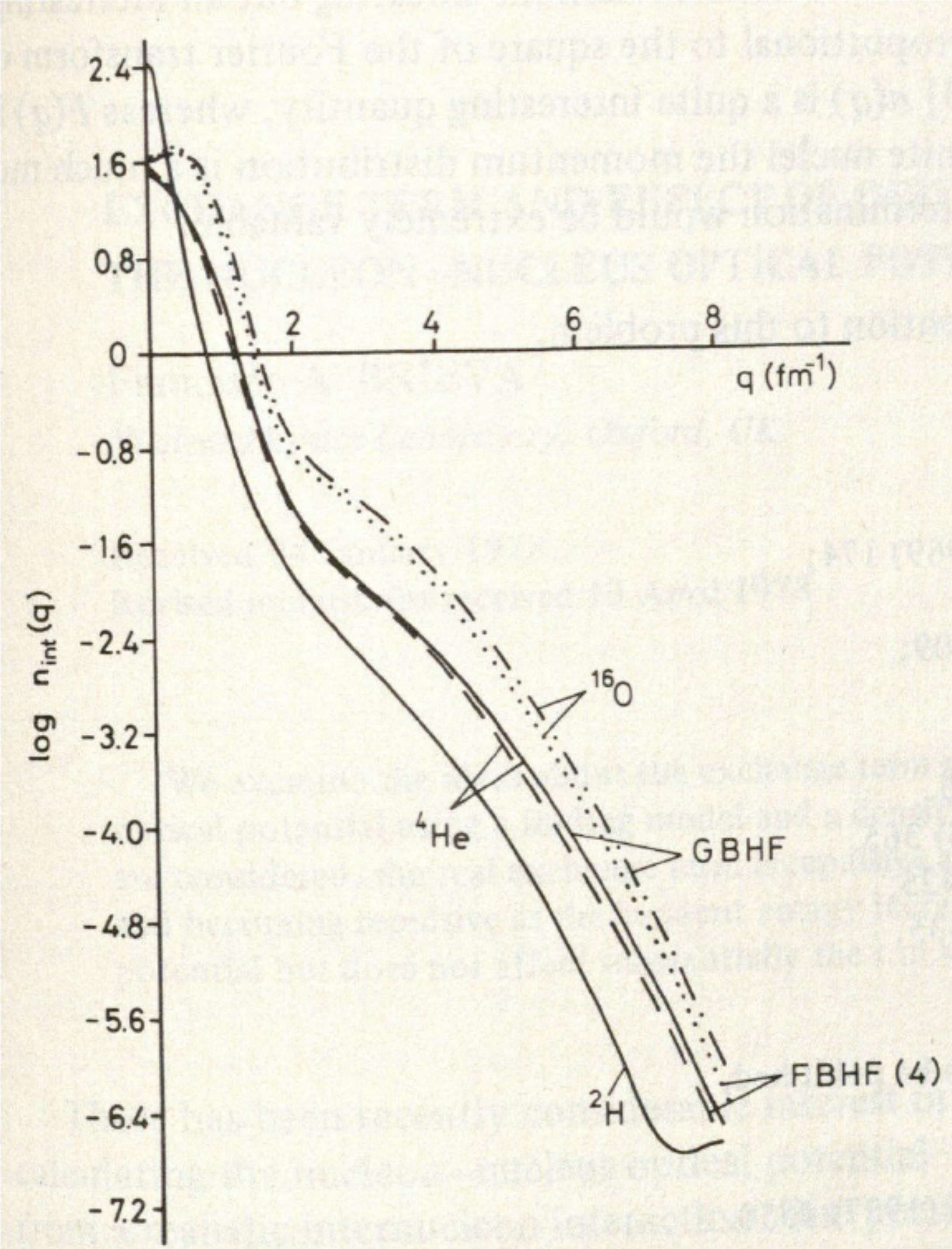


Fig. 3. Same as fig. 2, for ^{16}O.

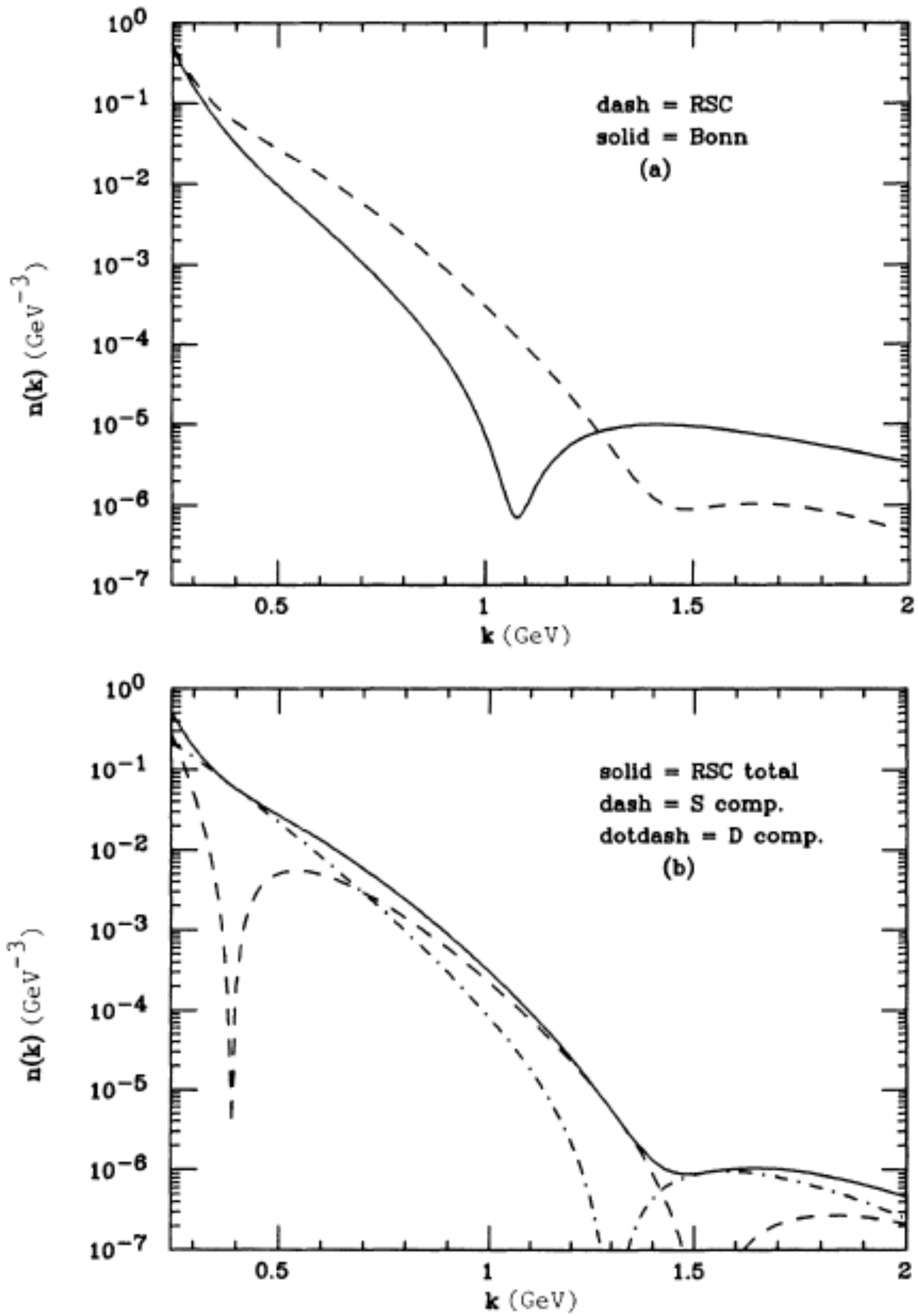
J.G. Zabolitzky and W. Ey, Phys Letts B76, 547 (1978)



J.G. Zabolitzky and W. Ey,
Phys Letts B76, 547 (1978)

Reid soft core NN interaction

GBHF: Coupled Cluster – NN only
FBHF: Coupled Cluster adding 3N and 4N terms



Sensitivity of nucleon momentum distributions In the Deuteron to intermediate range and short range correlations from competing NN interactions.

G. Yen, J.P. Vary, A. Harindranath and H.J. Pirner, Phys. Rev. C 42, 1665 (1990)

Tensor Forces and the Ground-State Structure of Nuclei

R. Schiavilla[1,2], R.B. Wiringa[3], Steven C. Pieper[3], and J. Carlson[4]

Phys. Rev. Lett. 98, 132501 (2007); arXiv: nucl-th 0611037

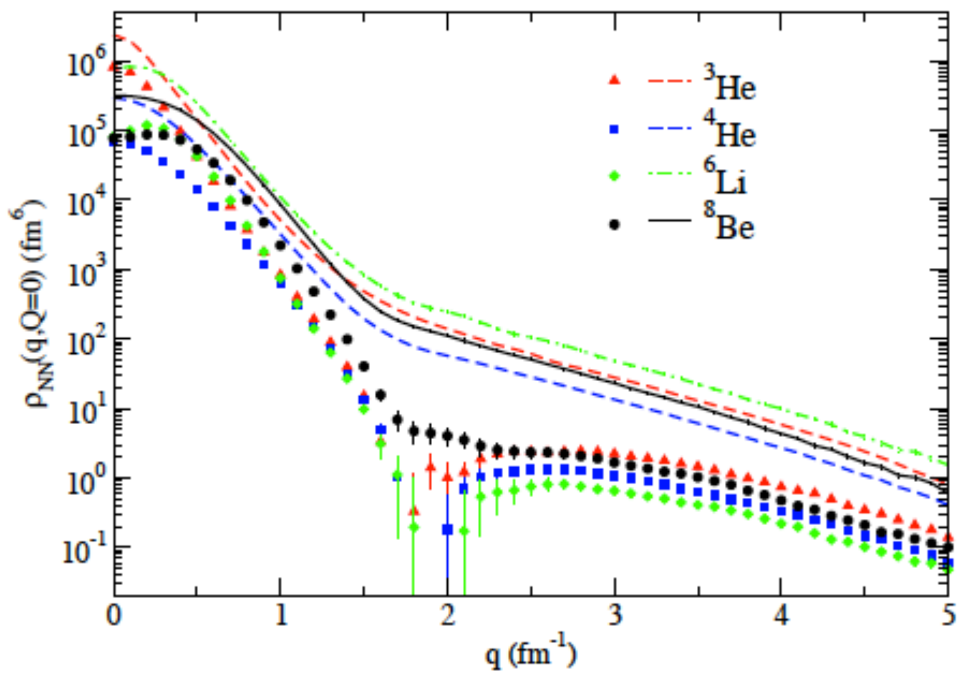


FIG. 1: (Color online) The *np* (lines) and *pp* (symbols) momentum distributions in various nuclei as functions of the relative momentum q at vanishing total pair momentum Q.

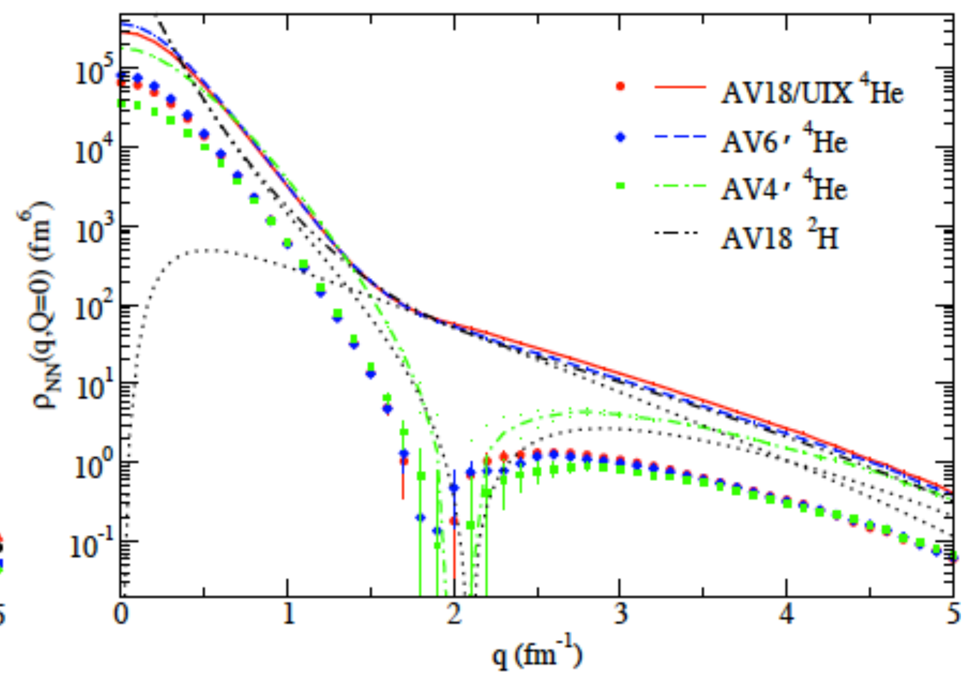
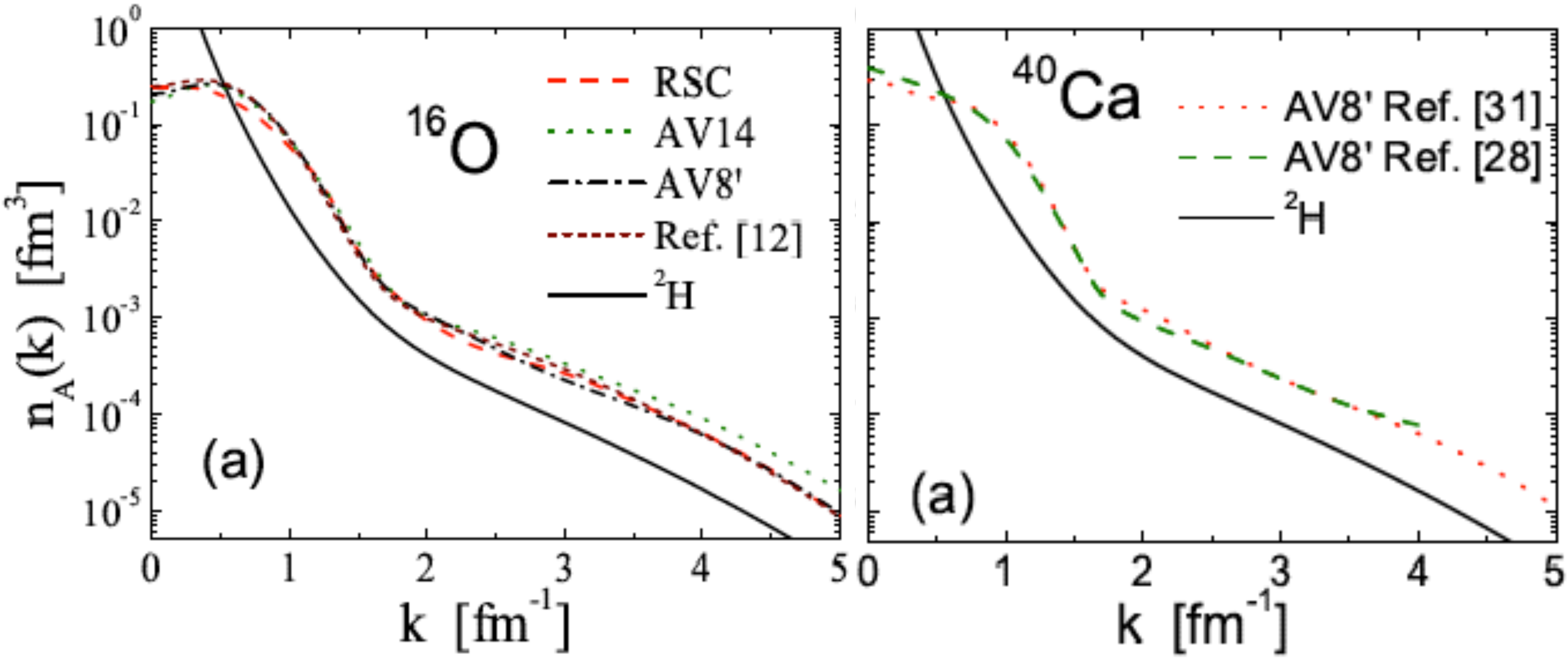


FIG. 2: (Color online) The *np* (lines) and *pp* (symbols) momentum distributions in ^{4}He obtained with different Hamiltonians. Also shown is the scaled momentum distribution for the AV18 deuteron; its separate S- and D-wave components are shown by dotted lines.

Universality of nucleon-nucleon short-range correlations: nucleon momentum distributions and their spin-isospin dependence

M. Alvioli,[1] C. Ciofi degli Atti,[2] L. P. Kaptari,[3,4] C. B. Mezzetti,[5,6] and H. Morita[7]



Nucleon-nucleon interaction in the *J*-matrix inverse scattering approach and few-nucleon systems

A. M. Shirokov*
Skobeltsyn Institute of Nuclear Physics, Moscow State University, Moscow, 119992, Russia

A. I. Mazur† and S. A. Zaytsev‡
Physics Department, Khabarovsk State Technical University, Tikhookeanskaya 136, Khabarovsk 680035, Russia

J. P. Vary§ and T. A. Weber‖
Department of Physics and Astronomy, Iowa State University, Ames, Iowa 50011-3160, USA

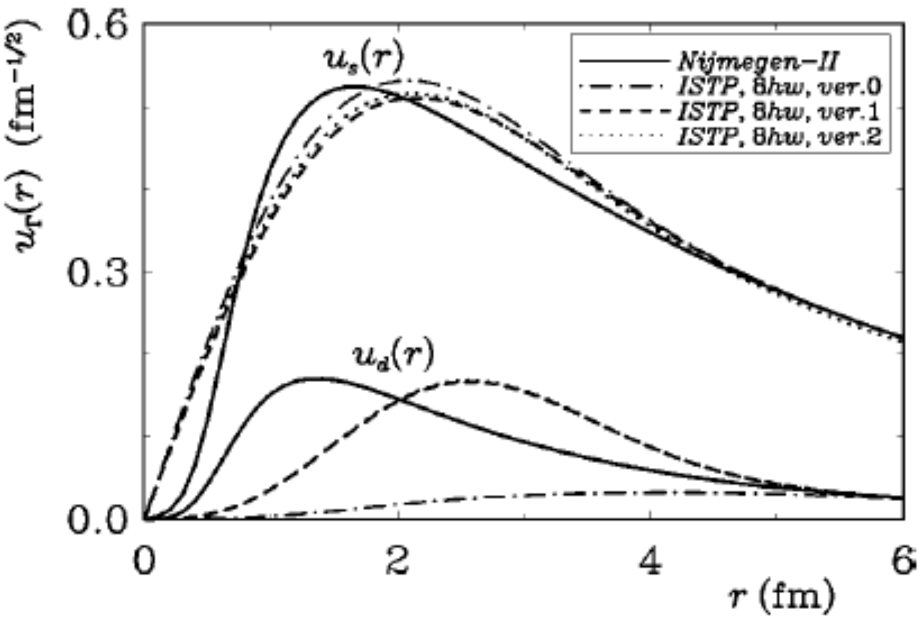
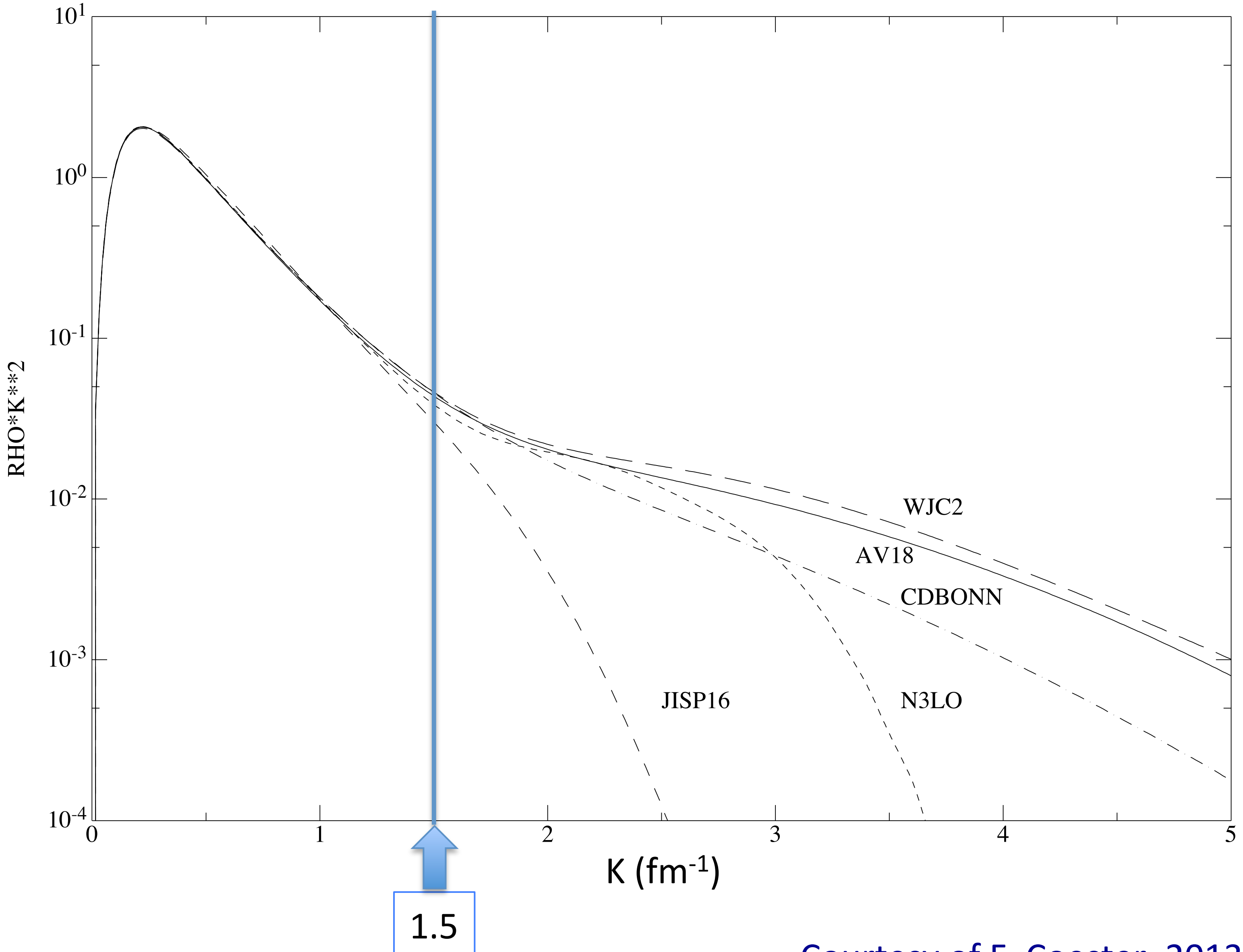


FIG. 34. Radial deuteron wave functions. Solid line—realistic meson exchange Nijmegen-II potential (See Ref. [3]) wave functions; dot-dash line—Version 0 ISTP wave functons; dashed line—Version 1 ISTP wave functions; dotted line—Version 2 ISTP wave functons.



Courtesy of F. Coester, 2013

Summary and Outlook

Ab initio nuclear structure/reactions has been developed rapidly

Advances in NN + NNN interactions based on chiral EFT (+ Deltas)
will underpin high precision investigations with controlled uncertainties
at low to moderate resolution scales

The UV scale will be set by regulators and renormalization (RR) procedures
(Furnstahl, . . . talks)

Consistent application of RR for structure and reactions will be critical to
have a controlled theory of nuclei at low and intermediate resolution.

Bridging these anticipated successful developments with the high-resolution
scale of nuclear phenomena remains an outstanding challenge.

Realtivistic QFT will be essential for high Q physics
(Stan Brodsky, Xingbo Zhao, . . . talks).

Many outstanding nuclear physics puzzles and discovery opportunities

Clustering phenomena

Origin of the successful nuclear shell model

Nuclear reactions and breakup

Astrophysical r/p processes & drip lines

Predictive theory of fission

Existence/stability of superheavy nuclei

Physics beyond the Standard Model

Possible lepton number violation

+ Many More!