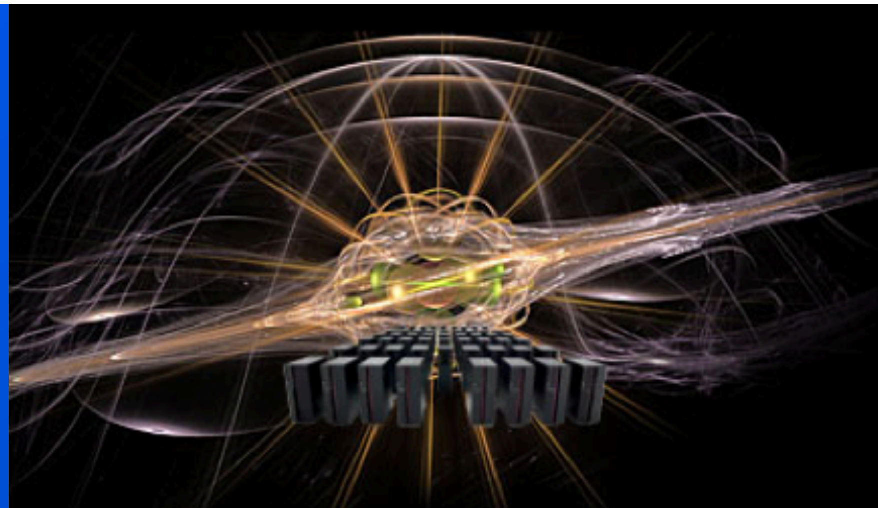

Recent physics insights from light nuclei and neutron drops

James P. Vary

Iowa State University

Progress in Ab Initio Techniques in Nuclear Physics

February 21-23, 2013

NUCLEI Nuclear Computational Low-Energy Initiative

U.S. DEPARTMENT OF ENERGY INCITE LEADERSHIP COMPUTING

National Science Foundation WHERE DISCOVERIES BEGIN

Selected insights of topics not already covered at this meeting

NCSM review paper published

B. R. Barrett, P. Navratil and J. P. Vary,
Prog. Part. Nucl. Phys., 69, 131 (2013).

New methods and applications (since review submitted)

(s) = submitted [3]; (a) = accepted [1]; (p) = published [5]

p-shell nuclei (see talk by Erich Ormand) (s)
A=7&8 in NCSM which chiral NN+NNN interactions (p)
Li-isotopes in NCFC (p) – some results cited in review paper
Neutron drops in NCFC (s)
Rotational states in the Be isotopes in NCFC (p)
Monte Carlo NCSM (MC-NCSM) (p)
Symmetry Adapted NCSM (SA-NCSM) (s)
Coulomb-Sturmian (CS) basis (p)
GPU accelerated decoupling of 3NF (a)

Progress in Particle and Nuclear Physics 69 (2013) 131–181

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Progress in Particle and Nuclear Physics

journal homepage: www.elsevier.com/locate/ppnp

Review

Ab initio no core shell model

Bruce R. Barrett [a], Petr Navrátil [b], James P. Vary [c,*]

[a] Department of Physics, University of Arizona, Tucson, AZ 85721, USA

[b] Theory Group, TRIUMF, Vancouver, BC V6T 2A3, Canada

[c] Department of Physics and Astronomy, Iowa State University, Ames, IA 50011, USA

Contents

Contents (Continued)

Comparison of theory and experiment for a suite of observables & predictions

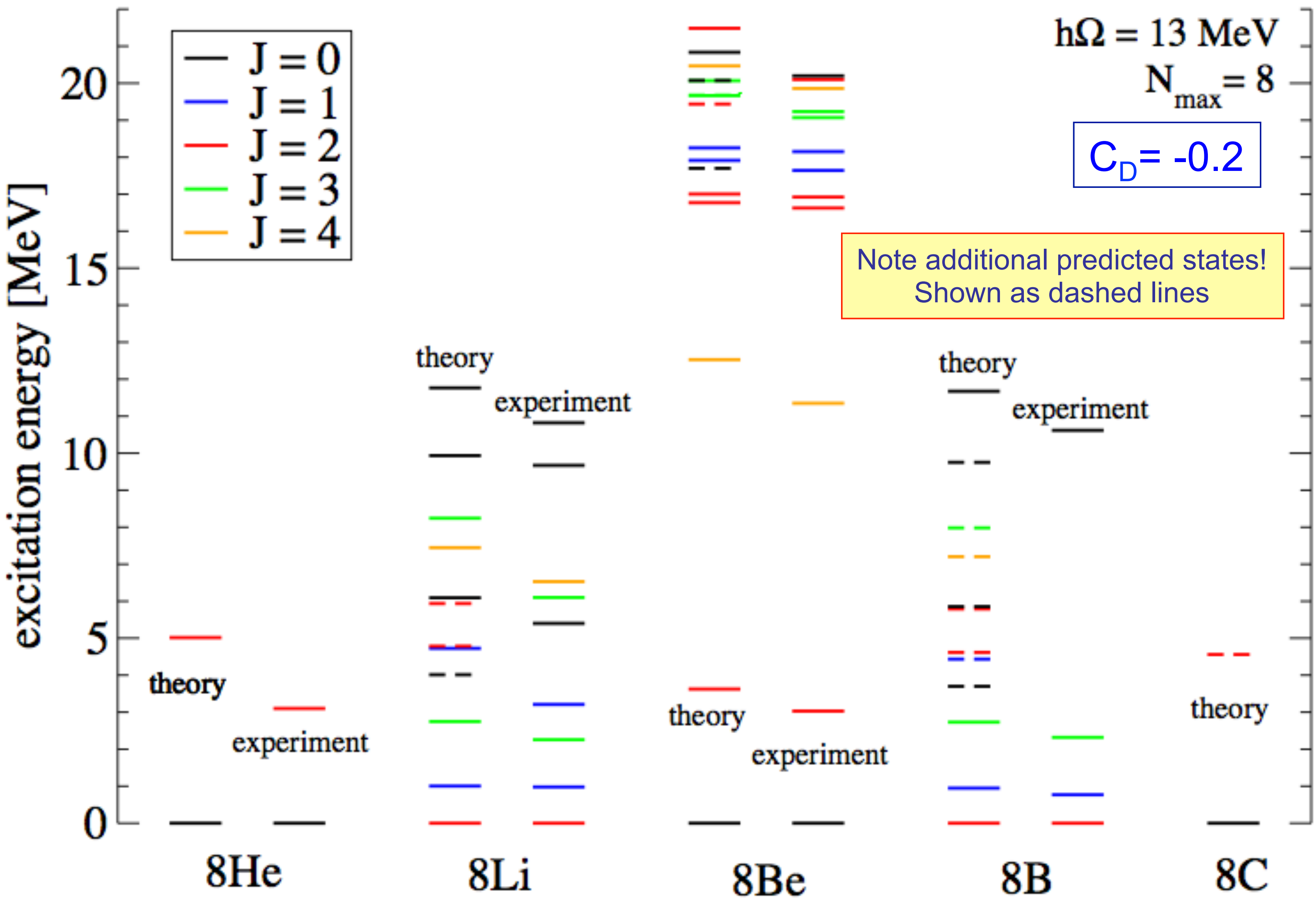
Note: Each observable has at least two theory results to compare with Expt

^{8}Li	Expt.	Chiral $NN + NNN$ Okubo–Lee–Suzuki	Chiral $NN + NNN$ SRG(0.08) $N_{max} = 8; 10$	AV18/IL2	JISP16	INOY	CD-B
$E_b(2^+)$	41.277	39.95(69)	39.90(1) ; 40.79(10)	41.9(2)	40.3(2)	41.3(5)	35.82
$\langle r^2_{pp} \rangle^{1/2}$	2.21(6)	2.09		2.09(1)	2.1	2.01	2.17
$E_x(1^+_1 1)$	0.981	1.00 (16;03)	1.027(2) ; 0.985(6)	1.4(3)	1.5(2)	1.26	0.86
$E_x(3^+_1 1)$	2.255(3)	2.75 (16;09)	2.608(3) ; 2.599(7)	2.5(3)	2.8(1)	2.87	3.02
$E_x(0^+_1 1)$	–	4.01 (84;20)	3.842(15) ; 3.537(40)			4.22	2.48
$E_x(1^+_2 1)$	3.210	4.73 (84;21)	4.632(16) ; 4.283(44)			4.90	3.25
$E_x(2^+_2 1)$	–	4.78 (44;12)	4.603(7) ; 4.443(23)			5.11	3.98
$E_x(2^+_3 1)$	–	5.94 (37;20)				6.07	5.29
$E_x(1^+_3 1)$	5.400	6.09 (70;22)				6.76	5.02
$E_x(4^+_1 1)$	6.53(20)	7.45 (36;15)		7.2(3)	7.0(3)	7.40	6.69
$E_x(3^+_2 1)$	–	8.24 (50;22)				8.92	7.57
$E_x(0^+_1 2)$	10.822	11.77 (27;29)				12.05	10.90
$Q(2^+)$	3.27(6)	2.65	2.73(1) ; 2.79(1)	3.2(1)	2.6	2.55	2.78
$Q(1^+)$	–	1.08	1.12(1) ; 1.12(1)		1.2		
$Q(3^+)$	–	−1.97	−1.92(1); −1.94(2)		−2.0		
$Q(4^+)$	–	−3.01			−3.4		
$\mu(2^+)$	1.654	1.49	–	1.65(1)	1.3(1)	1.42	1.24
$\mu(1^+)$	–	−2.27			−2.2(2)		
$\mu(3^+)$	–	2.13			2.0(1)		
$\mu(4^+)$	–	1.86			1.84(1)		
$B(E2;1^+)$	–	1.19			1.9		
$B(E2;3^+)$	–	3.70			4.6		
$B(E2;4^+)$	–	1.21			1.9		
$B(M1;1^+)$	5.0(16)	4.13	4.15(1) ; 4.14(1)		3.7(2)	4.56	4.39
$B(M1;3^+)$	0.52(23)	0.33	0.31(1) ; 0.30(1)		0.25(5)		

Note that some theory results have quantified uncertainties – see reference for details

B. R. Barrett, P. Navratil and J. P. Vary,
Prog. Part. Nucl. Phys., 69, 131 (2013).

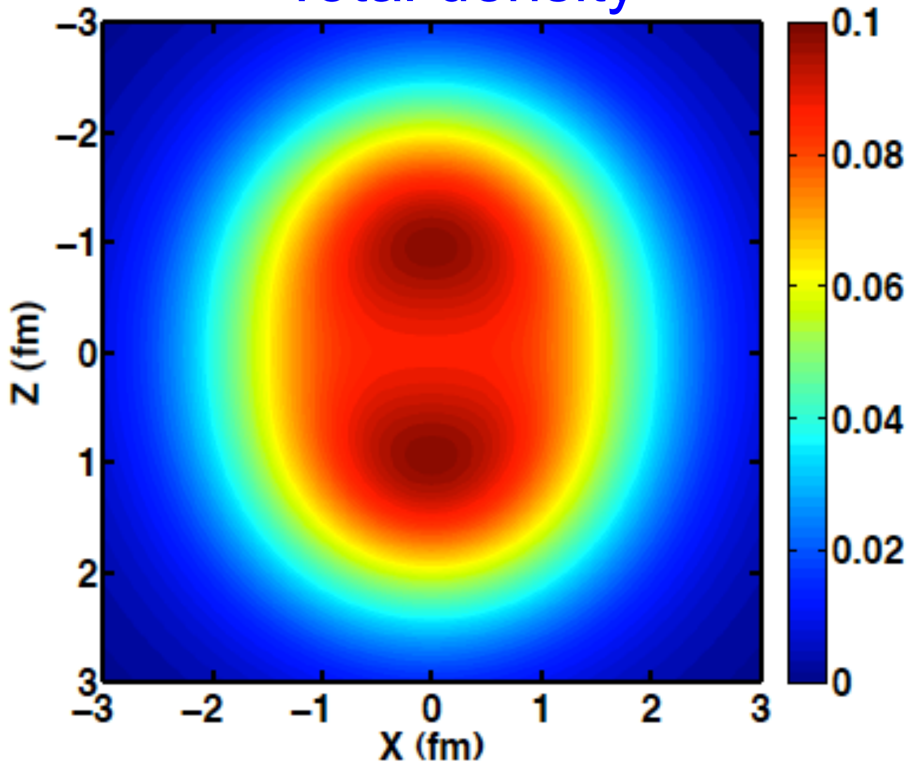
spectrum A=8 nuclei with N3LO 2-body + N2LO 3-body



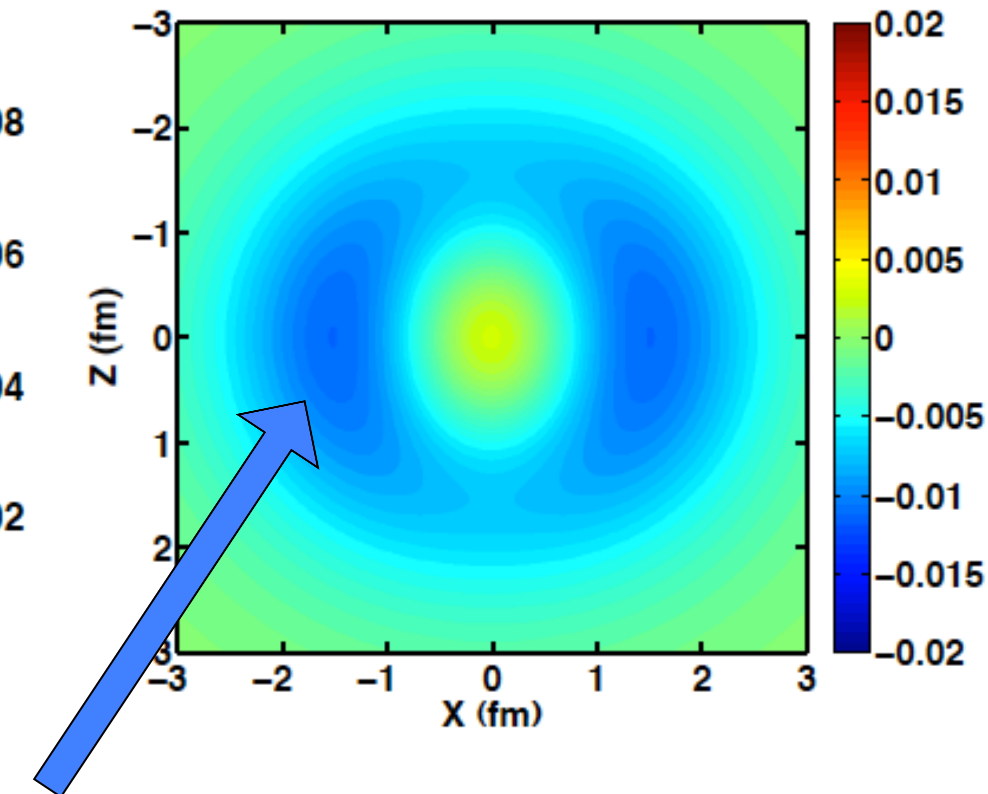
P. Maris, J. P. Vary and P. Navratil, Phys. Rev. C87, 014327 (2013); arXiv 1205.5686

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

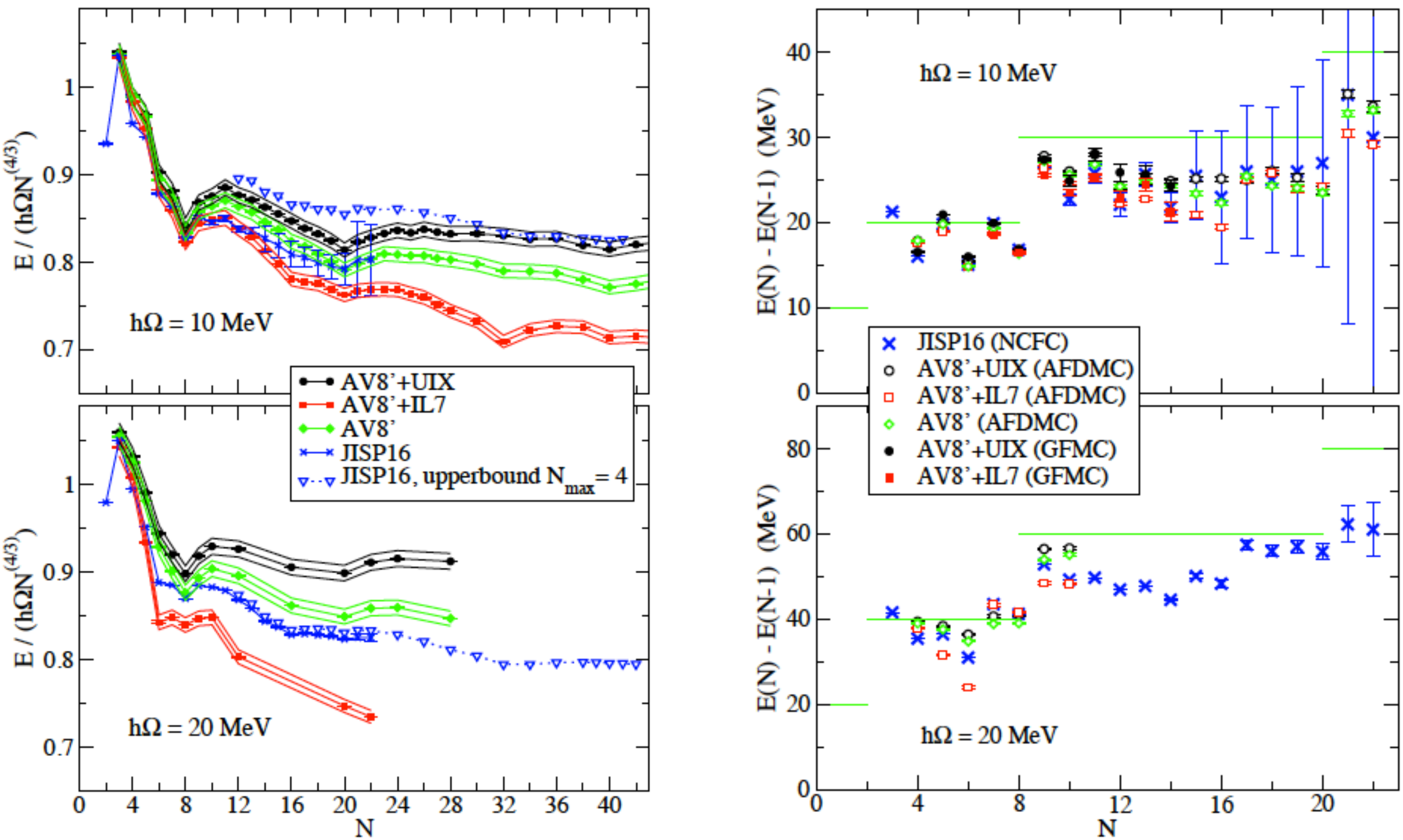
Properties of trapped neutrons interacting with realistic nuclear Hamiltonians

Pieter Maris and James P. Vary
Department of Physics and Astronomy, Iowa State University, Ames, IA, 50011

S. Gandolfi and J. Carlson
Theoretical Division, Los Alamos National Laboratory, Los Alamos, NM 87545

Steven C. Pieper
Physics Division, Argonne National Laboratory, Argonne, IL 60439
(Dated: February 7, 2013)

ArXiv: 1302.2089



Physics Letters B 719 (2013) 179–184

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Physics Letters B

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Emergence of rotational bands in *ab initio* no-core configuration interaction calculations of light nuclei

M.A. Caprio [a,*], P. Maris [b], J.P. Vary [b]

[a] Department of Physics, University of Notre Dame, Notre Dame, IN 46556-5670, USA
[b] Department of Physics and Astronomy, Iowa State University, Ames, IA 50011-3160, USA

Black line: Yrast band in collective model fit
Red line: excited band in collective model fit

Both natural and unnatural parity bands identified
Employed JISP16 interaction; N_{max} = 10 - 7

K=1/2 bands include Coriolis decoupling parameter:

$$E(J) = E_0 + A\left[J(J+1) + a(-)^{J+1/2}\left(J+\frac{1}{2}\right)\right],$$

$$Q(J) = \frac{3K^2 - J(J+1)}{(J+1)(2J+3)} Q_0,$$

$$B(E2; J_i \to J_f) = \frac{5}{16\pi}(J_i K 20 | J_f K)^2 (eQ_0)^2$$

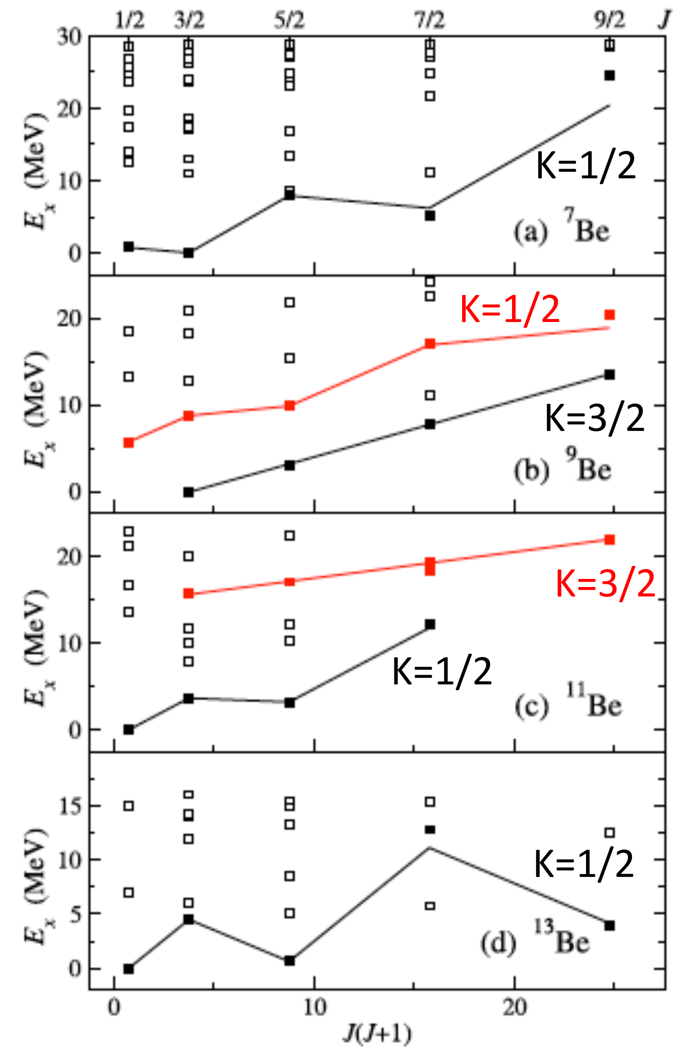


Fig. 1. Excitation energies obtained for states in the *natural* parity spaces of the odd-mass Be isotopes: (a) ^{7}Be, (b) ^{9}Be, (c) ^{11}Be, and (d) ^{13}Be. Energies are plotted with respect to $J(J+1)$ to facilitate identification of rotational energy patterns, while the J values themselves are indicated at top. Filled symbols indicate candidate rotational bandmembers (black for yrast states and red for excited states, in the web version of this Letter). The lines indicate the corresponding best fits for rotational energies. Where quadrupole transition strengths indicate significant two-state mixing (see text), more than one state of a given J is indicated as a bandmember.

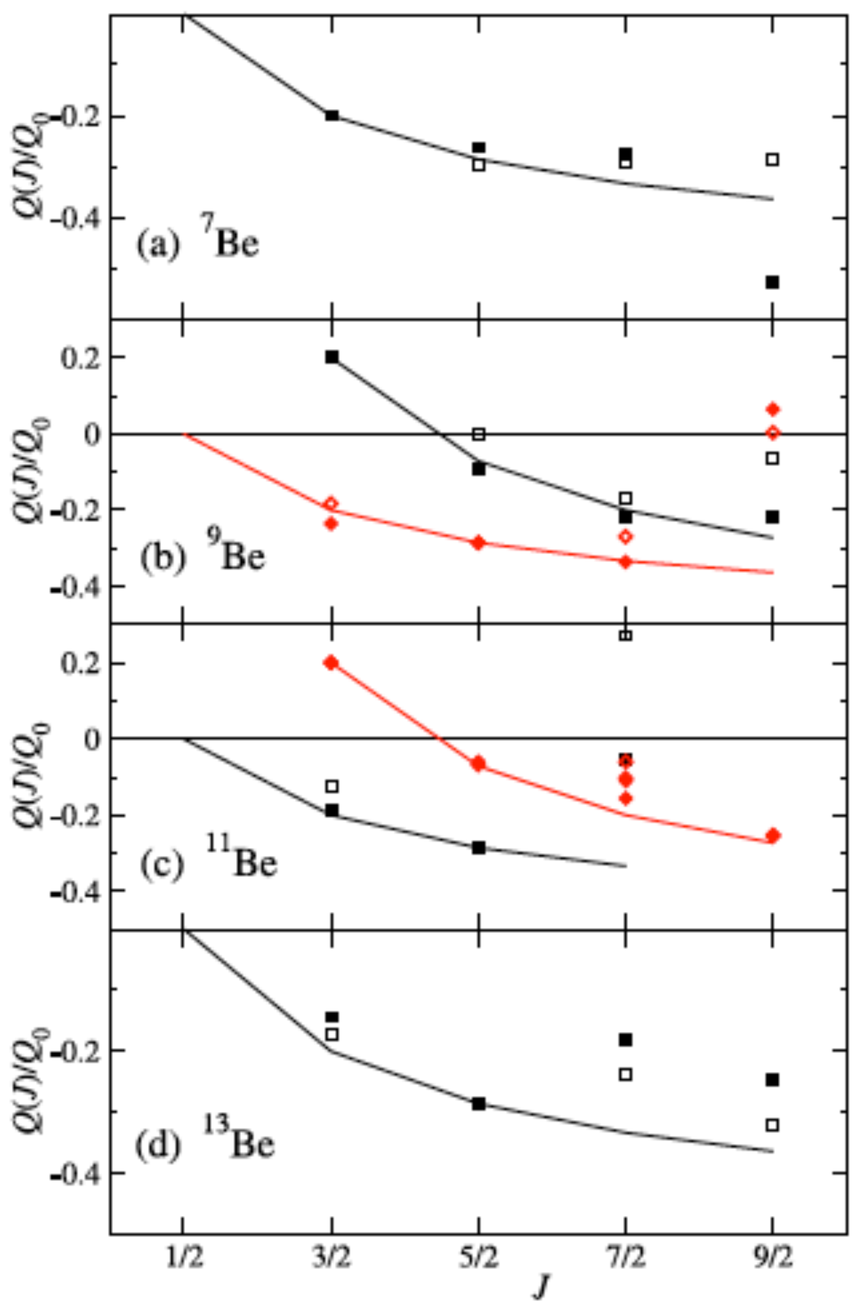


Fig. 3. Quadrupole moments calculated for candidate bandmembers in the *natural* parity spaces of the odd-mass Be isotopes: (a) ^{7}Be, (b) ^{9}Be, (c) ^{11}Be, and (d) ^{13}Be. The states are as identified in Fig. 1 and are shown as black squares for yrast states or red diamonds for excited states (color in the web version of this Letter). Filled symbols indicate proton quadrupole moments, and open symbols indicate neutron quadrupole moments. The curves indicate the theoretical values for a $K = 1/2$ or $K = 3/2$ rotational band, as appropriate, given by (4). Quadrupole moments are normalized to Q_0, which is defined by either the $J = 3/2$ or $J = 5/2$ bandmember (see text).

Note:
Although Q, B(E2) are slowly converging, the ratios within a rotational band appear remarkably stable

M.A. Caprio, P. Maris and J.P. Vary, Phys. Lett. B 719, 179 (2013)

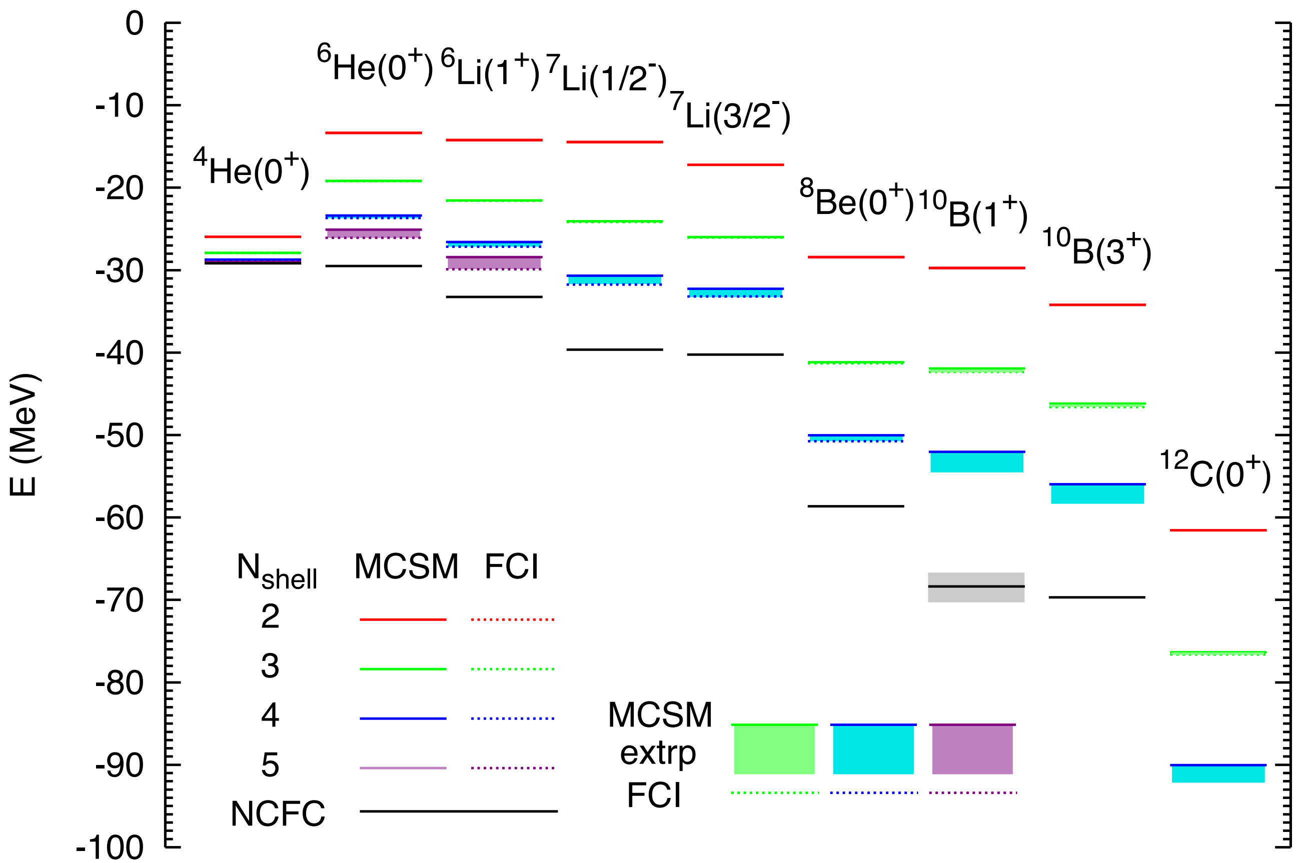
PHYSICAL REVIEW C 86, 054301 (2012)

Thanks to JUSTIPEN

Benchmarks of the full configuration interaction, Monte Carlo shell model, and no-core full configuration methods

T. Abe,[1] P. Maris,[2] T. Otsuka,[1,3,4] N. Shimizu,[1] Y. Utsuno,[5] and J. P. Vary[2]

arXiv:1204.1755



Notes:

Robust energy extrapolations based on energy variance

These MC-NCSM results are proof-of-principle

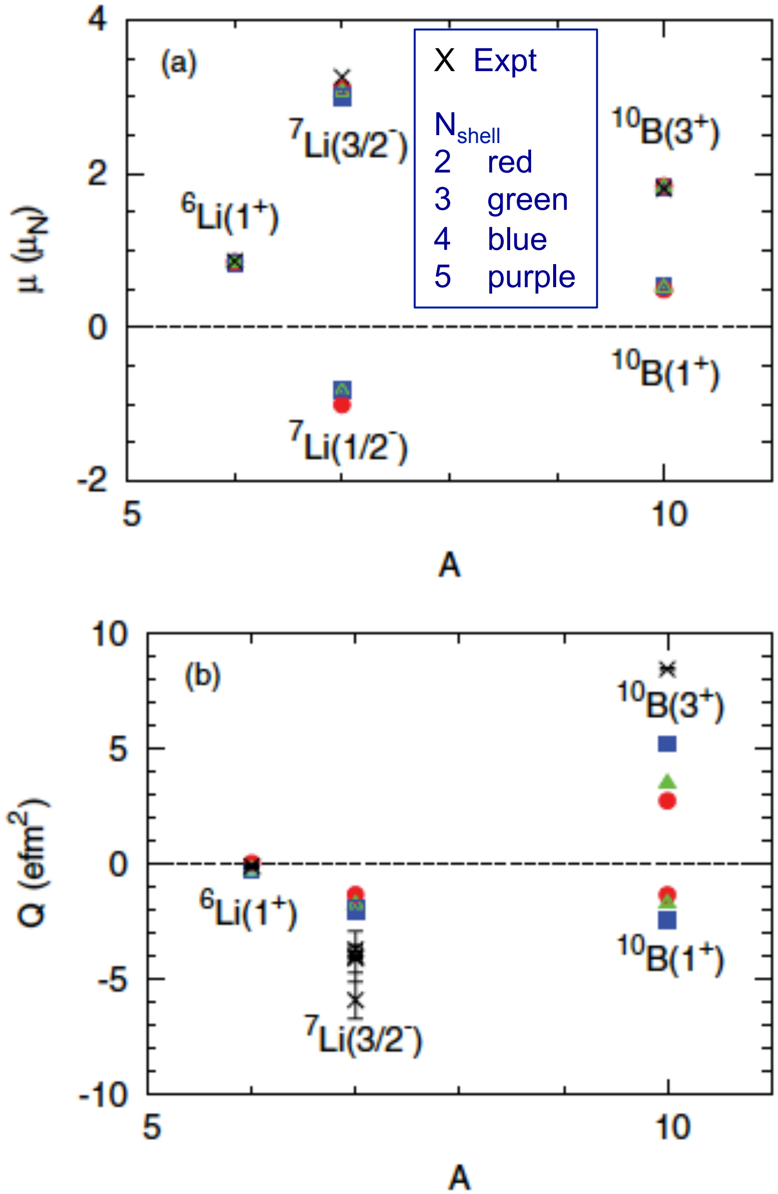


FIG. 10. (Color online) Comparisons between the extrapolated MCSM and FCI results for (a) the magnetic dipole moments, and (b) electric quadrupole moments. The conventions for the symbols are same as in Fig. 8; crosses indicate the experimental values for the ground states from Ref. [23].

MC-NCSM has superior scaling with A properties

Snapshot comparison	FCI	MCSM	NCFC
c.m. motion	approx.	approx.	exact
Spectra	OK	some	OK
wfns → observables	✓	✓	✓
Matrix dimension	$\lesssim 10^{10}$	$\lesssim 10^{20}$	$\lesssim 10^{10}$
Scaling with A	$A^{18\sim 20}$	$A^{3\sim 5}$	$A^{12\sim 14}$
No. parallel cores	10^5	10^5	10^5
Comp'l bottleneck	Memory	CPU time	Memory

T. Abe, P. Maris, T. Otsuka, N. Shimizu, Y. Utsuno and J.P. Vary, Phys. Rev. C 86, 054301 (2012)

Symmetry-adapted No-core Shell Model for Light Nuclei

K. D. Launey, T. Dytrych, J. P. Draayer, G. K. Tobin, M. C. Ferriss
Dept. of Physics and Astronomy, Louisiana State University, Baton Rouge, LA 70803, USA

D. Langr
Dept. of Computer Systems, Czech Technical University, Prague, Czech Republic

A. C. Dreyfuss
Keene State College, Keene, NH 03435, USA

C. Bahri
Dept. of Physics, University of Notre Dame, Notre Dame, IN 46556, USA

P. Maris and J. P. Vary
Dept. of Physics and Astronomy, Iowa State University, Ames, IA 50011, USA

Proceedings of the Sanibel ICFNS meeting, 2012 (to appear)

Model Space Dimensionality	$N_{\max} = 8[6]$-A 3.8%[a]	$N_{\max} = 8[6]$-B 9.2%[b]	$N_{\max} = 8$ 100%	Expt.
$E_{2_1^+}$ (MeV)	5.253	4.644	4.685	4.439
$E_{1_1^+}$ (MeV)		14.199	14.161	12.71
$E_{4_1^+}$ (MeV)	17.132	16.324	16.255	14.083
$r_m(0^+_{g.st.})$ (fm)	2.007	2.005	2.003	2.43(2)
$r_m(2_1^+)$ (fm)	2.027	2.023	2.024	N/A
$r_m(4_1^+)$ (fm)	2.058	2.055	2.061	N/A
$Q_{2_1^+}$ (e fm^2)	3.712	3.735	3.741	+6(3)
$Q_{4_1^+}$ (e fm^2)	4.826	4.845	4.864	N/A

Note: [a] Model space for all 0^+, 2^+, and 4^+ states in ^{12}C.
[b] Model space for all 0^+, 1^+, 2^+, and 4^+ states in ^{12}C.

The Coulomb-Sturmian basis for the nuclear many-body problem

M. A. Caprio

Department of Physics, University of Notre Dame,

Notre Dame, Indiana 46556-5670, USA

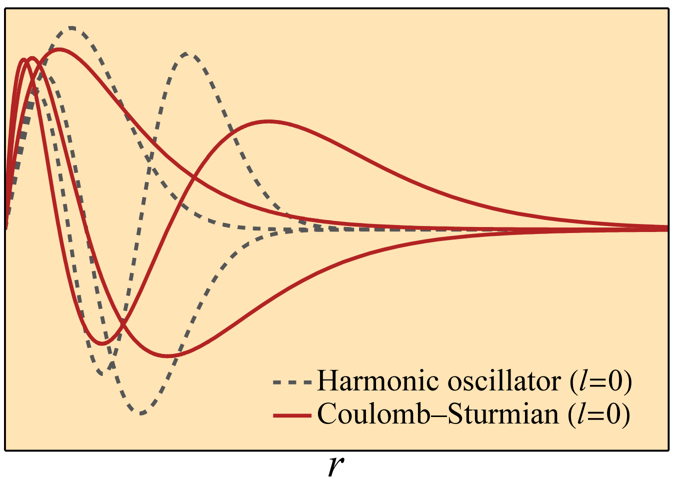
P. Maris and J. P. Vary

Department of Physics and Astronomy,

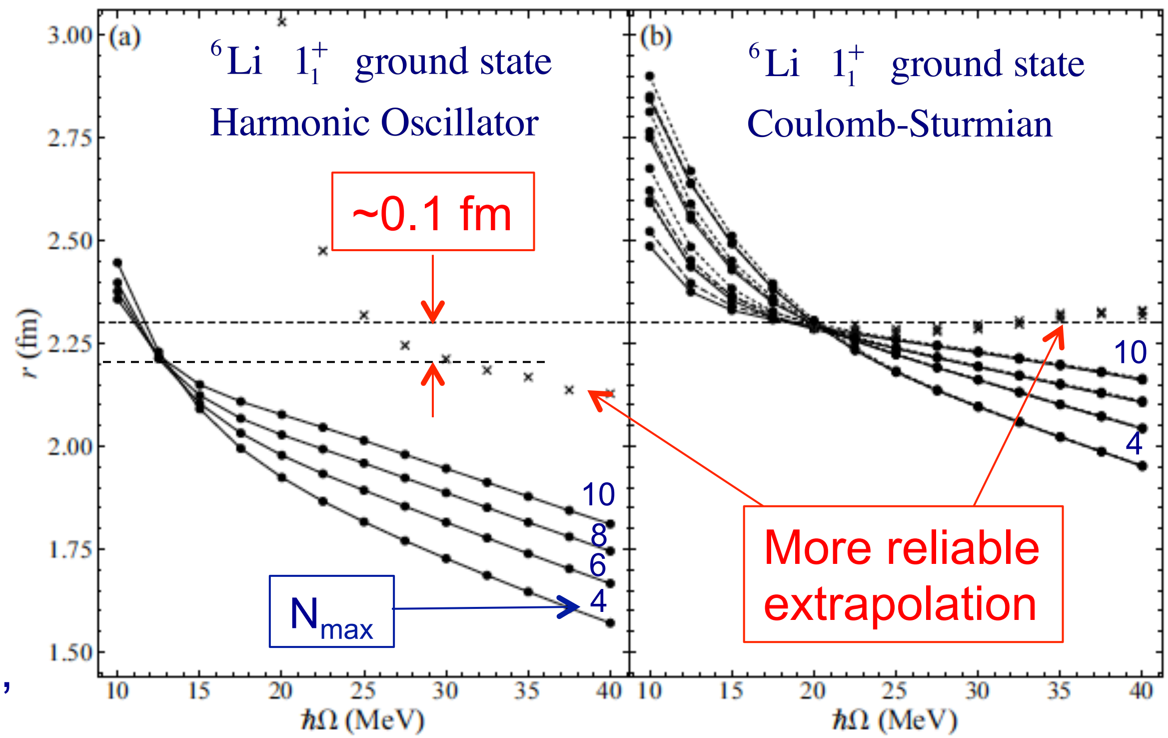
Iowa State University, Ames, Iowa 50011-3160, USA

Phys. Rev. C 86, 034312 (2012).; arXiv:1208.4156

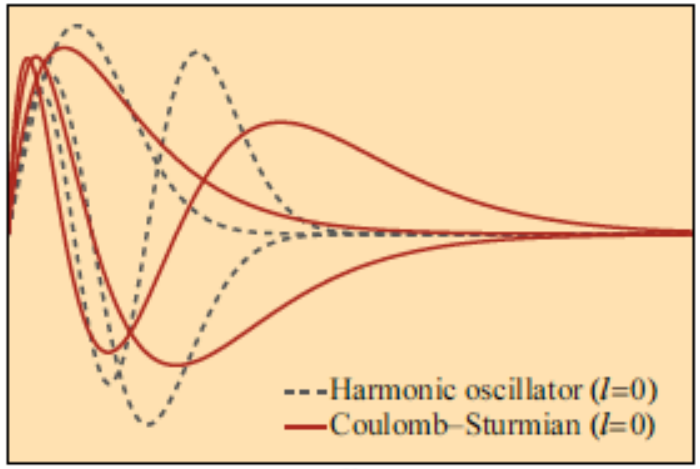
Goals: Improve the asymptotic wavefunctions and accelerate convergence of long-range observables (rms, Q, ANC, BE(2), M(2), etc)



- JISP16 used for these tests
- CS basis is not optimized
- rms = 2.3 fm from NCFC in C. Cockrell, J.P. Vary and P. Maris, Phys. Rev. C 86, 034325 (2012)



Coulomb-Sturmian radial wave functions



Coulomb

$$\psi_{nl}(r) \propto (2Zr)^{l+1} L_n^{(2l+1)}\left(\frac{2Zr}{n+l+1}\right) e^{-Zr/(n+l+1)}$$

Schrödinger solutions only form complete set if continuum states included…

Coulomb-Sturmian

$$\phi_{nl}(r) \propto (2r/b)^{l+1} L_n^{(2l+1)}(2r/b) e^{-r/b} \qquad (n+l+1)/Z \to b$$

Sturm-Liouville solutions form complete, discrete set, orthogonal under weight $1/r$…

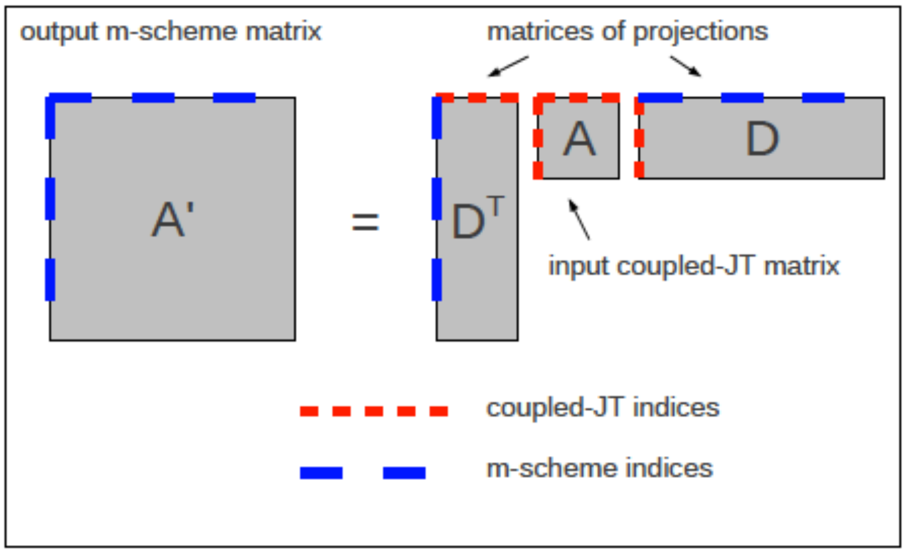
$$S_{nl}(r) \propto (2r/b)^{l+1} L_n^{(2l+2)}(2r/b) e^{-r/b} \qquad l \to l+1/2$$

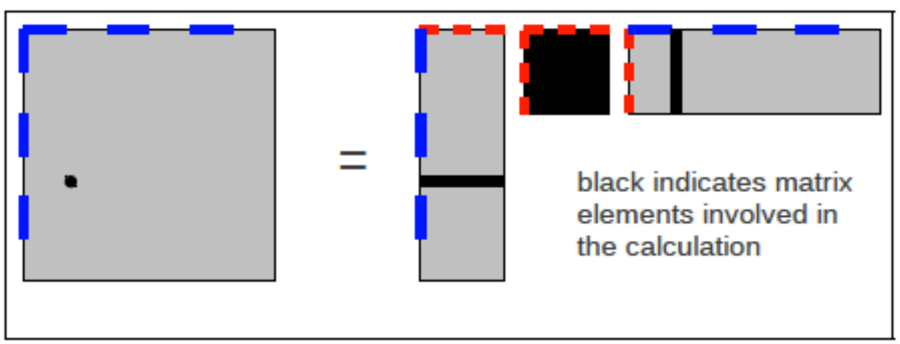
Complete, discrete, orthogonal set, for expansion of square-integrable functions…

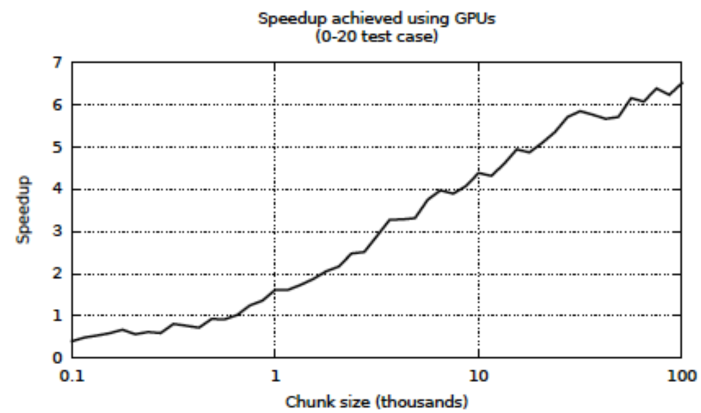
Leveraging GPUs in Ab Initio Nuclear Physics Calculations

Dossay Oryspayev[*], Hugh Potter[†], Pieter Maris[†], Masha Sosonkina[*‡], James P. Vary[†], Sven Binder[§], Angelo Calci[§], Joachim Langhammer[§], and Robert Roth[§]
[*]*Department of Electrical and Computer Engineering, Iowa State University, Ames, IA 50011, USA*
[†]*Department of Physics and Astronomy, Iowa State University, Ames, IA 50011, USA*
[‡]*Department of Modeling, Simulation and Visualization Engineering, Old Dominion University, Norfolk, VA 23529, USA*
[§]*Institut für Kernphysik, Technische Universität Darmstadt, 64289 Darmstadt, Germany*

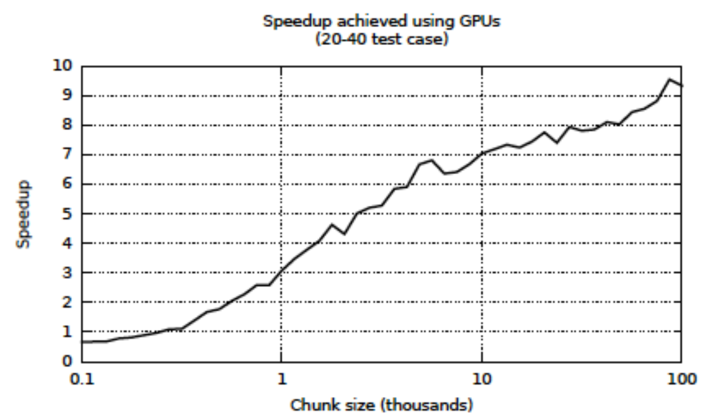
Accepted for publication in IEEE conference PDSEC-13 proceedings







(a) 0-20 test case



(b) 20-40 test case

Many recent insights obtained:

Collective modes in light nuclei accessible with ab initio approach
3NFs continue to play an important role in many observables
Neutron drop results show (sub)shell closures
IR and UV convergence in HO basis (Coon, Papenbrock)
Alternative basis spaces could relieve IR shortcomings of HO basis
Alternative MB methods could access clustering, halo physics regions
Computer Science and Applied Math collaborations invaluable
Generous allocations of computer resources essential to progress