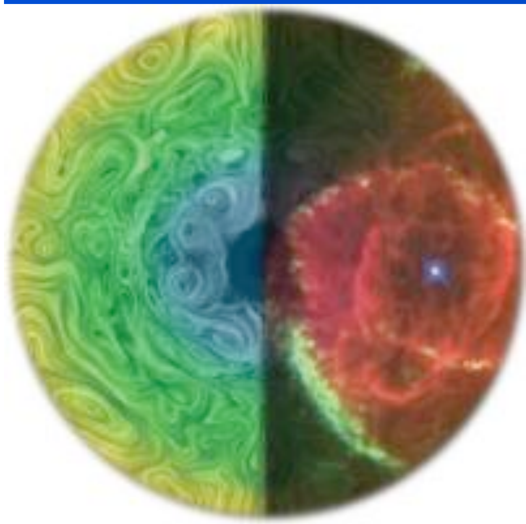
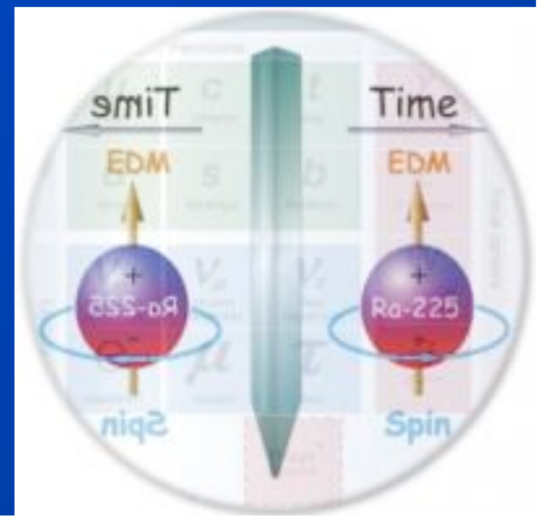
Computational Quantum Hamiltonian Physics
Finite Nuclei with Strong Interactions

James P. Vary, Iowa State University



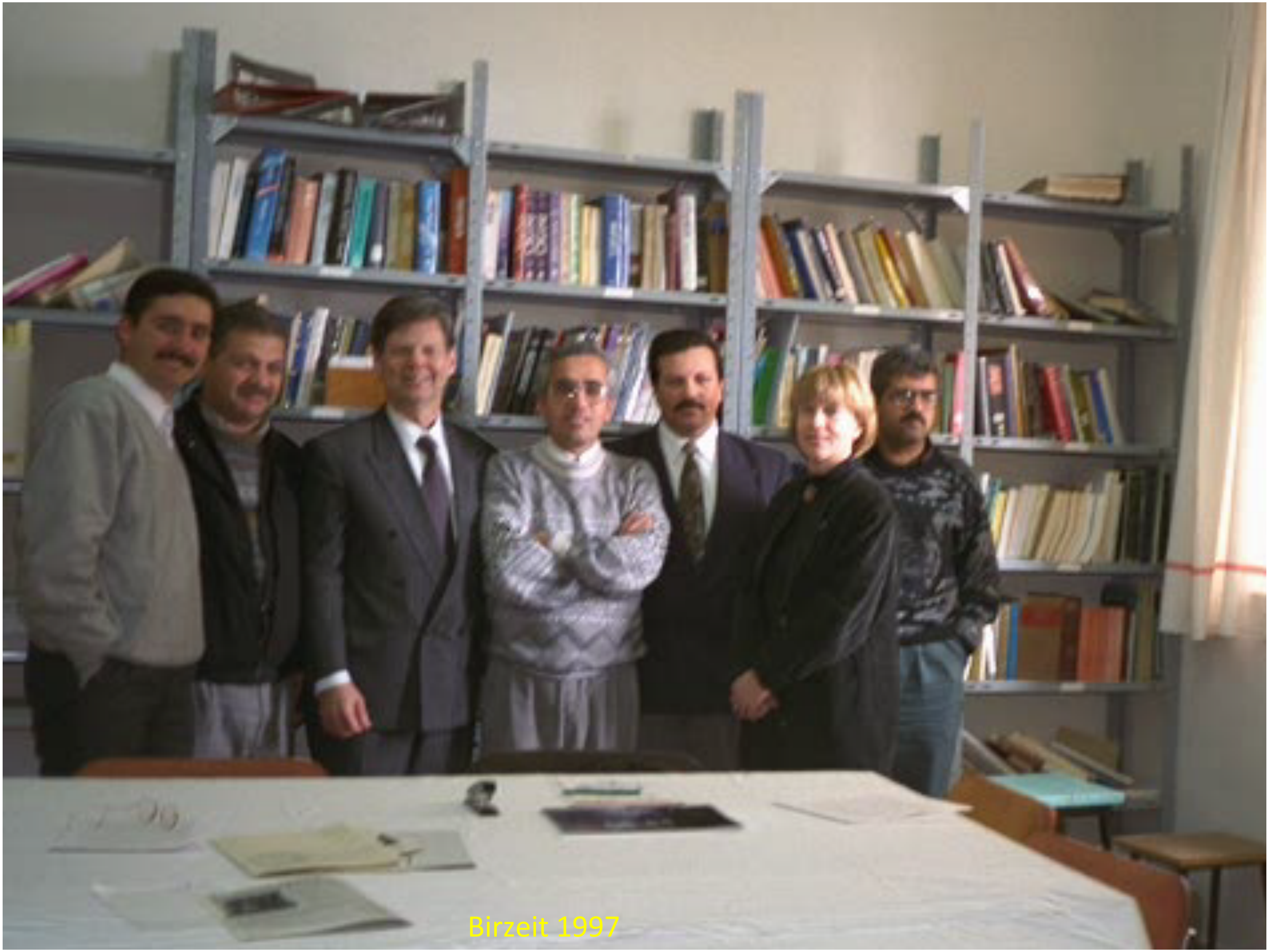



1997
An-Najah 1997


Al-Quds 1997

Al-Quds 1997


Birzeit 1997


Birzeit 1997

Fundamental questions of nuclear physics => discovery potential

- What controls nuclear saturation?
- How shell and collective properties emerge 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?
- Can we solve QCD to describe hadronic structures and interactions?

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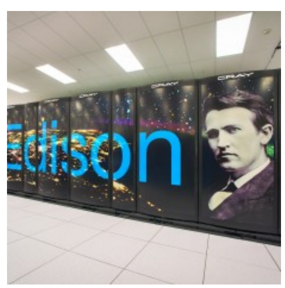
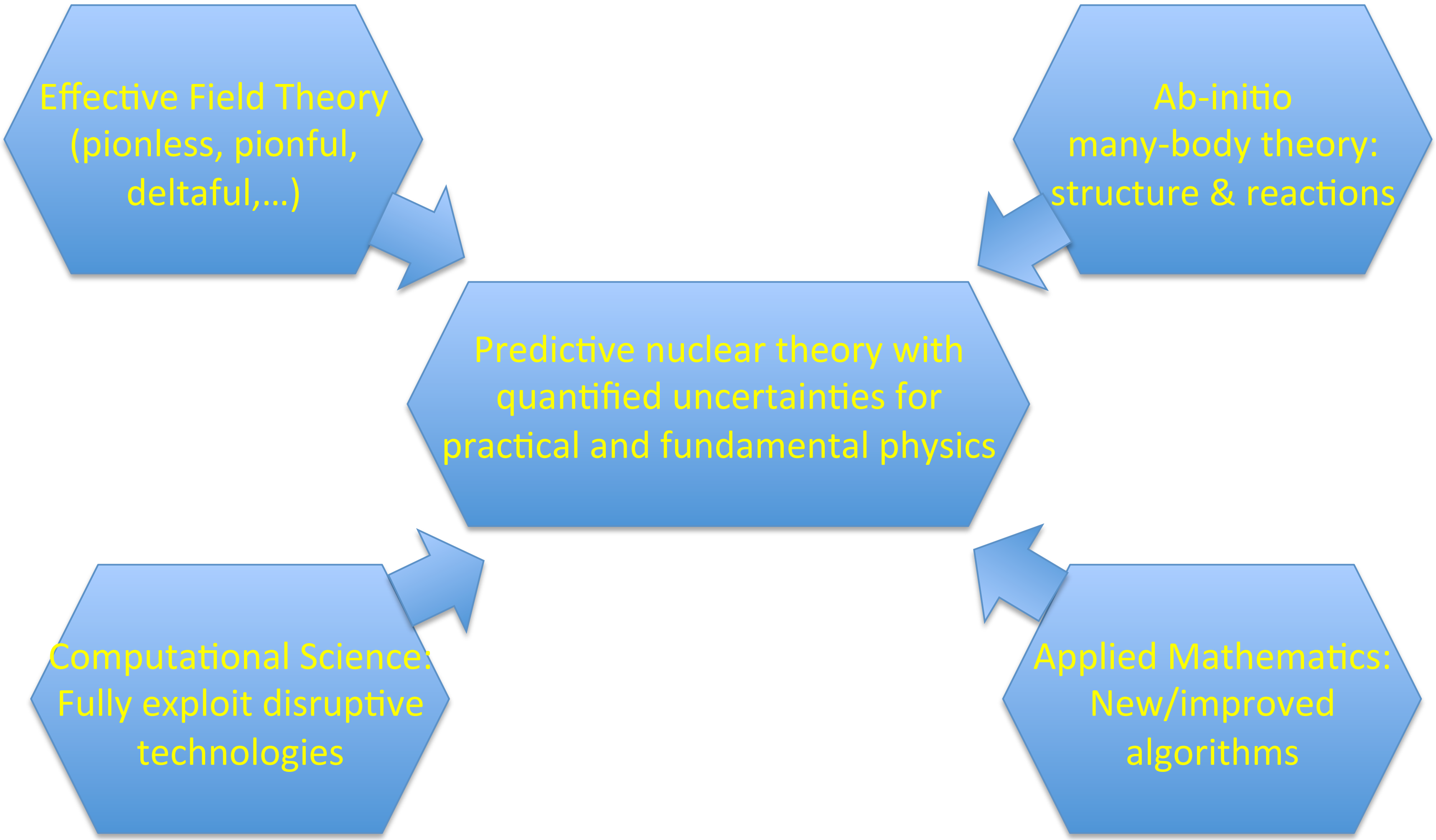


+ K-super.
+ Blue Waters
+ TianHe II
+ Tachyon-II

Strategy for discovering the solutions to these fundamental problems



The Nuclear Many-Body Problem

The many-body Schroedinger equation for bound states consists of $2\binom{A}{Z}$ 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**)

Meson Exchg interactions

Featured results here

Hamiltonian matrix in basis function space
No Core Configuration Interaction (**NCSM/NCFC**)

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

Lattice Nuclear Chiral EFT, MB Greens Function, MB Perturbation Theory, . . . approaches

Chiral EFT interactions

Comments

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

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 bookkeepping 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=16 (40) today with largest computers available

Physics Letters B 719, 179 (2013)

Contents lists available at SciVerse ScienceDirect

Physics Letters B

www.elsevier.com/locate/physletb

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:

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

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

$$B(E2; J_i \to J_f) = \frac{5}{16\pi}(J_i K 2 0 | J_f K)^2 (eQ_0)^2$$

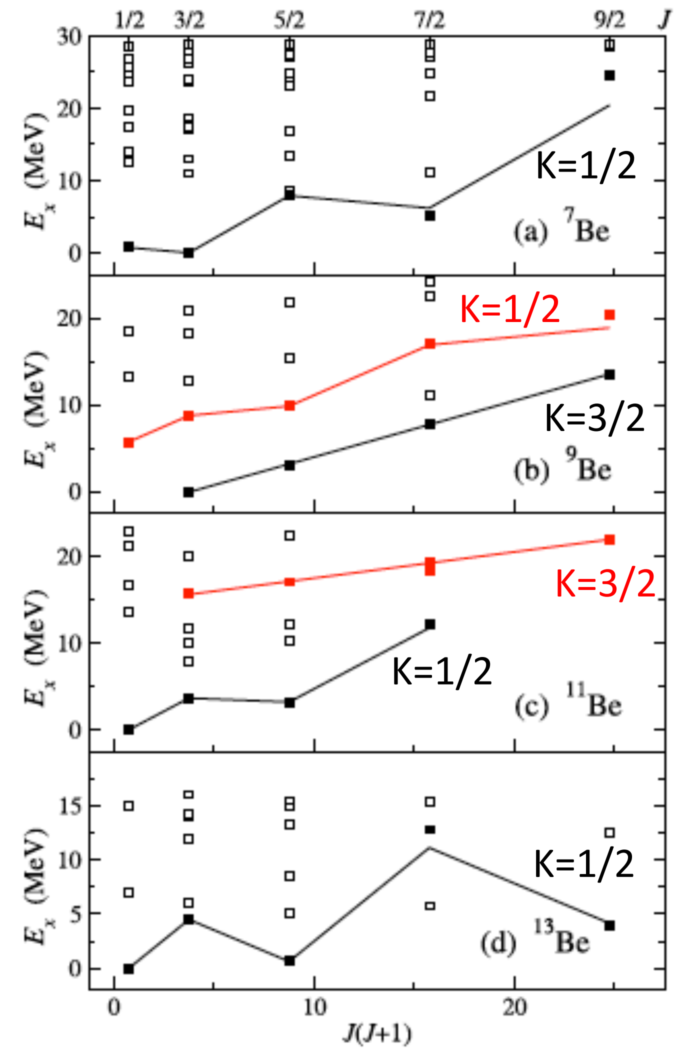
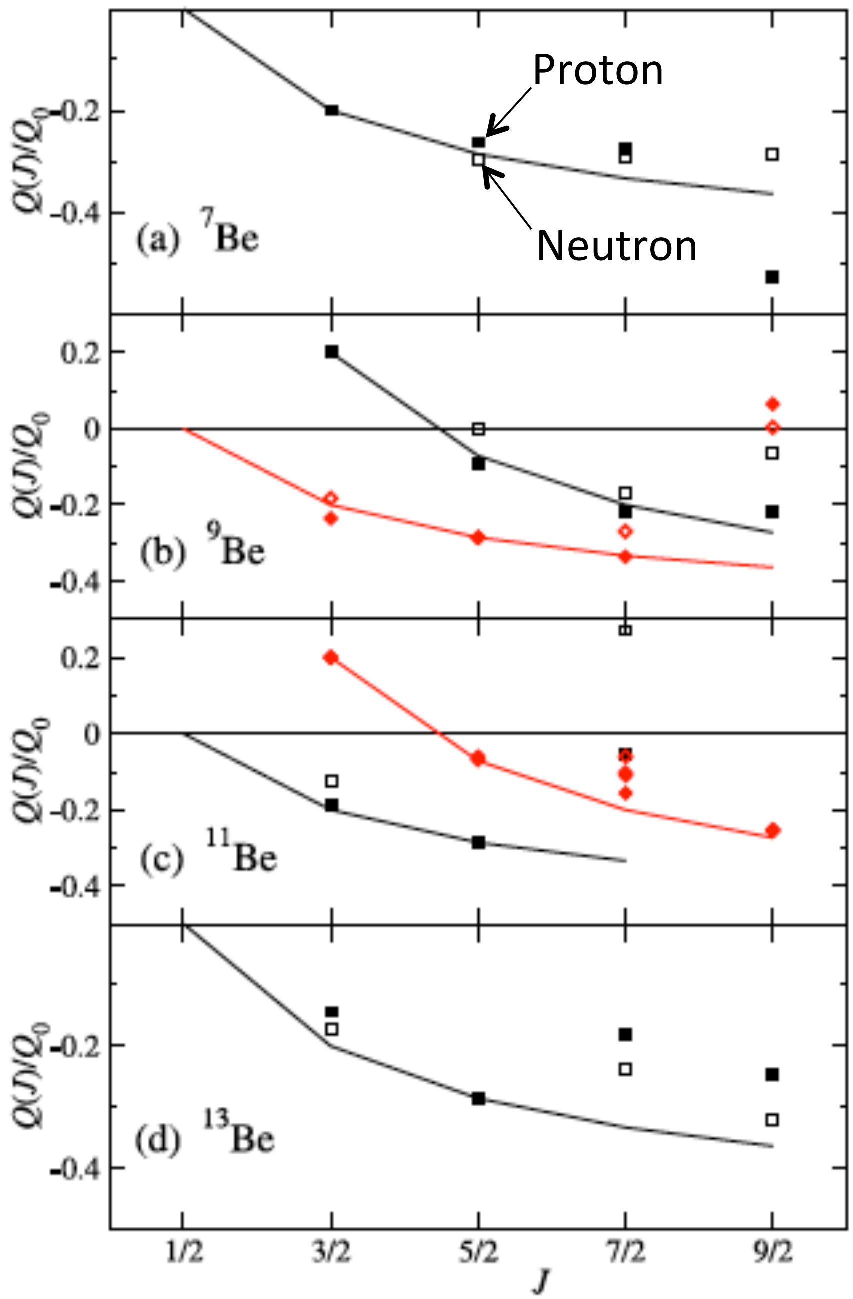


Fig. 1. Excitation energies obtained for states in the *natural* parity spaces of the odd-mass Be isotopes: (a) ^{7}Be, (b) ^{9}Be, (c) ^{11}Be, and (d) ^{13}Be. Energies are plotted with respect to $J(J+1)$ to facilitate identification of rotational energy patterns, while the J values themselves are 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.



Collective model:

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

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

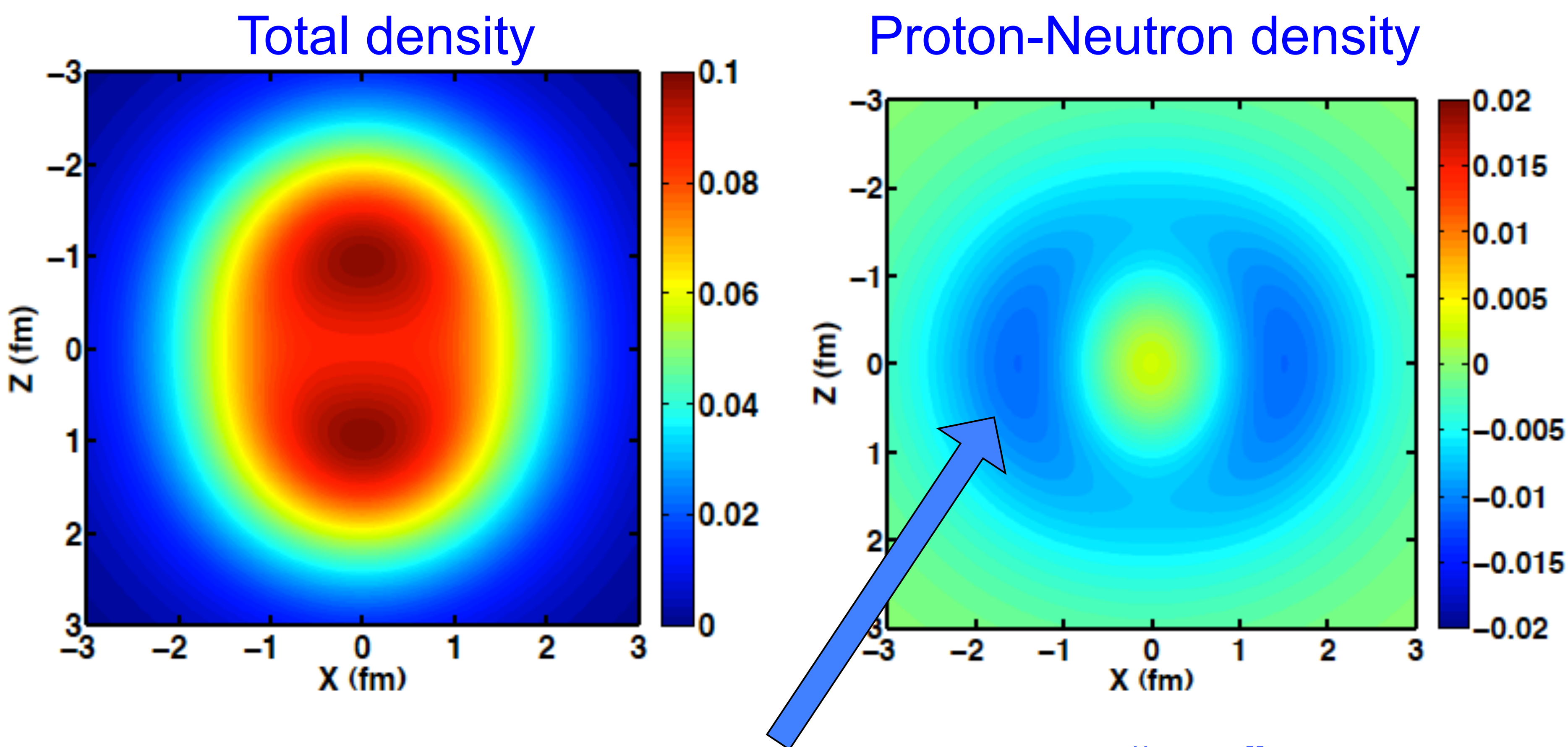
Fig. 3. Quadrupole moments calculated for candidate bandmembers in the *natural* parity spaces of the odd-mass Be isotopes: (a) ^{7}Be, (b) ^{9}Be, (c) ^{11}Be, and (d) ^{13}Be. The states are as identified in Fig. 1 and are shown as black squares for yrast states or red diamonds for excited states (color 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

Next challenge: Investigate same phenomena with Chiral EFT interactions

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

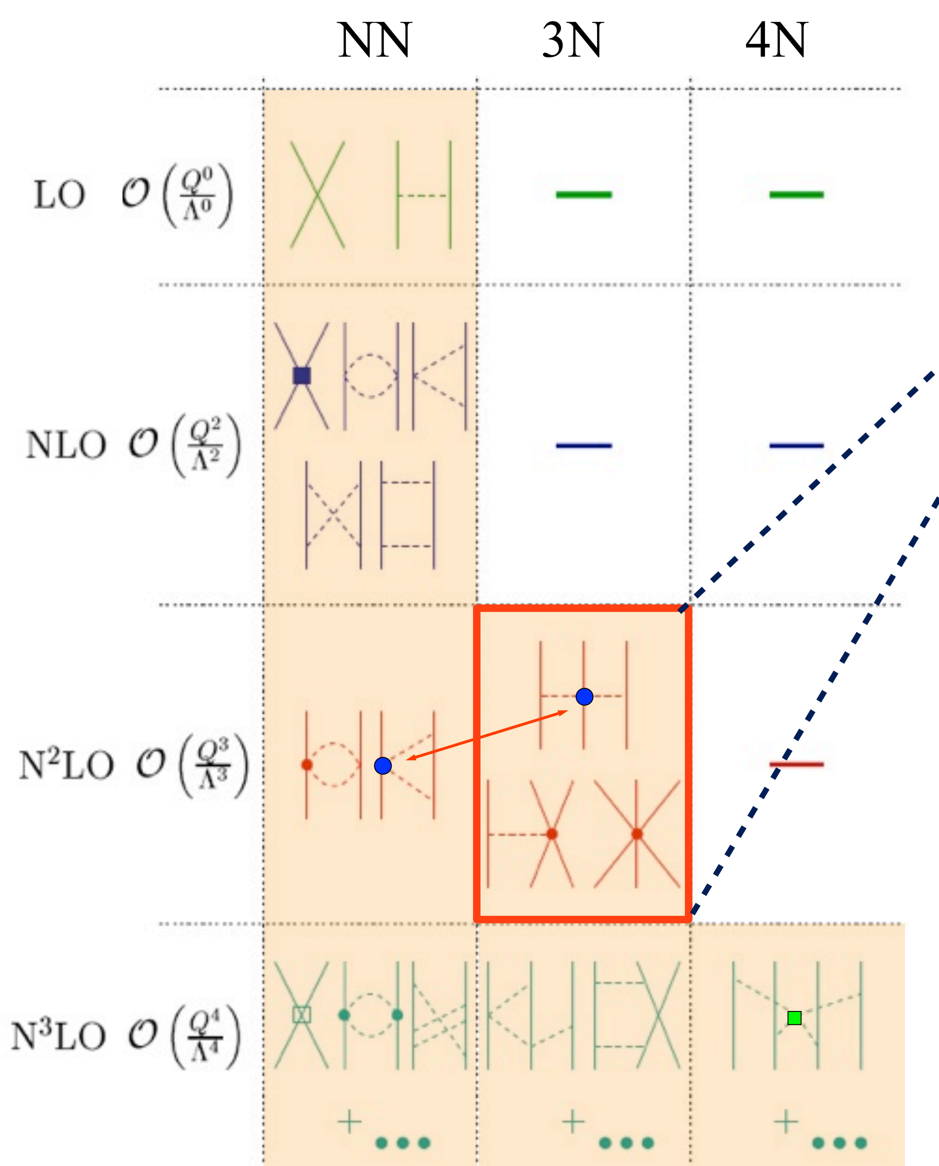
9Be Translationally invariant gs density
Full 3D densities = rotate around the vertical axis

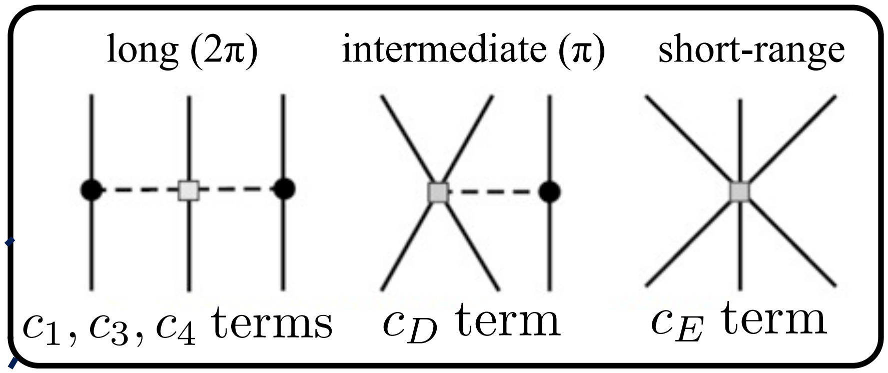


Shows that one neutron provides a “ring” cloud around two alpha clusters binding them together

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

Chiral EFT for nuclear forces, leading order 3N forces





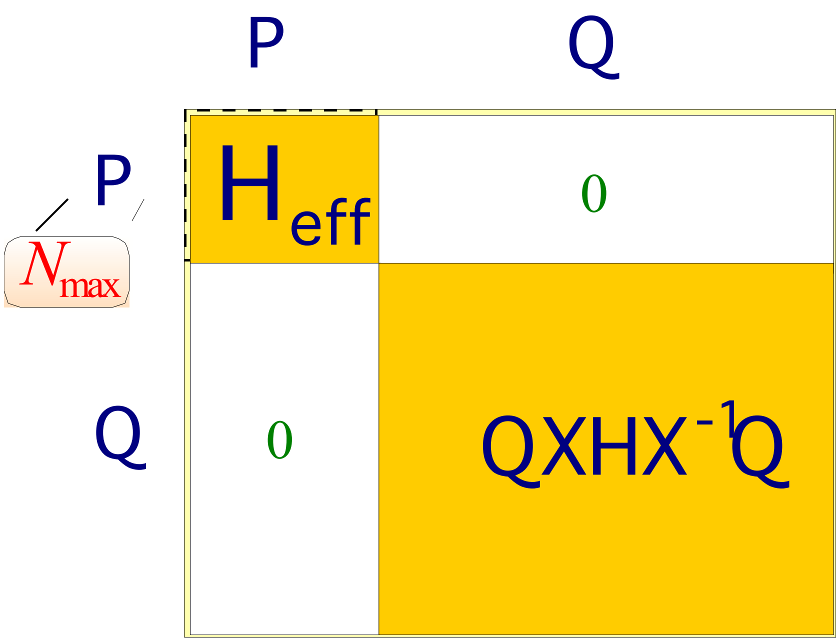
large uncertainties in coupling constants at present:

$$c_1 = -0.9^{+0.2}_{-0.5}\ , \ c_3 = -4.7^{+1.5}_{-1.0}\ , \ c_4 = 3.5^{+0.5}_{-0.2}$$

lead to theoretical uncertainties in many-body observables

Adapted from Kai Hebeler, ECT* workshop May 2014

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



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

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

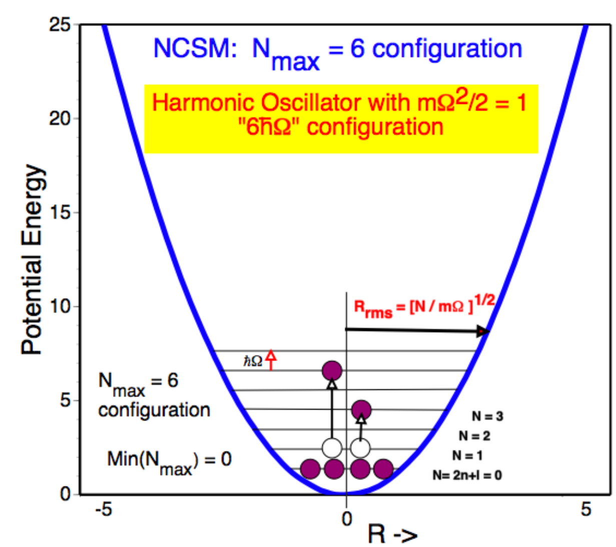
model space dimension

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

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

unitary $X = \exp[-\mathrm{arctan\,h}(\omega^+ - \omega)]$

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

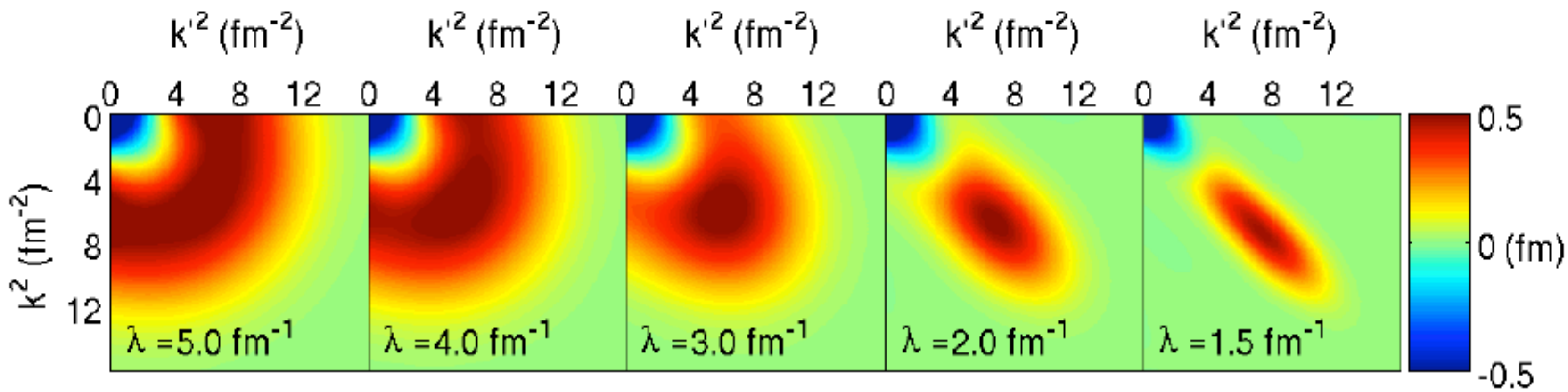


Adapted from Petr Navratil

Similarity Renormalization Group – NN interaction

- SRG evolution

Bogner, Furnstahl, Perry, PRC 75 (2007) 061001



  - drives interaction towards band-diagonal structure
  - SRG shifts strength between 2-body and many-body forces

- Initial chiral EFT Hamiltonian
  power-counting hierarchy A-body forces

$$V_{NN} \gg V_{NNN} \gg V_{NNNN}$$

Both OLS and SRG derivations of H_{eff} will be used in applications here

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

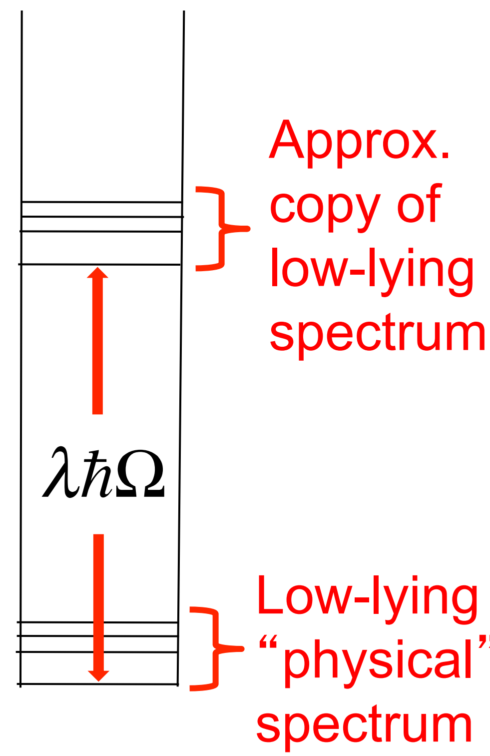
Add a Lagrange multiplier term acting on the cm alone so as not to interfere with the internal motion dynamics

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

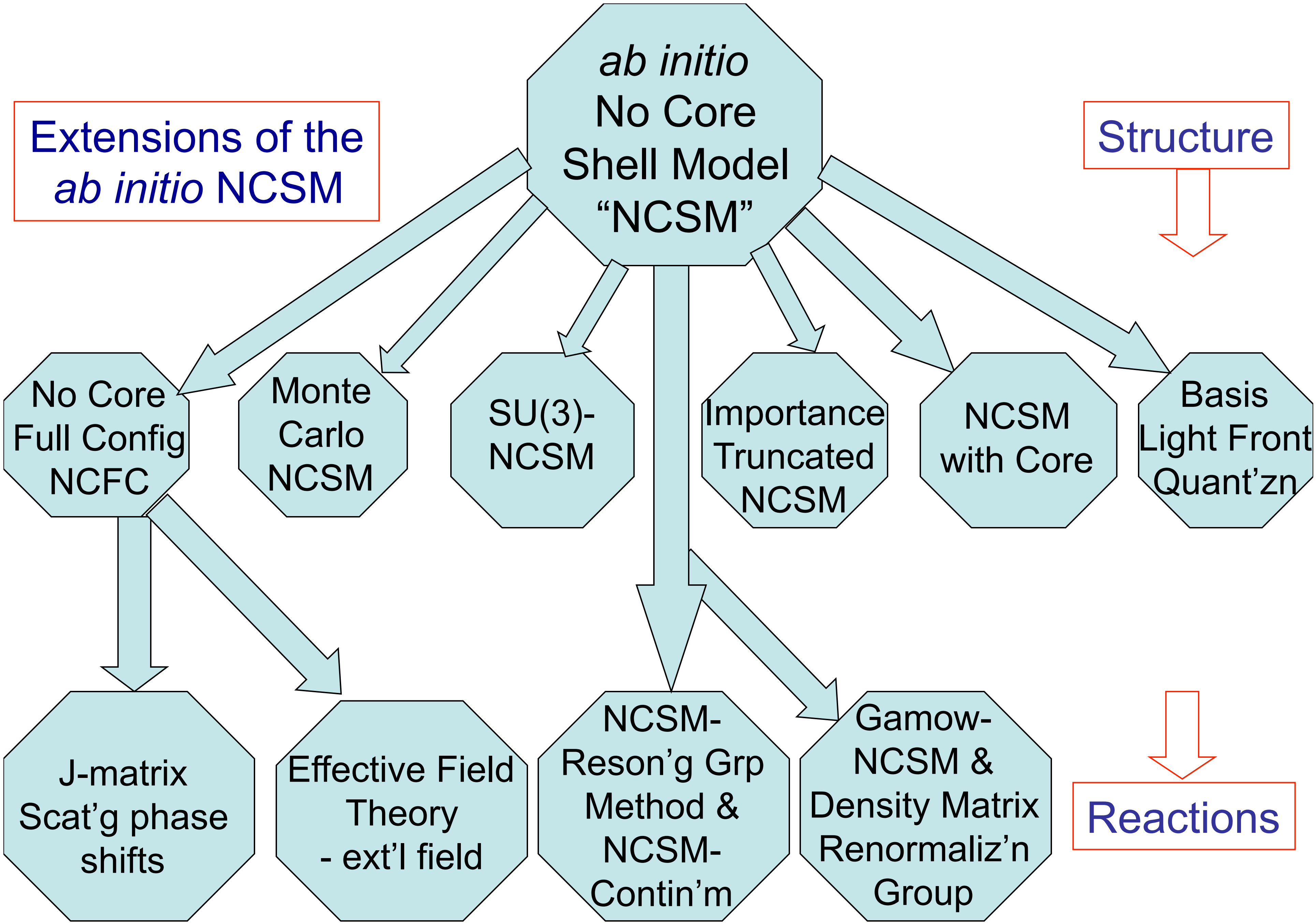
$$H = H_{eff}\left(N_{\max},\hbar\Omega\right) + \lambda H_{cm}$$

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

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



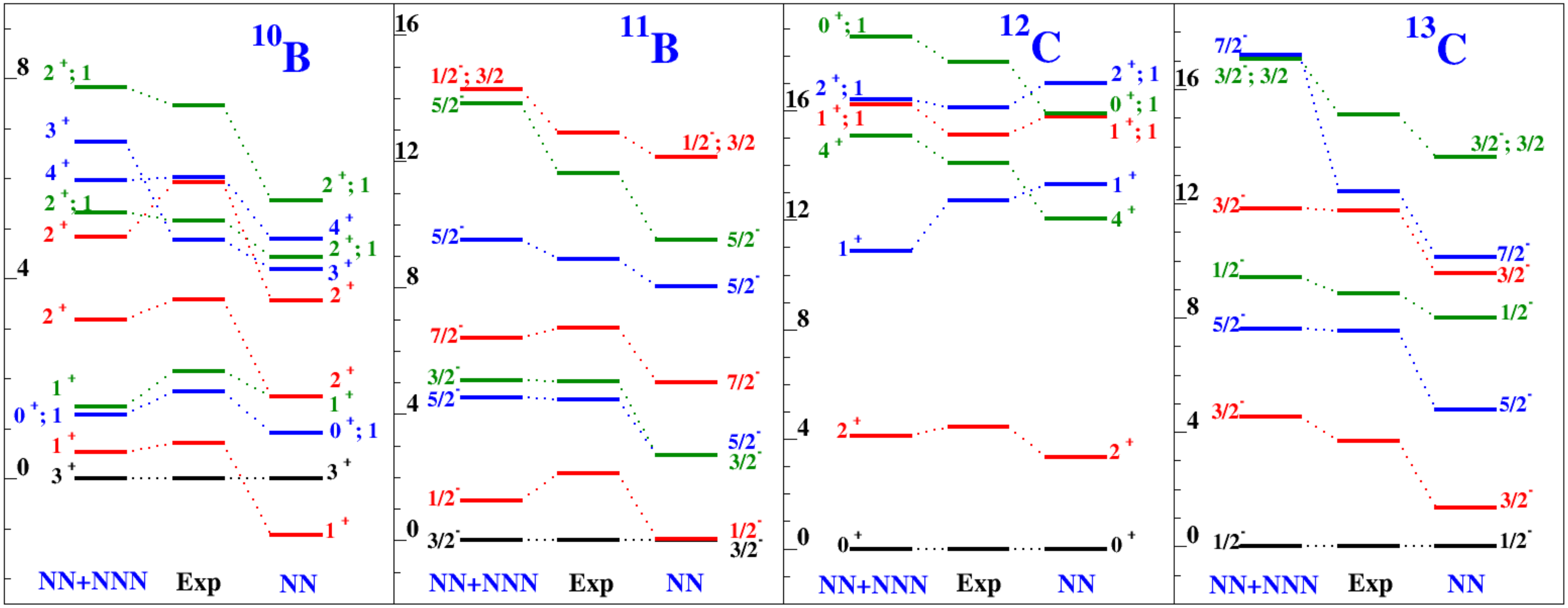
Along with the N_{max} truncation in the HO basis, the Lagrange multiplier term guarantees that all low-lying solutions have eigenfunctions that factorize into a 0s HO wavefunction for the cm times a translationaly invariant wavefunction.



Extensions of the
ab initio NCSM
ab initio
No Core
Shell Model
“NCSM”
Structure
No Core
Full Config
NCFC
Monte
Carlo
NCSM
SU(3)-
NCSM
Importance
Truncated
NCSM
NCSM
with Core
Basis
Light Front
Quant’zn
J-matrix
Scat’g phase
shifts
Effective Field
Theory
- ext’l field
NCSM-
Reson’g Grp
Method &
NCSM-
Contin’m
Gamow-
NCSM &
Density Matrix
Renormaliz’n
Group
Reactions

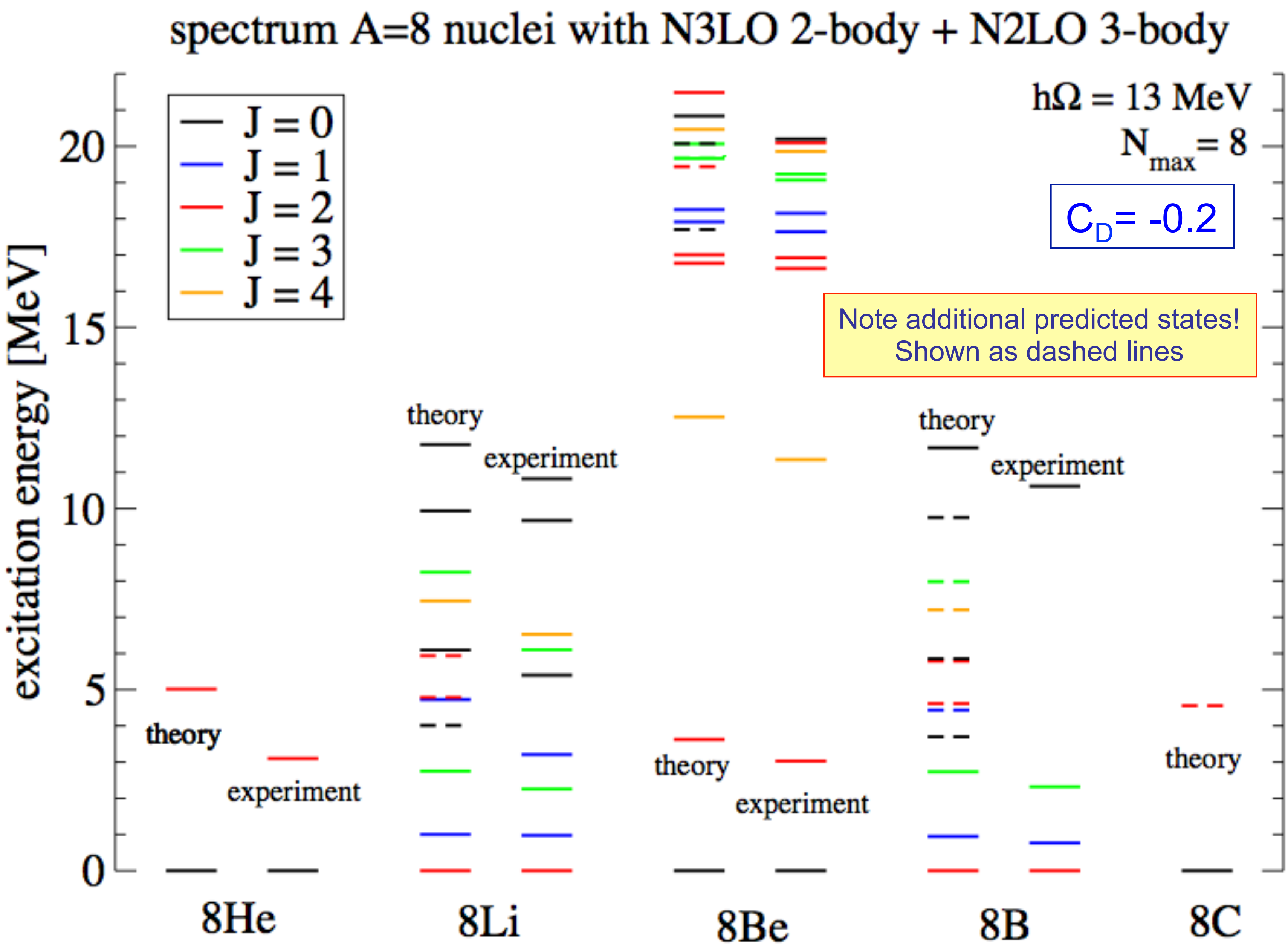
ab initio NCSM with χ_{EFT} Interactions

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

^{8}Be

No Core CI calculations for light nuclei with chiral 2- and 3-body forces

Pieter Maris[1], H Metin Aktulga[2], Sven Binder[3], Angelo Calci[3], Ümit V Çatalyürek[4,5], Joachim Langhammer[3], Esmond Ng[2], Erik Saule[4], Robert Roth[3], James P Vary[1] and Chao Yang[2]

J. Phys. Conf. Ser. 454, 012063 (2013)

SRG Renormalization scale invariance, convergence & agreement with experiment

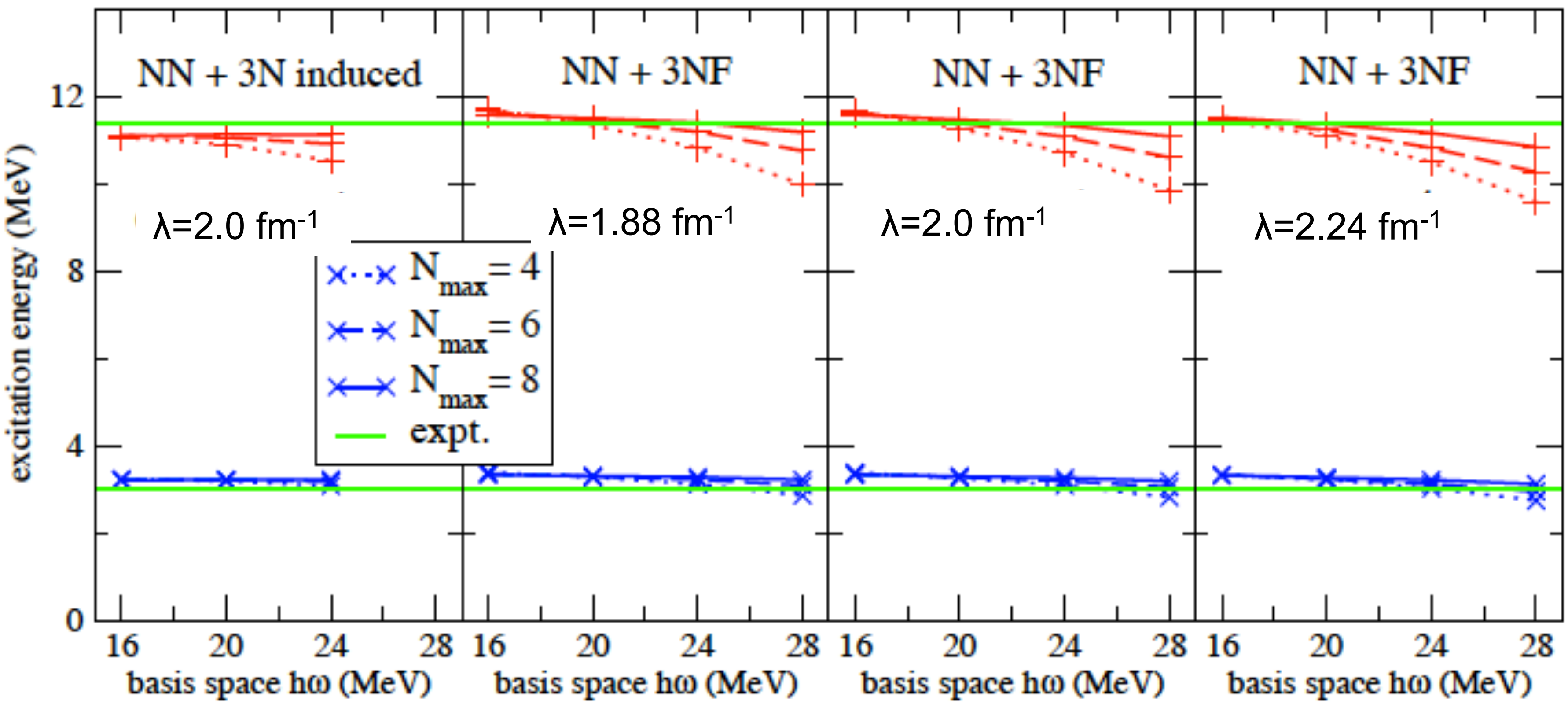
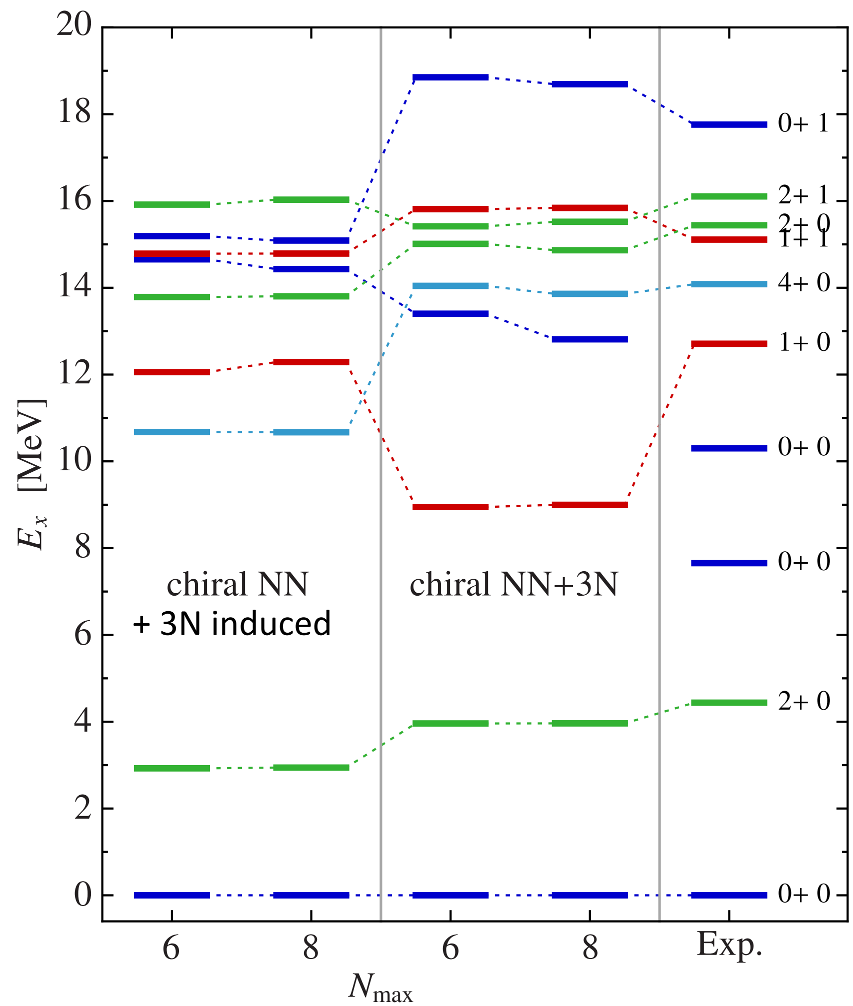


Figure 5. Excitation energies of the 2^+ (blue crosses) and 4^+ states (red plusses) for ^{8}Be with SRG evolved chiral N^{3}LO 2NF plus induced 3NF at $\alpha = 0.0625$ fm^4 (left-most panel) and with SRG evolved chiral N^{3}LO 2NF plus chiral N^{2}LO 3NF. Experimental values are indicated by the horizontal green lines.

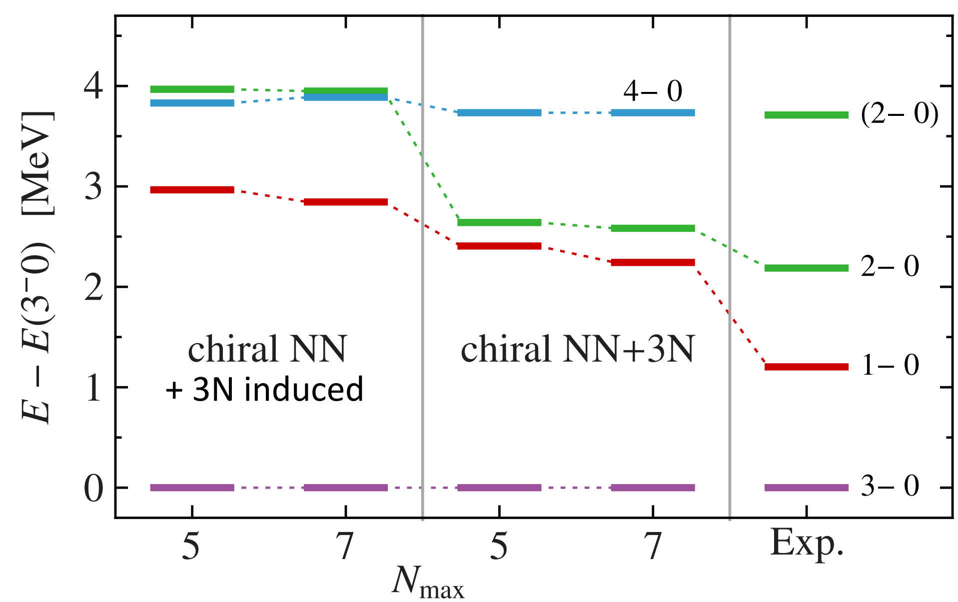
NCSM excitation spectra for ^{12}C with chiral NN(N3LO) (+3N induced) and NN(N3LO) + 3N(N2LO) interactions



$\alpha = 0.0625\ \mathrm{fm}^4$

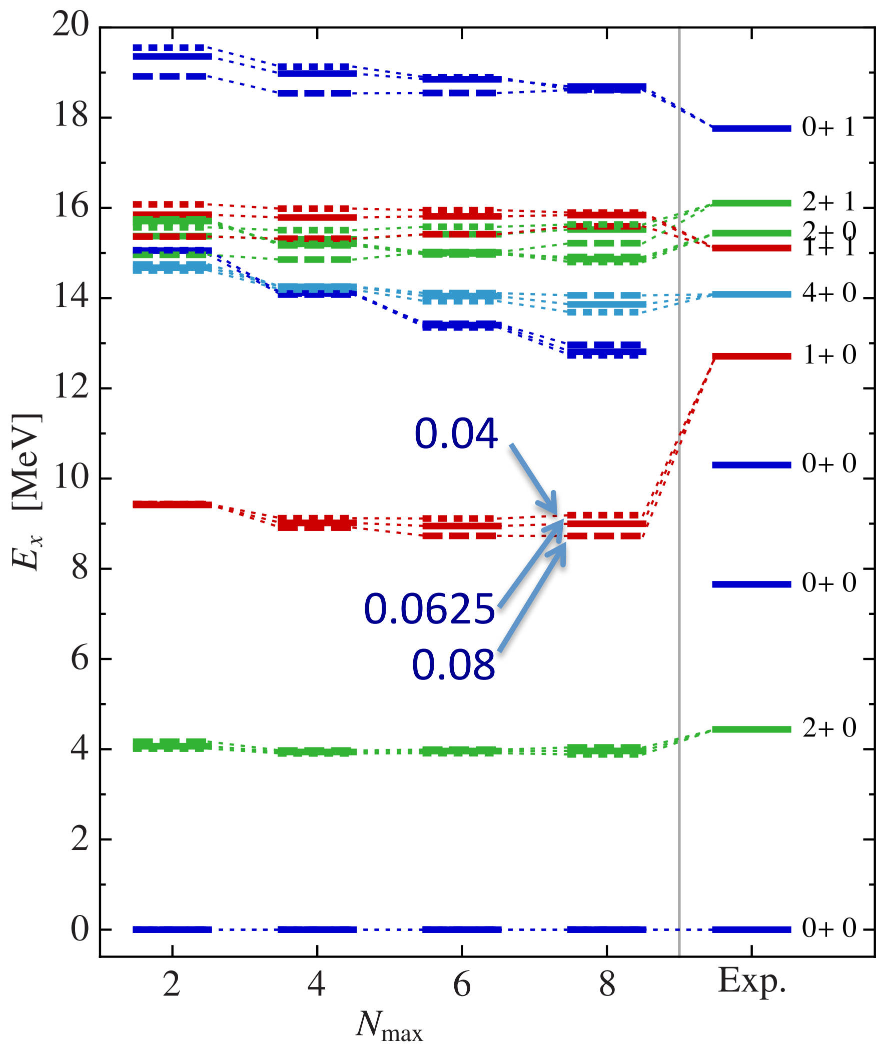
$\lambda = 2.0\ \mathrm{fm}^{-1}$

$\hbar\Omega = 20\ \mathrm{MeV}$

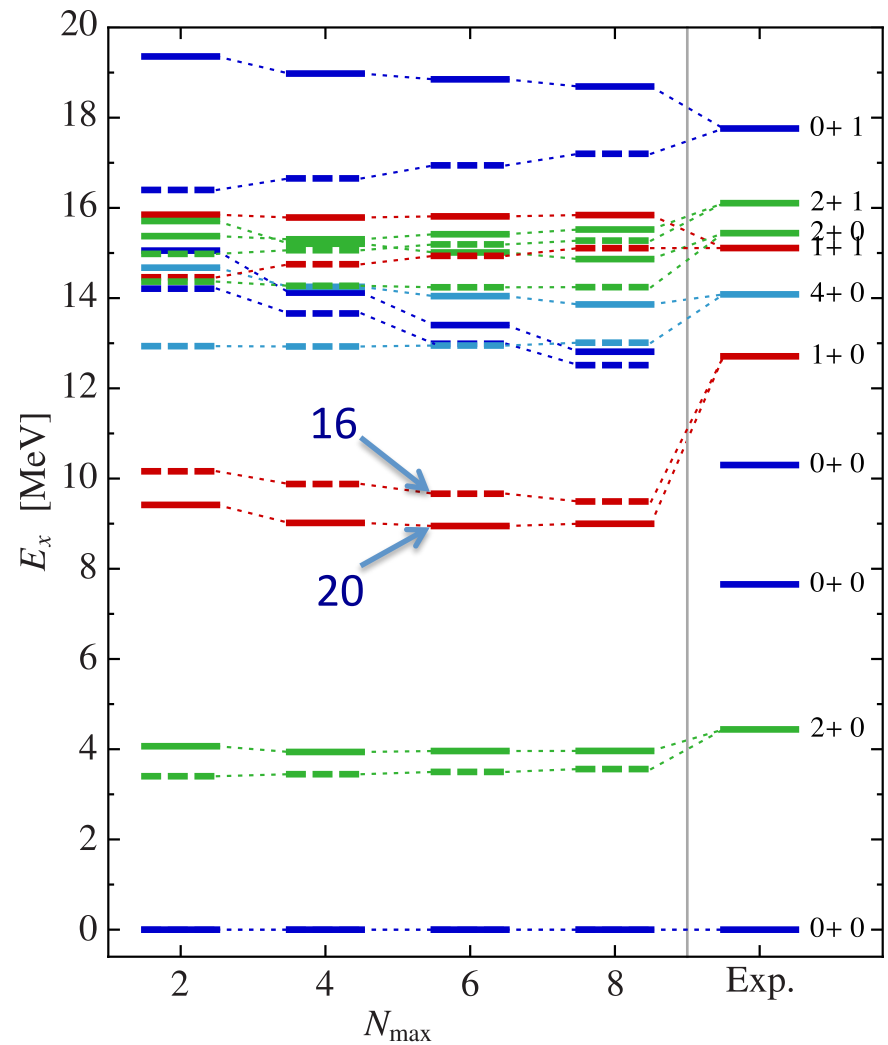


P. Maris, J.P. Vary, A. Calci, J. Langhammer, S. Binder and R. Roth, Phys. Rev. C 90, 014314 (2014); arXiv 1405.1331

NCSM excitation spectra for ^{12}C with chiral NN(N3LO) + 3N(N2LO) interaction



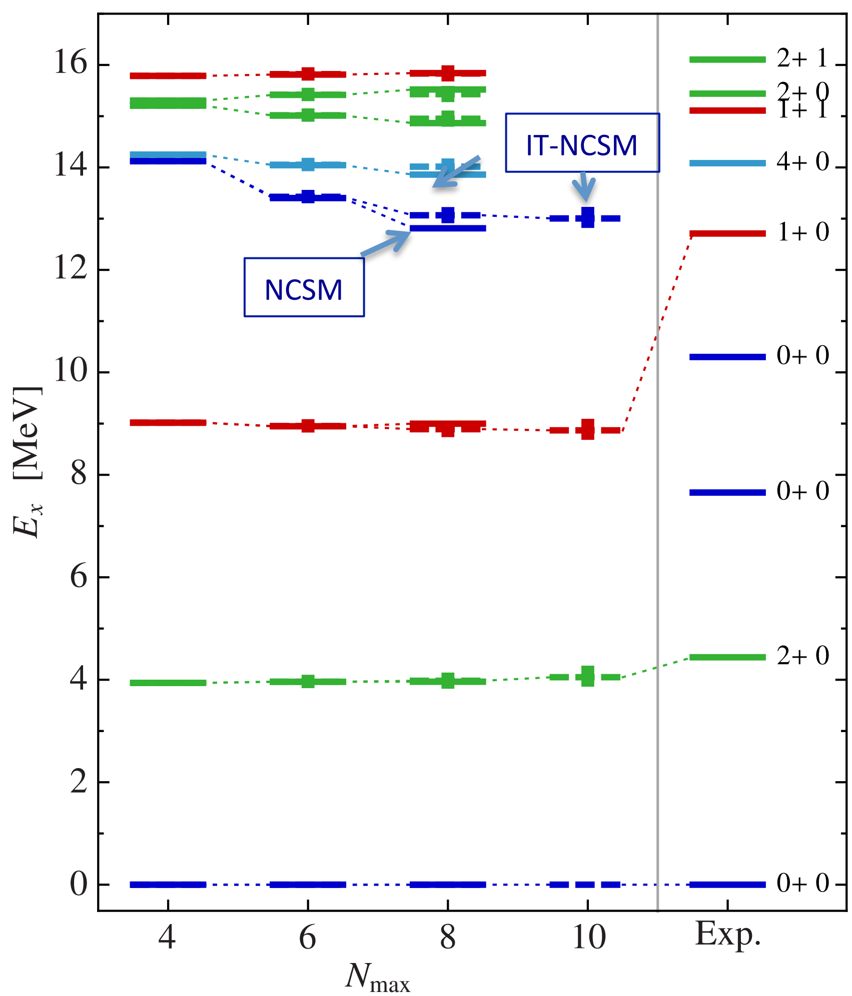
SRG evolution scale (in fm4) dependence



HO frequency (in MeV) dependence

P. Maris, J.P. Vary, A. Calci, J. Langhammer, S. Binder and R. Roth, Phys. Rev. C 90, 014314 (2014); arXiv 1405.1331

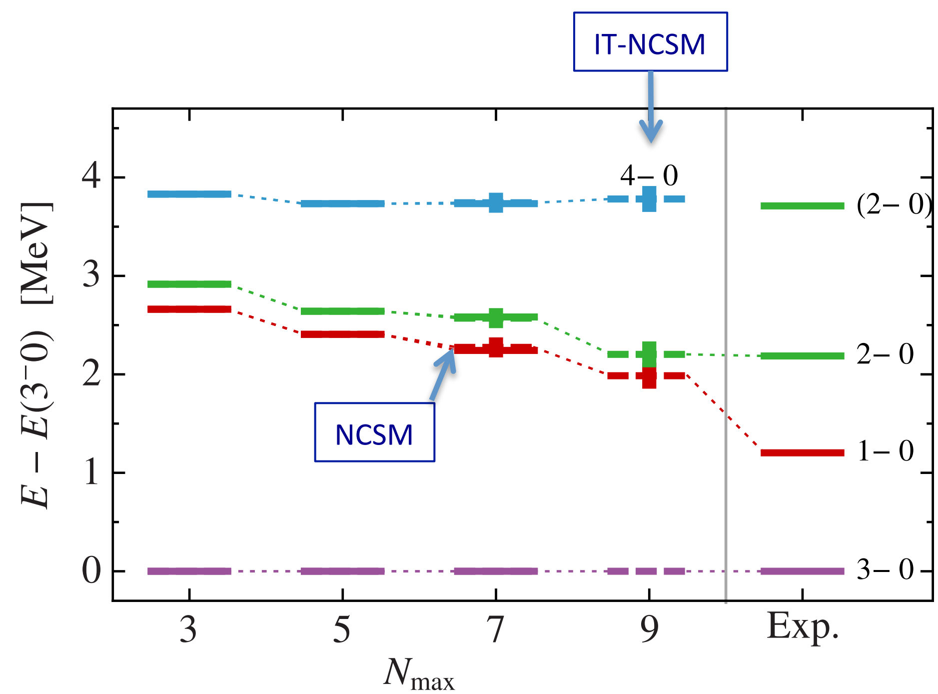
Convergence rates of excitation spectra for SRG evolved chiral NN(N3LO) + 3N(N2LO)



$$\alpha = 0.0625\ \text{fm}^4$$

$$\lambda = 2.0\ \text{fm}^{-1}$$

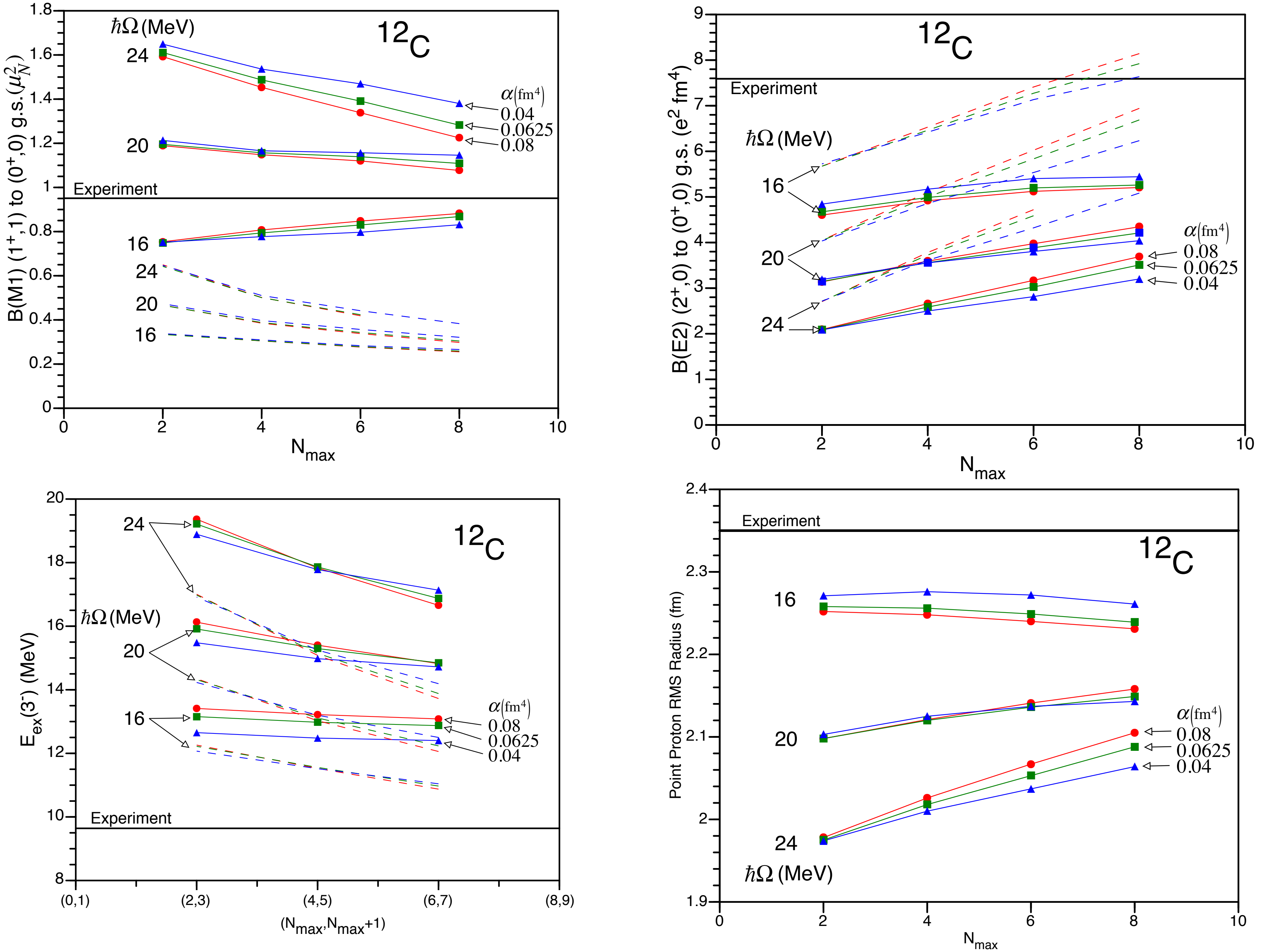
$$\hbar\Omega = 20\ \text{MeV}$$



Boxes indicate threshold-extrapolation uncertainties for IT-NCSM

P. Maris, J.P. Vary, A. Calci, J. Langhammer, S. Binder and R. Roth, Phys. Rev. C 90, 014314 (2014); arXiv 1405.1331

Convergence rates of selected observables for SRG evolved chiral NN(N3LO) + 3N(N2LO)



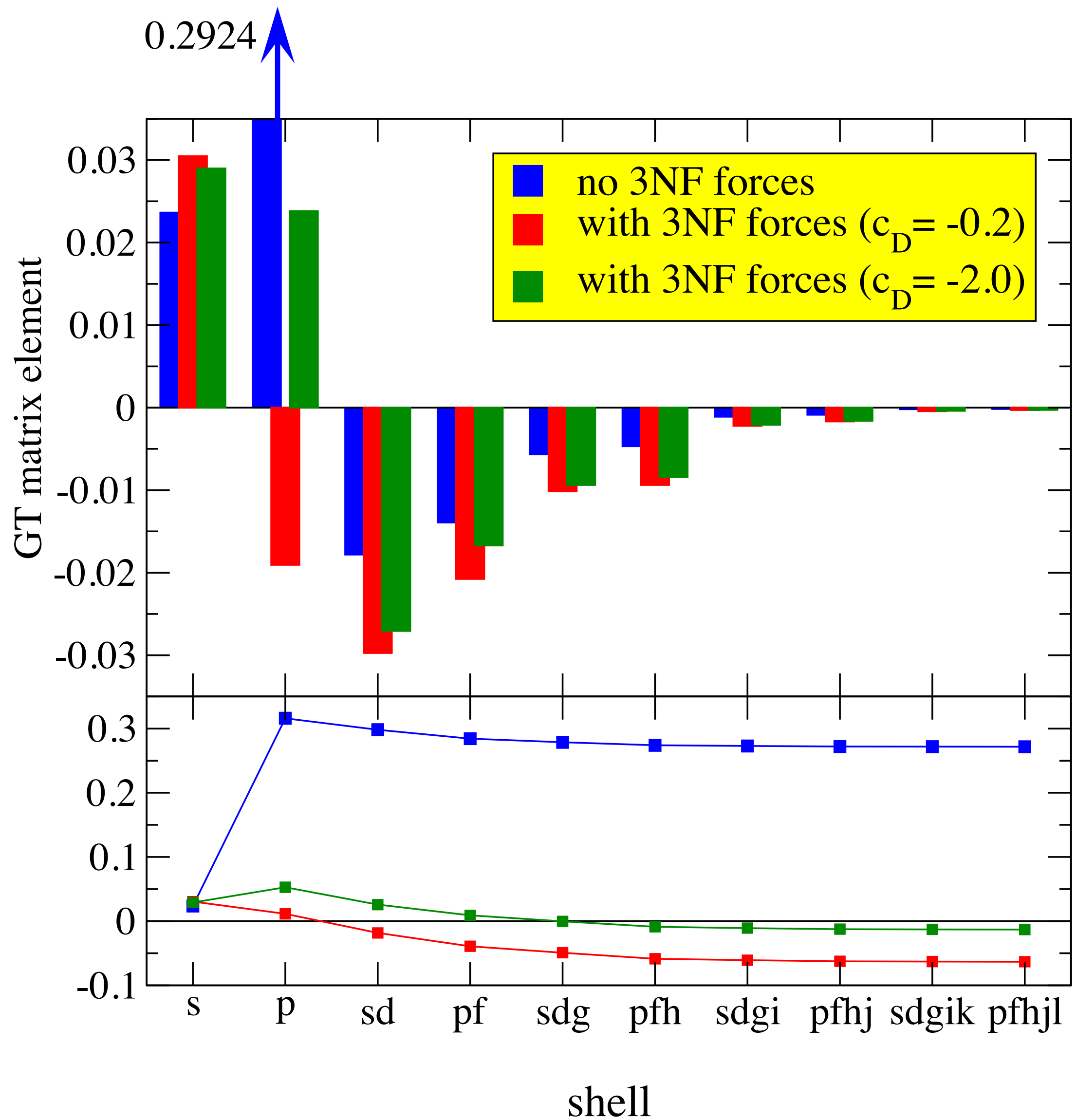
P. Maris, J.P. Vary, A. Calci, J. Langhammer, S. Binder and R. Roth, Phys. Rev. C 90, 014314 (2014); arXiv 1405.1331

Next Generation Ab Initio Structure Applications – Aim for Precision

Electroweak processes
Beyond the Standard Model tests (e.g. CKM unitarity => v_{ud} determination)
Neutrinoful and neutrinoless double beta-decay
?

Each puts major demands on theory, algorithms and computational resources
Growing demands => larger collaborating teams, growing computational resources,
Increase in the multi-disciplinary character, . . .

Origin of the anomalously long life-time of ^{14}C



- near-complete cancellations between dominant contributions within p-shell
- very sensitive to details

Maris, Vary, Navratil, Ormand, Nam, Dean, PRL106, 202502 (2011)

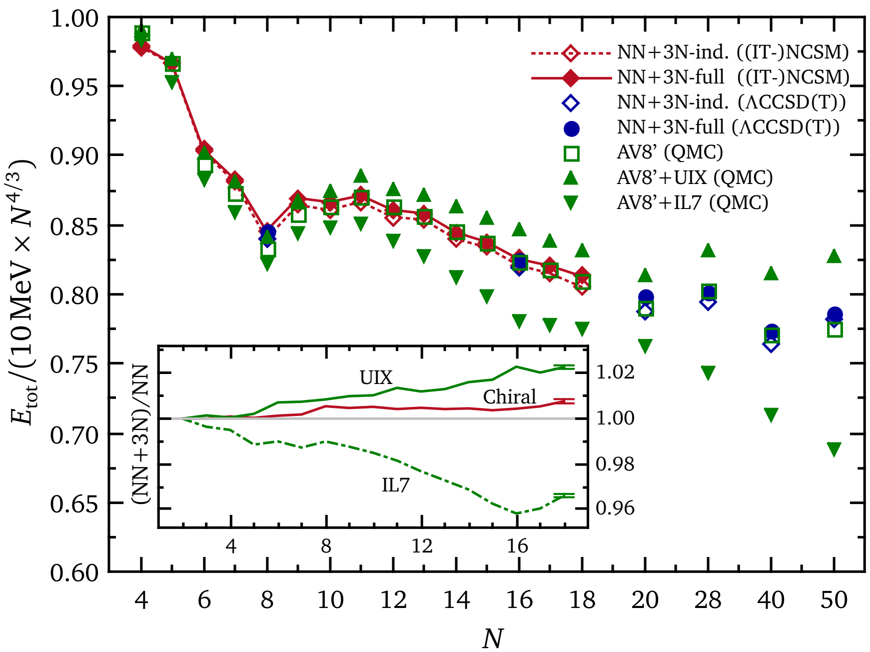
Ab initio Extreme Neutron Matter

Objectives

- Predict properties of neutron-rich systems which relate to exotic nuclei and nuclear astrophysics
- Determine how well high-precision phenomenological strong interactions compare with effective field theory based on QCD
- Produce accurate predictions with quantified uncertainties

Impact

- Improve nuclear energy density functionals used in extensive applications such as fission calculations
- Demonstrate the predictive power of *ab initio* nuclear theory for exotic nuclei with quantified uncertainties
- Guide future experiments at DOE-sponsored rare isotope production facilities



Comparison of ground state energies of systems with N neutrons trapped in a harmonic oscillator with strength 10 MeV. Solid red diamonds and blue dots signify new results with two-nucleon (NN) plus three-nucleon (3N) interactions derived from chiral effective field theory related to QCD. Inset displays the ratio of NN+3N to NN alone for the different interactions. Note that with increasing N, the chiral predictions lie between results from different high-precision phenomenological interactions, i.e. between AV8'+UIX and AV8'+IL7.

Accomplishments

1. Demonstrates predictive power of *ab initio* nuclear structure theory.
2. Provides results for next generation nuclear energy density functionals
3. Leads to improved predictions for astrophysical reactions
4. Demonstrates that the role of three-nucleon (3N) interactions in extreme neutron systems is significantly weaker than predicted from high-precision phenomemological interactions

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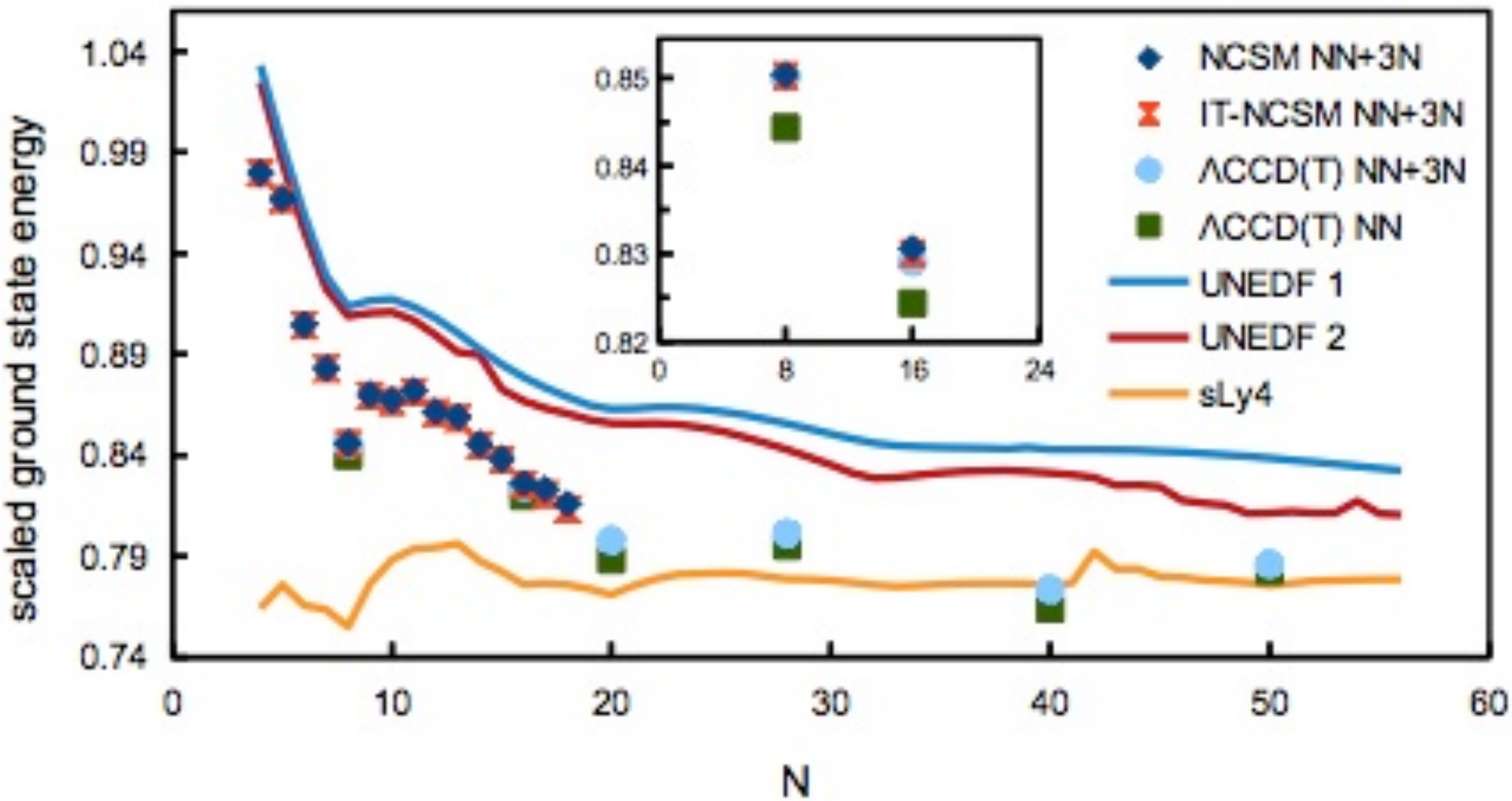
NUCLEI Nuclear Computational Low-Energy Initiative

References: P. Maris, J.P. Vary, S. Gandolfi, J. Carlson, S.C. Pieper, Phys. Rev. C87, 054318 (2013); H. Potter, S. Fischer, P. Maris, J.P. Vary, S. Binder, A. Calci, J. Langhammer and R.Roth, arXiv:1406.1160; Contact: jvary@iastate.edu

Neutron drops in 10 MeV harmonic trap
with Chiral NN and Chiral NN + 3N interactions

NCSM, IT-NCSM, CC and HFB results



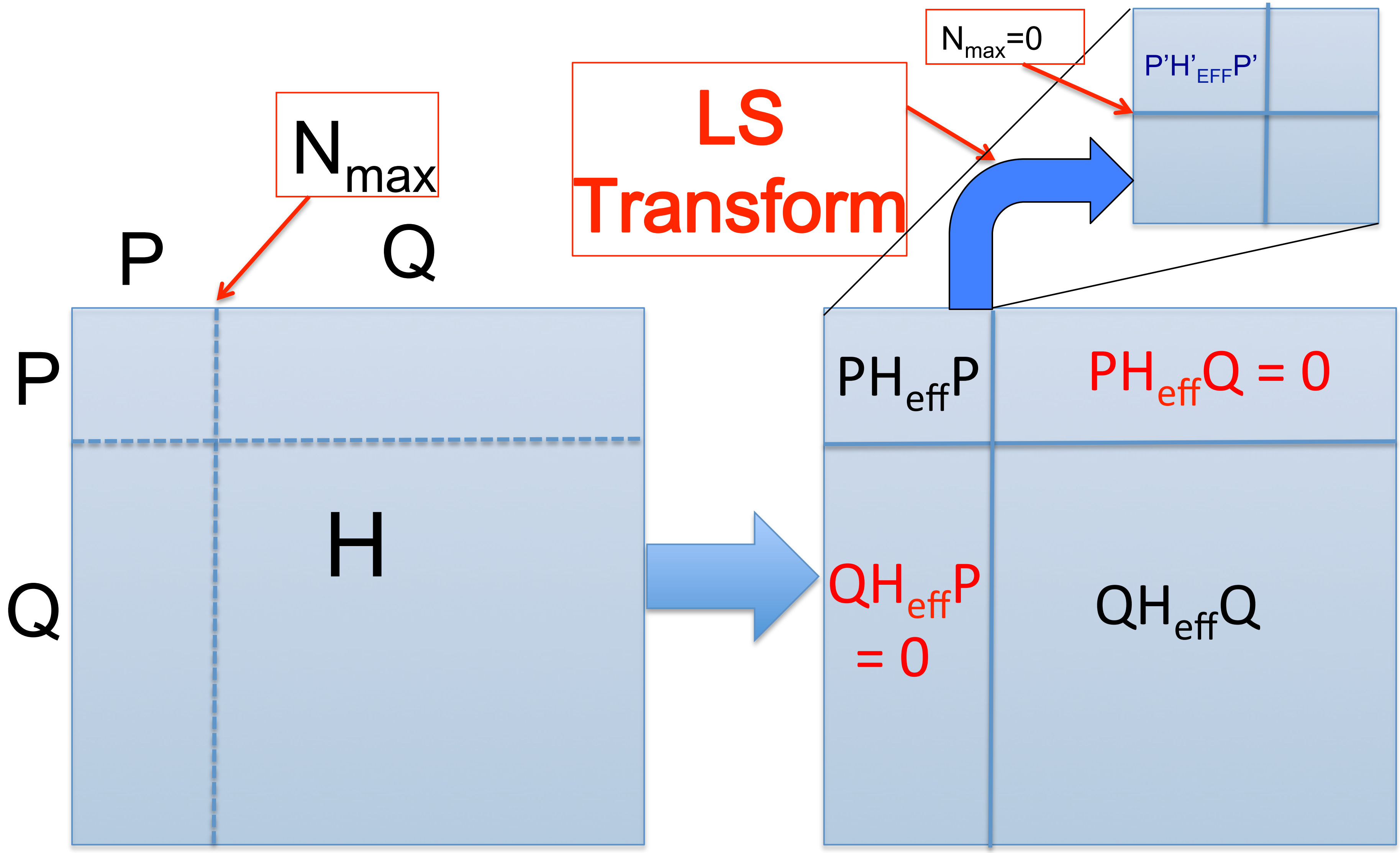
H.D. Potter, PhD project, Iowa State University
Iowa State – Darmstadt Collaboration; arXiv 1406:1160

Observables in light nuclei known to be sensitive to 3NFs based on chiral NN (N3LO) + 3N (N2LO) [Lambda = 500 MeV]

Binding energies (through Oxygen)and subshell closures (through Calcium)
Spectral properties having spin-orbit sensitivity
Electroweak moments and transitions (M1, E2, F, GT}
Ratio of B(E2)'s [GS -> 1_1^+ over GS -> 1_2^+] in ^{10}B
^{10}B ground state spin
^{14}C anomalous half-life

Established challenges – possible roles for improved 3NFs (LENPIC)

Gaps between natural & unnatural parity spectra
The energy of J = 1+, T=0 state in 12C
Two low-lying 2+ states in 10Be with radically different B(E2)'s
Level crossing of J = 5/2 and J = 1/2 states in 9Be
Spectra of 14N
Overbinding of Ca isotopes and above
RMS radii too small in ~all nuclei above 4He
Extra GT transitions (intruders, clusters, . . .) in p-shell nuclei
How JISP16 and NNLO_opt are able to simulate 3NF effects



The "double Lee-Suzuki transform" for valence H_{eff}

Effective interactions in *sd*-shell from *ab-initio* shell model with a core

Preliminary Results

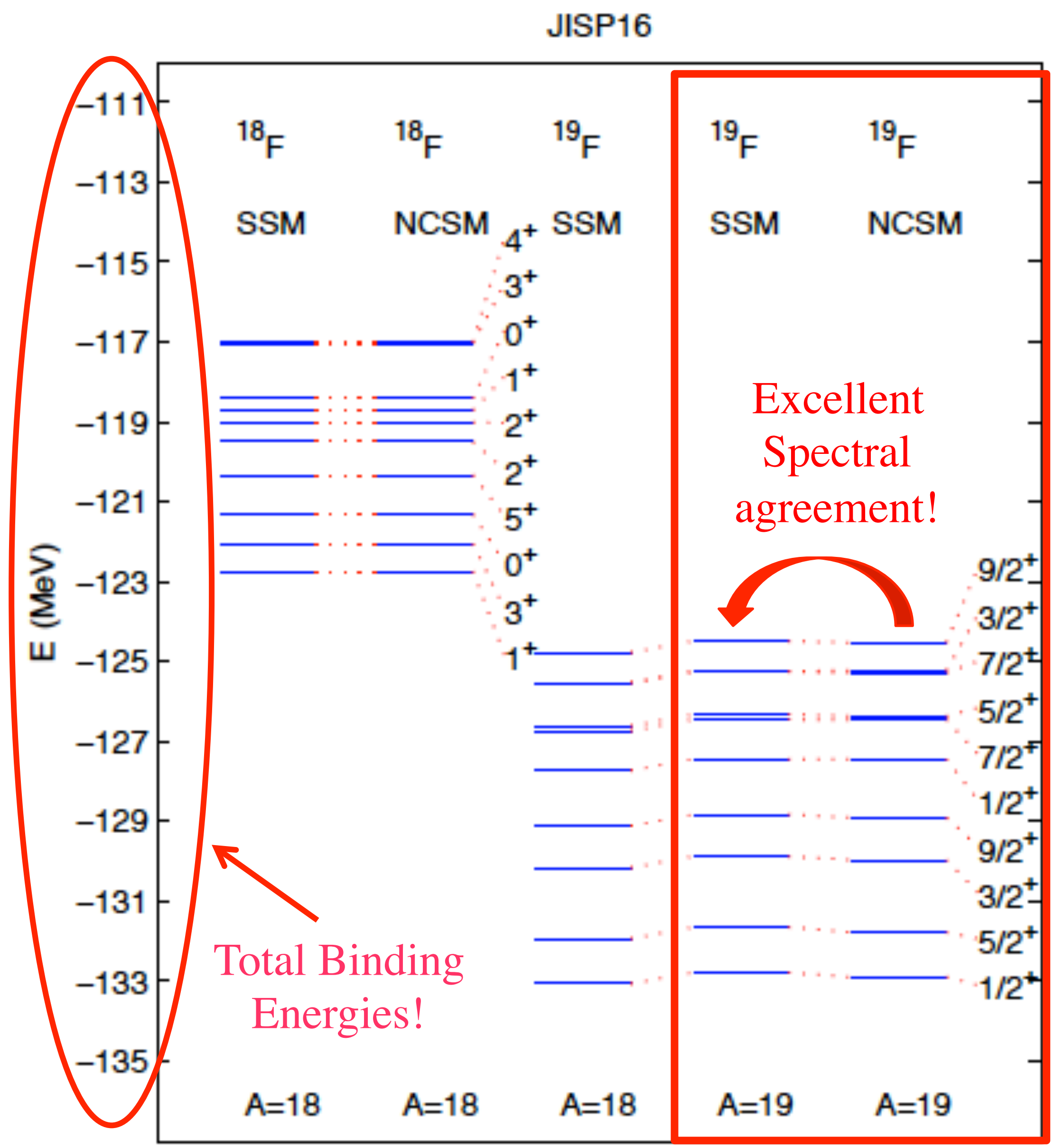
E. Dikmen,[1,2,*] A. F. Lisetskiy,[2,†] B. R. Barrett,[2] P. Maris,[3] A. M. Shirokov,[3,4,5] and J. P. Vary[3]

Aim: Regain valence-core separation but retain full ab initio NCSM

=> "Double OLS" Approach

Now extend to s-d shell the successful p-shell applications

p-shell application:
A. F. Lisetskiy, B. R. Barrett, M. K. G. Kruse, P. Navratil, I. Stetcu, J. P. Vary, Phys. Rev. C. 78, 044302 (2008); arXiv:0808.2187

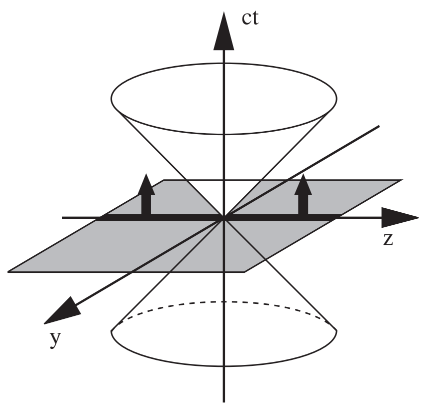


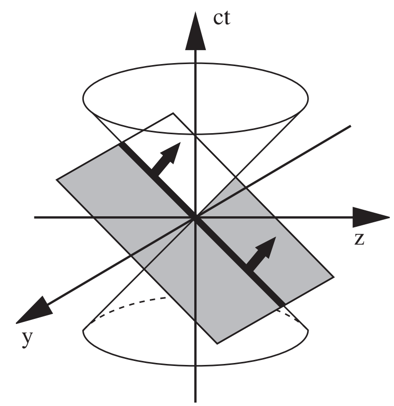
Basis Light-Front Quantization Approach

[Dirac 1949]

- Basic idea: solve generalized wave eq. for quantum field evolution

equal time quantization	VS	light front quantization
$i\frac{\partial}{\partial t}\lvert\varphi(t)\rangle = H\lvert\varphi(t)\rangle$		$i\frac{\partial}{\partial x^+}\lvert\varphi(x^+)\rangle = P_+\lvert\varphi(x^+)\rangle$



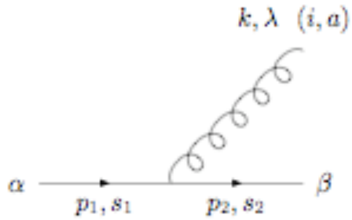


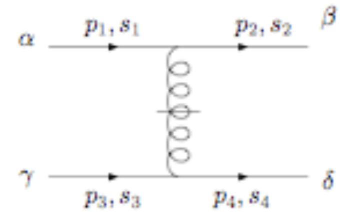
- Time: $t \equiv x^0$ $\qquad$ $t \equiv x^+ = x^0 + x^3$
- Hamiltonian: $H \equiv P^0$ $\qquad$ $H \equiv P_+ = \frac{P^0 - P^3}{2}$

Derived from Lagrangian with gauge fixing

- On-shell condition: $P^0 = \sqrt{m^2 + P_\perp^2 + P_3^2}$ $\qquad$ $P_+ = \frac{m^2 + P_\perp^2}{2P^+}$

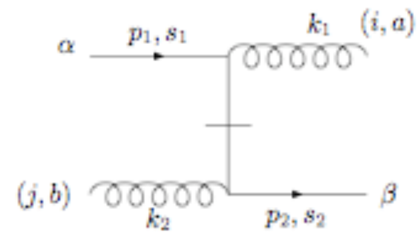
Light Front (LF) Hamiltonian defined by its elementary vertices in LF gauge

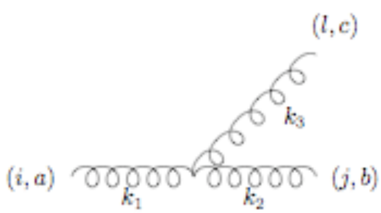


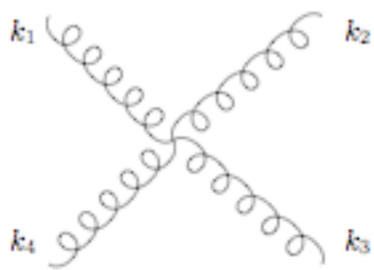


QED & QCD

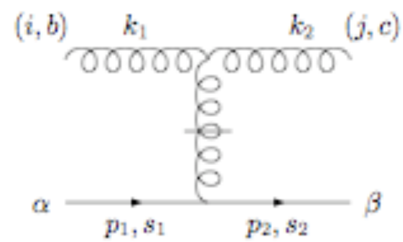
H_{qqgg1}

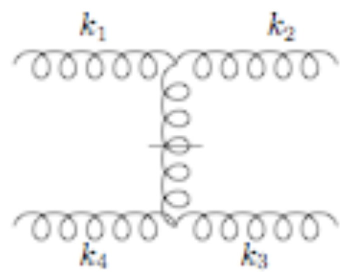






H_{qqgg2}





QCD

$$
\begin{aligned}
H = & \frac{1}{2}\int d^3x \overline{\widetilde{\psi}} \gamma^+ \frac{(\mathrm{i}\partial^\perp)^2 + m^2}{\mathrm{i}\partial^+} \widetilde{\psi} - A^i_a (\mathrm{i}\partial^\perp)^2 A_{ia} \\
& - \frac{1}{2} g^2 \int d^3x \mathbf{Tr} \left[\widetilde{A}^\mu, \widetilde{A}^\nu\right] \left[\widetilde{A}_\mu, \widetilde{A}_\nu\right] \\
& + \frac{1}{2} g^2 \int d^3x \overline{\widetilde{\psi}} \gamma^+ T^a \widetilde{\psi} \frac{1}{(\mathrm{i}\partial^+)^2} \overline{\widetilde{\psi}} \gamma^+ T^a \widetilde{\psi} \\
& - g^2 \int d^3x \overline{\widetilde{\psi}} \gamma^+ \left(\frac{1}{(\mathrm{i}\partial^+)^2} \left[\mathrm{i}\partial^+ \widetilde{A}^\kappa, \widetilde{A}_\kappa\right] \right) \widetilde{\psi} \\
& + g^2 \int d^3x \mathbf{Tr} \left(\left[\mathrm{i}\partial^+ \widetilde{A}^\kappa, \widetilde{A}_\kappa\right] \frac{1}{(\mathrm{i}\partial^+)^2} \left[\mathrm{i}\partial^+ \widetilde{A}^\kappa, \widetilde{A}_\kappa\right] \right) \\
& + \frac{1}{2} g^2 \int d^3x \overline{\widetilde{\psi}} \widetilde{\not{A}} \frac{\gamma^+}{\mathrm{i}\partial^+} \widetilde{\not{A}} \widetilde{\psi} \\
& + g \int d^3x \overline{\widetilde{\psi}} \widetilde{\not{A}} \widetilde{\psi} \\
& + 2g \int d^3x \mathbf{Tr} \left(\mathrm{i}\partial^\mu \widetilde{A}^\nu \left[\widetilde{A}_\mu, \widetilde{A}_\nu\right] \right)
\end{aligned}
$$

Discretized Light Cone Quantization

Pauli & Brodsky c1985

⇩

Basis Light Front Quantization*

$$\phi(\vec{x}) = \sum_{\alpha} \left[f_\alpha(\vec{x}) a_\alpha^+ + f_\alpha^*(\vec{x}) a_\alpha \right]$$

where $\{a_\alpha\}$ satisfy usual (anti-) commutation rules.

Furthermore, $f_\alpha(\vec{x})$ are arbitrary except for conditions:

Orthonormal: $\int f_\alpha(\vec{x}) f_{\alpha'}^*(\vec{x}) d^3x = \delta_{\alpha\alpha'}$

Complete: $\sum_{\alpha} f_\alpha(\vec{x}) f_\alpha^*(\vec{x}') = \delta^3(\vec{x} - \vec{x}')$

=> Wide range of choices for $f_a(\vec{x})$ and our initial choice is

$$f_\alpha(\vec{x}) = N e^{ik^+x^-} \Psi_{n,m}(\rho,\varphi) = N e^{ik^+x^-} f_{n,m}(\rho) \chi_m(\varphi)$$

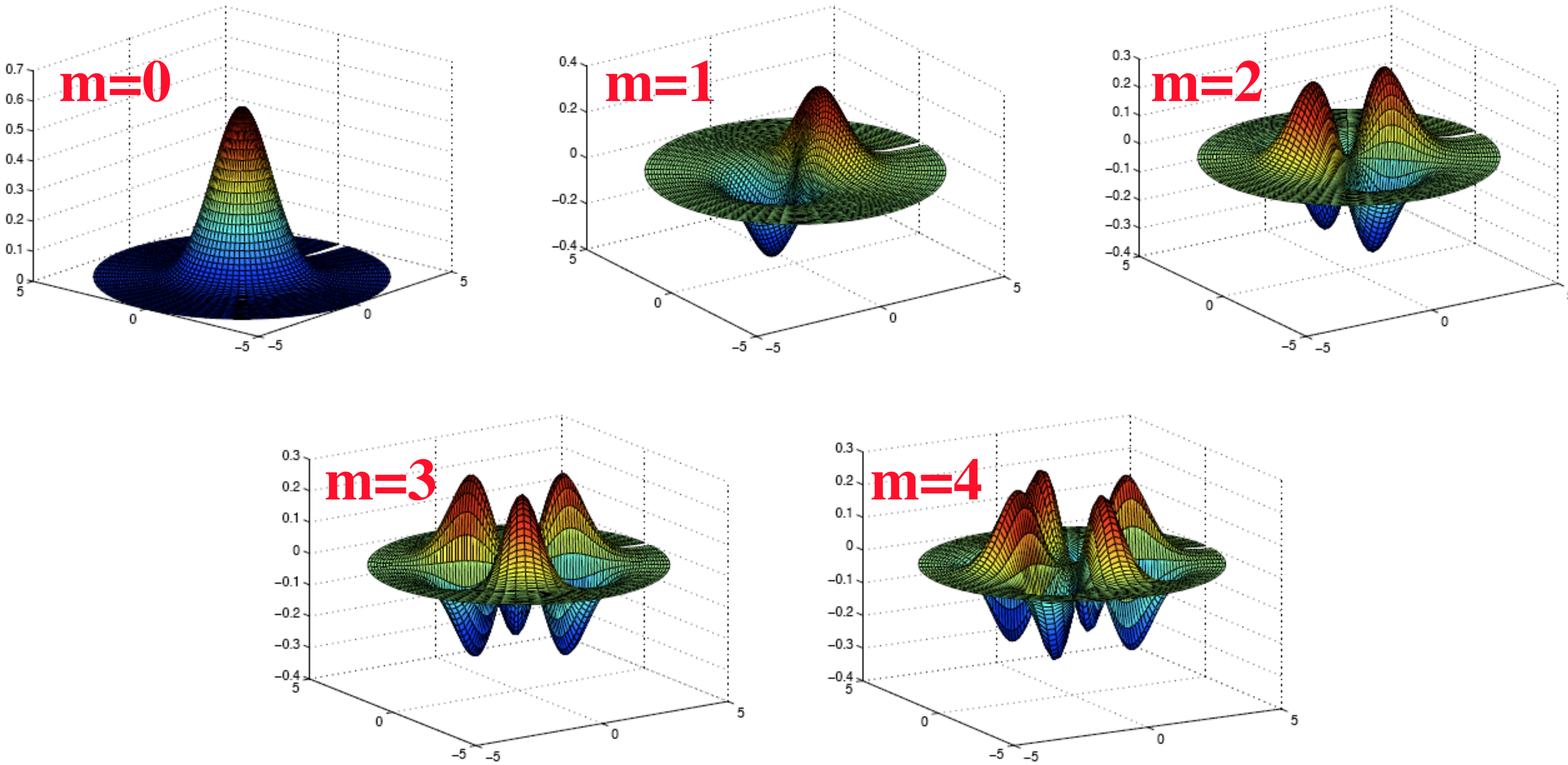
*J.P. Vary, H. Honkanen, J. Li, P. Maris, S.J. Brodsky, A. Harindranath, G.F. de Teramond, P. Sternberg, E.G. Ng and C. Yang, PRC 81, 035205 (2010). ArXiv:0905:1411

The properly normalized wavefunctions $\Psi_{n,m}(\rho,\phi) = f_{n,m}(\rho)\chi_m(\phi)$ are given by

$$f_{n,m}(\rho) \;=\; \sqrt{2\,M\,\Omega}\,\sqrt{\frac{n!}{(n+|m|)!}}\;\mathrm{e}^{-M\,\Omega\,\rho^2/2}\;\left(\sqrt{M\,\Omega}\;\rho\right)^{|m|}\;L_n^{|m|}(M\,\Omega\,\rho^2)$$

$$\chi_m(\phi) \;=\; \frac{1}{\sqrt{2\pi}}\,\mathrm{e}^{i\,m\,\phi}$$

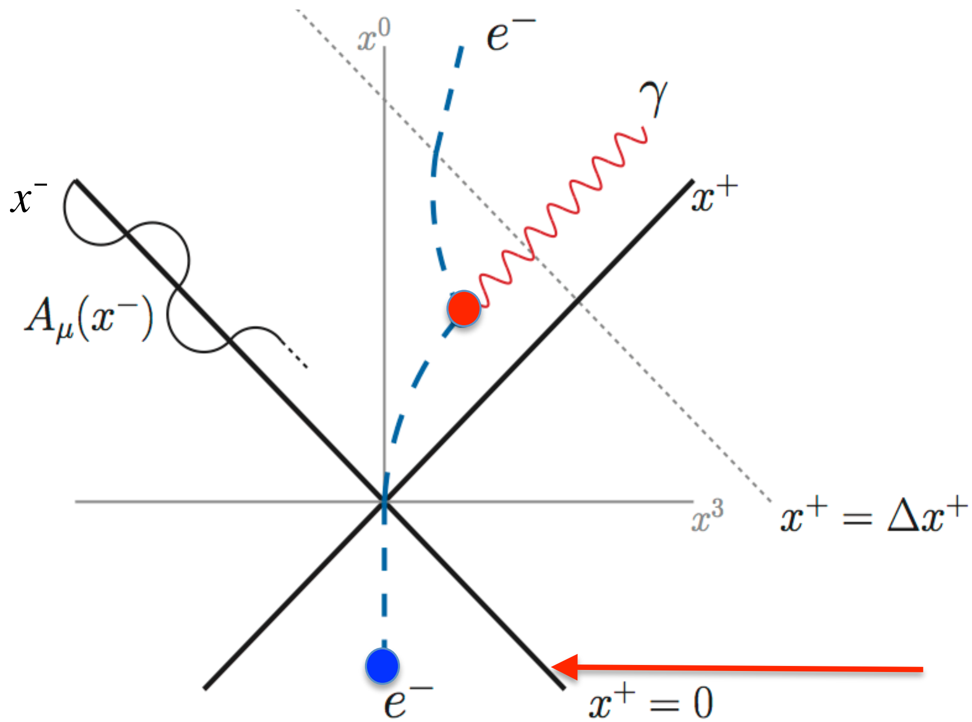
Set of transverse 2D HO modes for n=0



J.P. Vary, H. Honkanen, J. Li, P. Maris, S.J. Brodsky, A. Harindranath,
G.F. de Teramond, P. Sternberg, E.G. Ng and C. Yang, PRC 81, 035205 (2010).

tBLFQ: Nonlinear Compton Scattering

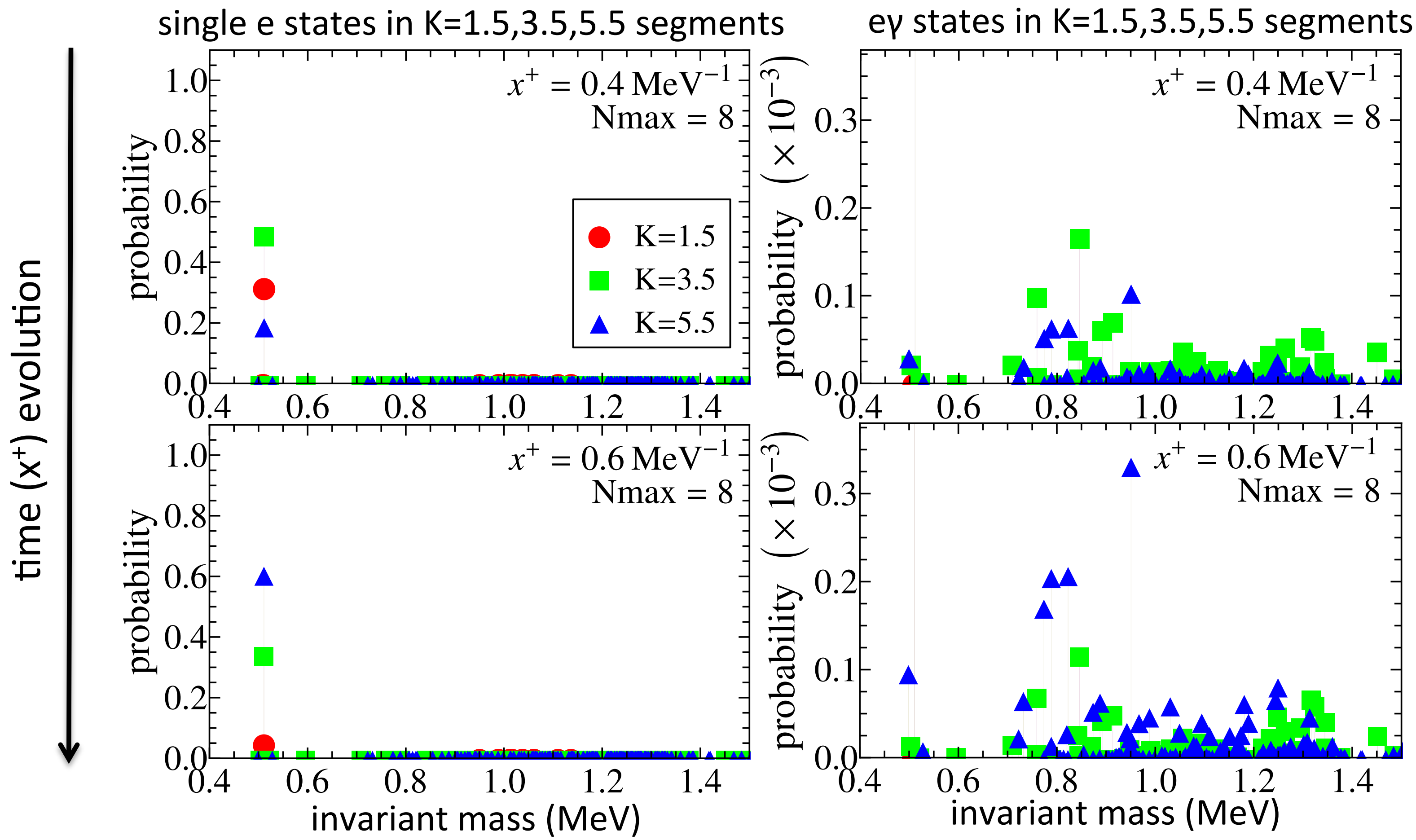
- Space-time structure



- Two effects: acceleration and radiation

Xingbo Zhao, Anton Ilderton, Pieter Maris and James P. Vary, Phys. Rev. D 88, 065014 (2013); arXiv 1303.3237; and Phys. Letts B 726, 856 (2013); arXiv 1309.5338

Results: Nonlinear Compton Scattering

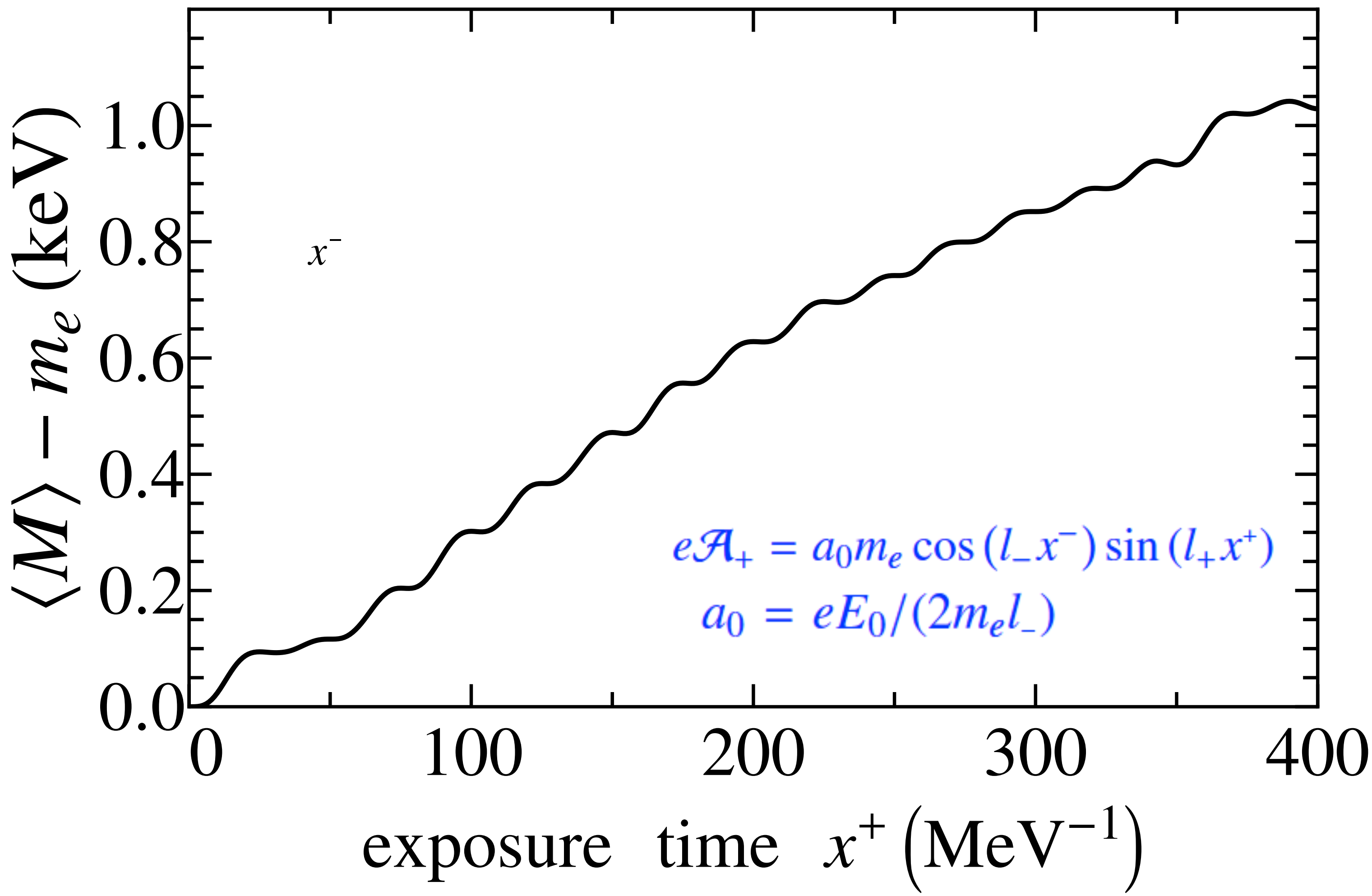


- Acceleration and radiation are treated in the same Hilbert space
- Entire process is nonperturbative (initial state changes significantly)

X. Zhao, A. Ilderton, P. Maris, J.P. Vary PRD 88 065014 (2013)

tBLFQ: Nonlinear Compton Scattering

Average invariant mass depends on exposure time

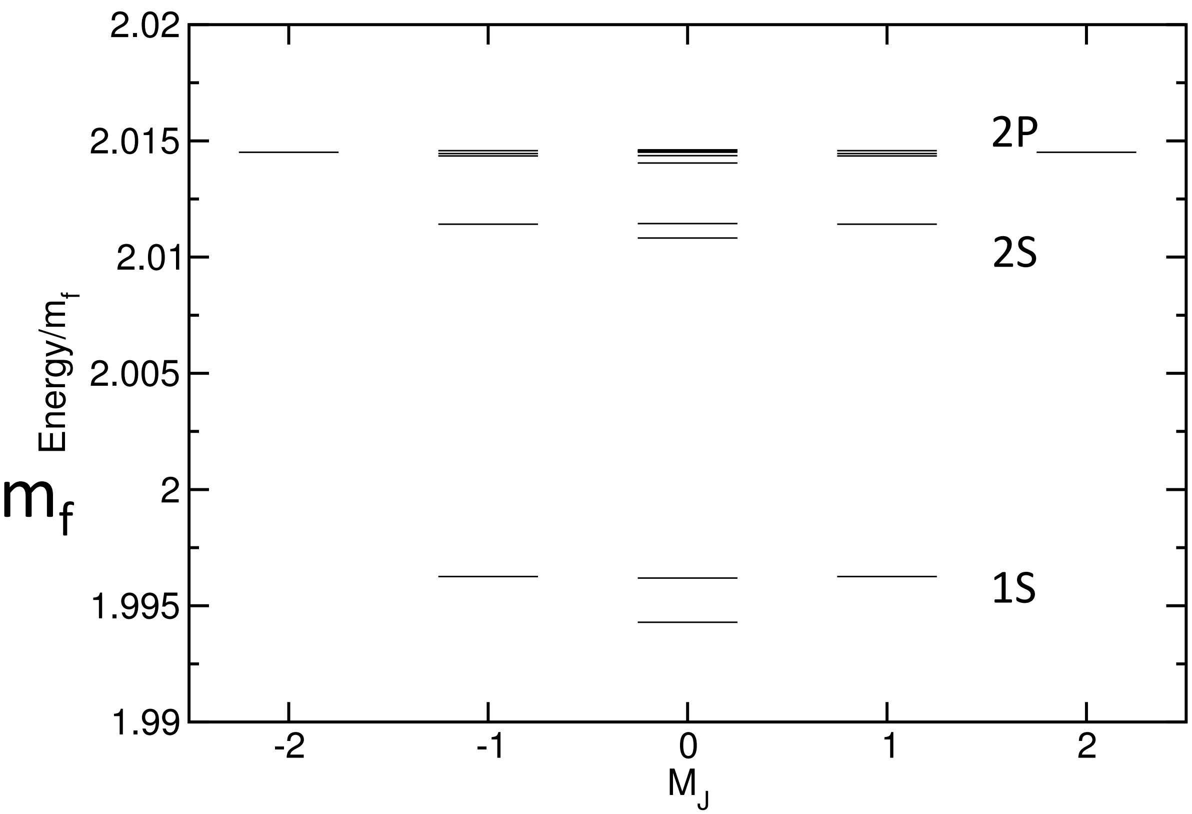


Xingbo Zhao, Anton Ilderton, Pieter Maris and James P. Vary, Phys. Rev. D 88, 065014 (2013); arXiv 1303.3237; and Phys. Letts B 726, 856 (2013); arXiv 1309.5338

Positronium in BLFQ

- Fock sector truncation: $|e^+e^-\rangle_{\rm phys} = a\,|e^+e^-\rangle + b\,|e^+e^-\gamma\rangle$
  - Fermion self-energy neglected

- Spectrum:
  - α=0.3
  - $K=N_{max}=19$
  - $b = \mu = 0.1\ m_f$



Lowest 8 states obtained as expected. Additional higher states not plotted.

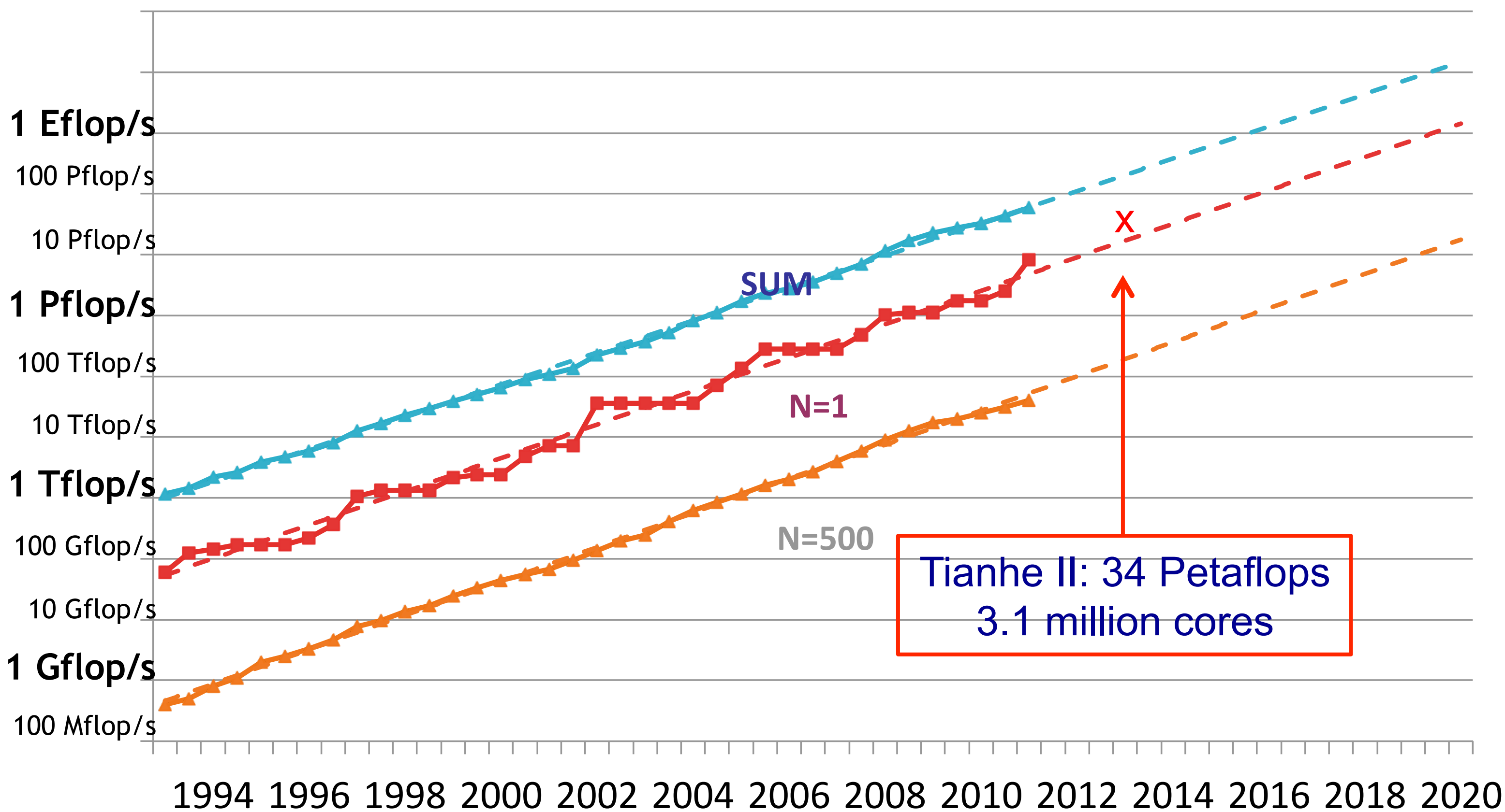
P. Wiecki, Y. Li, X. Zhao, P. Maris and J.P. Vary arXiv 1404.6234

- Hardware advances: Moore's Law
- Theory/Algorithms/Software advances: Doubles Moore's Law

Discovery potential increases geometrically

Role of Supercomputers

Projected Performance Development

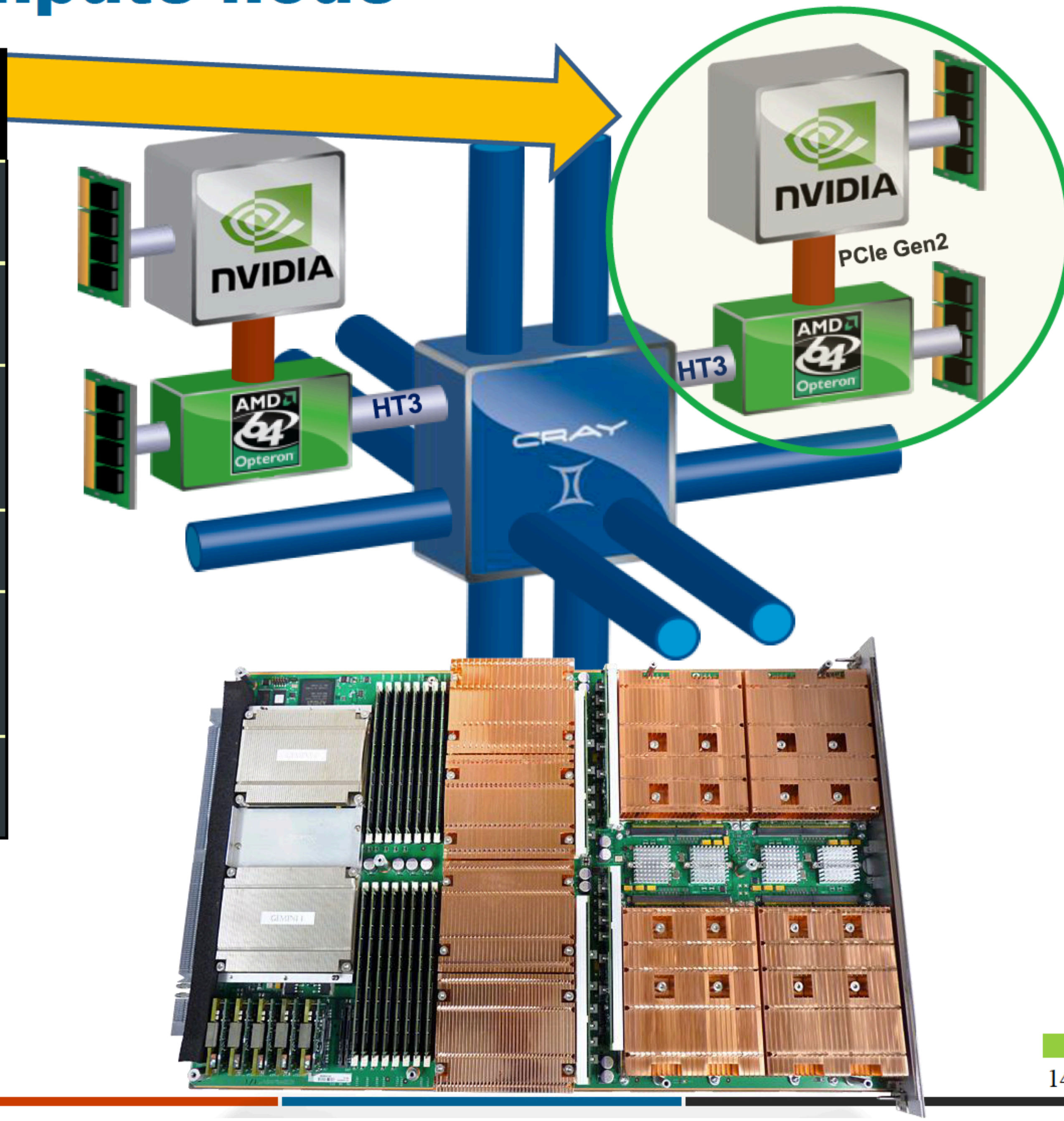


Titan at Oak Ridge National Laboratory is the world's second most powerful supercomputer with a theoretical peak performance exceeding 20 petaflops (quadrillion calculations per second).

That kind of computational capability—almost unimaginable—is on par with each of the world's 7 billion people being able to carry out 3 million calculations per second.

Cray XK6 compute node

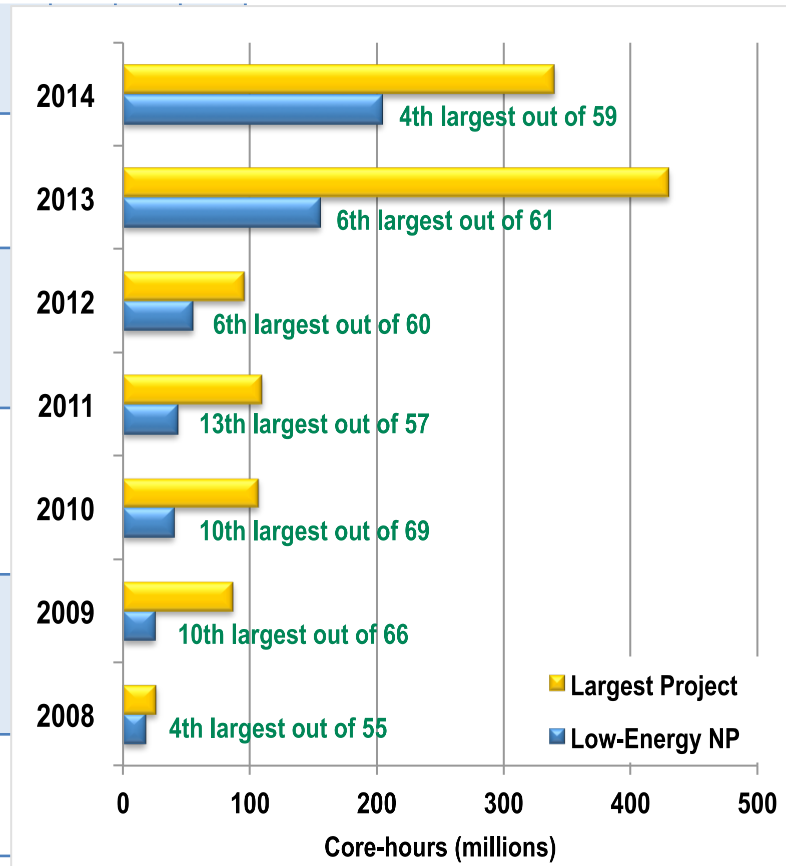
XK6 Compute Node Characteristics
AMD Opteron 6200 "Interlagos" 16 core processor @ 2.2GHz
Tesla M2090 "Fermi" @ 665 GF with 6GB GDDR5 memory
Host Memory 32GB 1600 MHz DDR3
Gemini High Speed Interconnect
Upgradeable to NVIDIA's next generation "Kepler" processor in 2012
Four compute nodes per XK6 blade. 24 blades per rack



Low Energy NP Application Areas

Application	Production Run Sizes	Resource	Dense Linear Alg.	Sparse Linear Alg.	Monte Carlo
AGFMC: Argonne Green's Function Monte Carlo	262,144 cores @ 10 hrs	Mira			X
MFDn: Many Fermion Dynamics - nuclear	260K cores @ 4 hrs 500K cores @ 1.33 hrs	Titan Mira		X	
NUCCOR: Nuclear Coupled-Cluster Oak Ridge, m-scheme & spherical	100K cores @ 5 hrs (1 nucleus, multiple parameters)	Titan		X	
DFT Code Suite: Density Functional Theory, mean-field methods	100K cores @ 10 hrs (entire mass table, fission barriers)	Titan	X		
MADNESS: Schroedinger, Lippman-Schwinger and DFT	40,000 cores @ 12 hrs (extreme asymmetric functions)	Titan	X	X	
NCSM_RGM: Resonating Group Method for scattering	98,304 cores @ 8 hrs	Titan	X	X	

- Ab initio Methods (CC, GFMC, NCSM) →pushing the limits to calculate larger nuclei
- Density Functional Theory → reasonable time to solution to calculate the entire mass table



Slide by Hai Ah Nam, ORNL

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
Spin content of the proton
+ Many More!

Conclusions/Outlook

- ✧ Impressive recent progress in deriving NN and NNN interactions from QCD
- ✧ Much work needs to be done to improve upon these interactions and the many-body approaches that employ them
- ✧ We will continue to apply these interactions to nuclei as they are developed
- ✧ Collaborations of Chiral EFT theorists and ab-initio many-body theorists needed to improve the properties of the Chiral EFT interactions
- ✧ Collaborations of nuclear theorists with computer scientists and applied mathematicians must continue
- ✧ Increasing computational resources needed (3NFs, 4NFs are major challenges)
- ✧ Increased manpower needed to achieve these goals in larger collaborating teams

Recent Collaborators

United States

ISU: Pieter Maris, George Papadimitriou, Chase Cockrell, Hugh Potter, Alina Negoita
LLNL: Erich Ormand, Tom Luu, Eric Jurgenson, Michael Kruse
ORNL/UT: David Dean, Hai Ah Nam, Markus Kortelainen, Witek Nazarewicz, Gaute Hagen,Thomas Papenbrock
OSU: Dick Furnstahl, students
MSU: Scott Bogner, Heiko Hergert
Notre Dame: Mark Caprio
ANL: Harry Lee, Steve Pieper, Fritz Coester
LANL: Joe Carlson, Stefano Gandolfi
UA: Bruce Barrett, Sid A. Coon, Bira van Kolck, Matthew Avetian, Alexander Lisetskiy
LSU: Jerry Draayer, Tomas Dytrych, Kristina Sviratcheva, Chairul Bahri
UW: Martin Savage

International

Canada: Petr Navratil
Russia: Andrey Shirokov, Alexander Mazur, Eugene Mazur, Sergey Zaytsev, Vasily Kulikov
Sweden: Christian Forssen, Jimmy Rotureau
Japan: Takashi Abe, Takaharu Otsuka, Yutaka Utsuno, Noritaka Shimizu
Germany: Achim Schwenk, Robert Roth, Kai Hebeler, students
South Korea: Youngman Kim, Ik Jae Shin
Turkey: Erdal Dikman

Computer Science/ Applied Math

ODU/Ames Lab: Masha Sosonkina, Dossay Oryspayev
LBNL: Esmond Ng, Chao Yang, Hasan Metin Aktulga
ANL: Stefan Wild, Rusty Lusk
OSU: Umit Catalyurek, Eric Saule

Quantum Field Theory

ISU: Xingbo Zhao, Pieter Maris, Paul Wiecki, Yang Li, Kirill Tuchin, John Spence
Stanford: Stan Brodsky
Penn State: Heli Honkanen
Russia: Vladimir Karmanov

Germany: Hans-Juergen Pirner
Costa Rica: Guy de Teramond
India: Avaroth Harindranath, Usha Kulshreshtha, Daya Kulshreshtha, Asmita Mukherjee, Dipankar Chakrabarti, Ravi Manohar