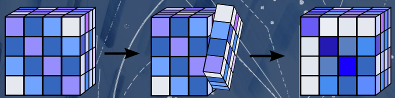
Canada's national laboratory
for particle and nuclear physics
and accelerator-based science

Can the shell model be truly ab initio?
and other questions

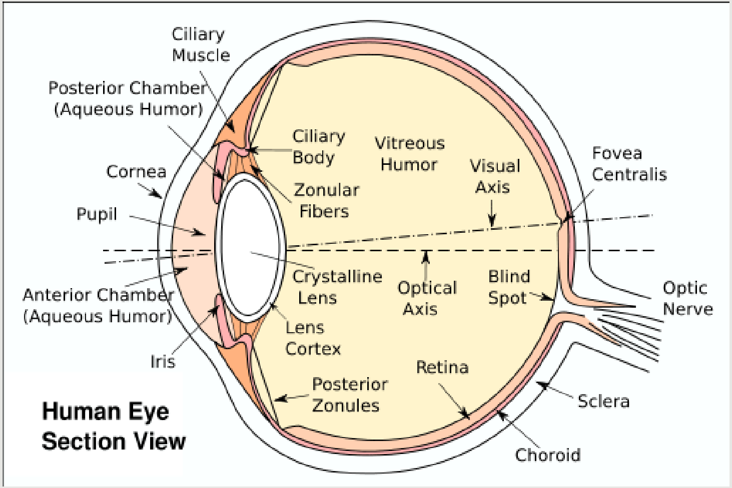
Ragnar Stroberg

TRIUMF

The tower of effective field theories
and the emergence of nuclear phenemena
CEA Saclay
January 19, 2017



Irreducible complexity?



Reductionism

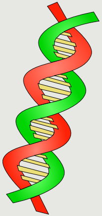
The underlying physical laws necessary for the mathematical theory of a large part of physics and the whole of chemistry are thus completely known, and the difficulty is only that the exact application of these laws leads to equations much too complicated to be soluble.

–Paul Dirac, 1929

$$i\partial\!\!\!/\psi = m\psi$$

$$\Downarrow$$

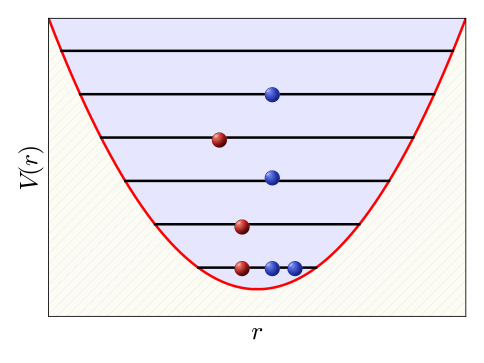
$$V = \frac{e^2}{r} + \ldots \Rightarrow$$



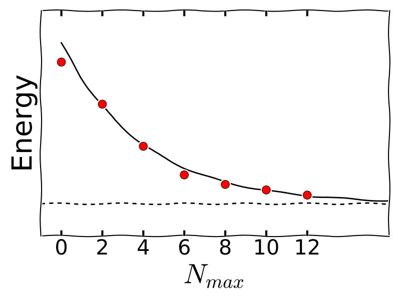
Outline

1. What is the shell model?
2. Is the shell model ab initio?
3. Can the shell model be derived from an underlying theory?
4. Can the shell model be formulated as an effective theory?
5. One magical chiral (-inspired) interaction, and hope for mankind

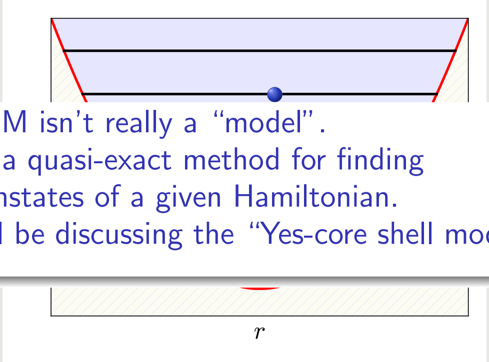
No core shell model



- Explicitly use harmonic oscillator basis
- HO forms complete basis
- Diagonalize with all nucleons active
- Extrapolate to infinite model space (variational principle)



No core shell model



NCSM isn't really a "model".
It is a quasi-exact method for finding eigenstates of a given Hamiltonian.
I will be discussing the "Yes-core shell model".

- Explicitly use harmonic oscillator basis
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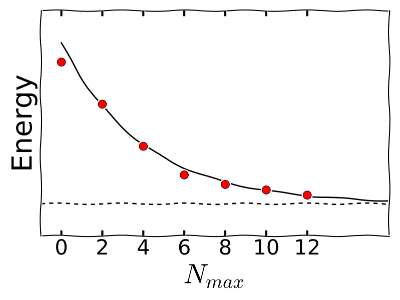
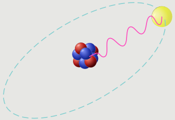
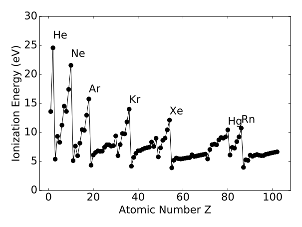
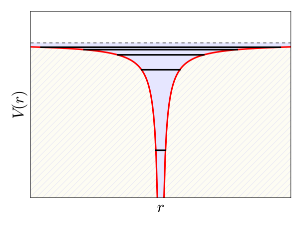
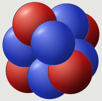


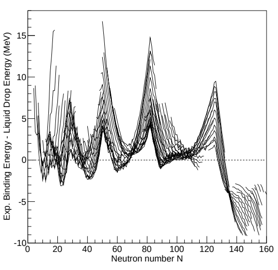
Analogy with atomic theory

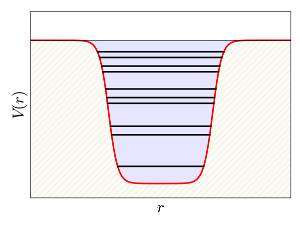




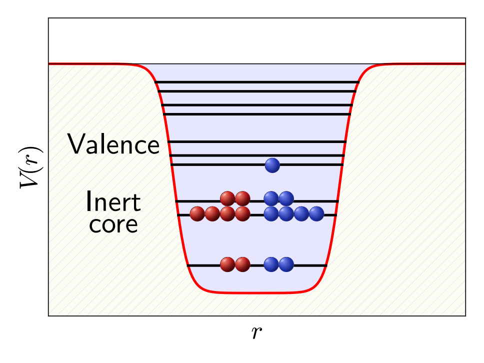








The nuclear shell model



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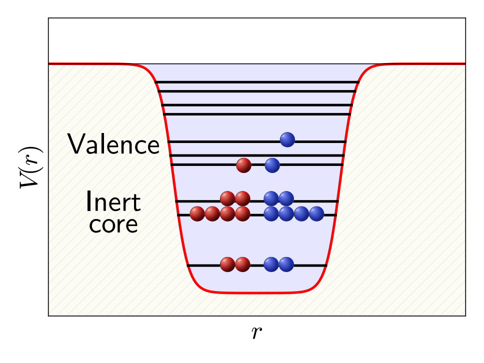

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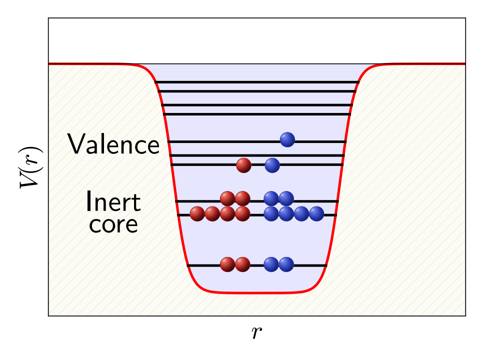
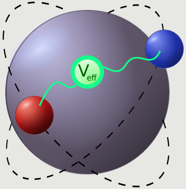
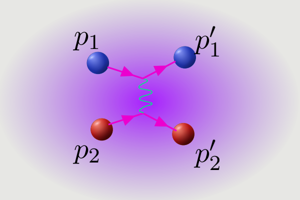


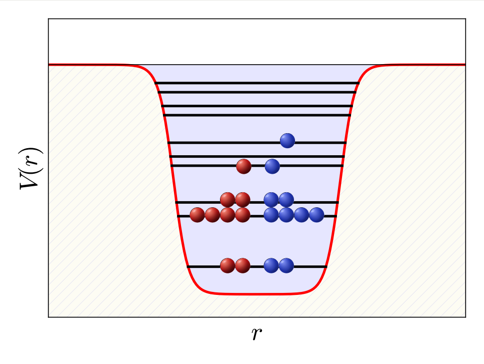
- Large gap suppresses core excitations
- Structure due to valence particles
- Core provides static mean field
- Valence particles interact via V_{eff}
- 19-body problem $\Rightarrow$ 3-body problem
- But what is V_{eff}?



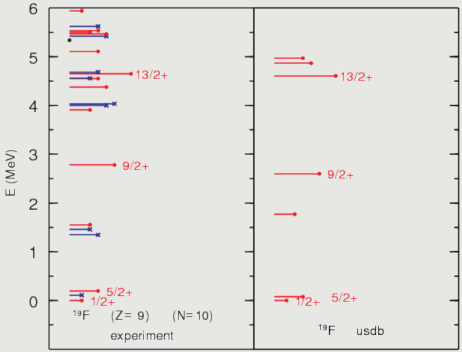


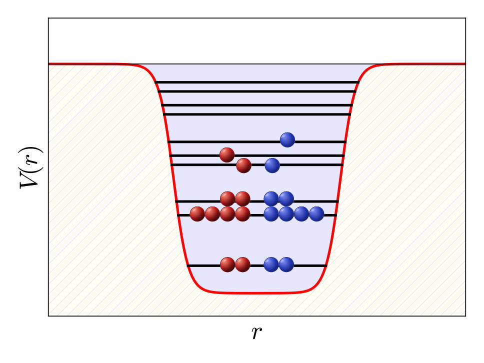
Pauli blocked

The nuclear shell model

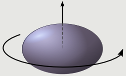


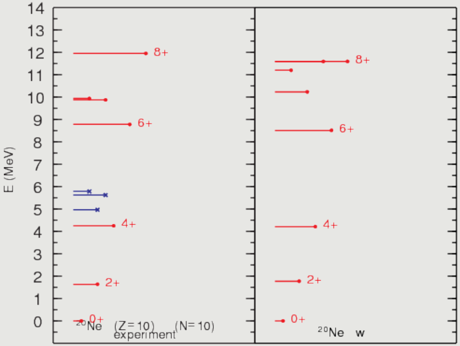
USD interaction: global fit to data yields spectroscopy with rms deviation 126 keV for sd shell nuclei.





Rotational band in ^{20}Ne





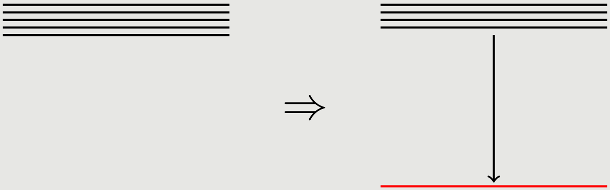
How does collectivity emerge in the shell model?

Simple example: a maximally coherent state

$$H_{N\times N} = \begin{pmatrix} -1 & -1 & \dots & -1 \\ -1 & -1 & \dots & -1 \\ \vdots & \vdots & \ddots & \vdots \\ -1 & -1 & \dots & -1 \end{pmatrix}$$

Eigenvalues: $\{-N, 0, 0, \dots, 0\}$

Lowest eigenvector: $\frac{1}{\sqrt{N}}(1, 1, \dots, 1)$



Is the shell model ab initio?

ab initio:

"Exact" solution of "exact" problem

1. Degrees of freedom must be fully specified (e.g. free nucleons)
2. Hamiltonian is "fundamental", i.e. not tailored to patch over deficiencies of the method
3. Solution method is exact (within estimated error)

Allen and Karo, Rev. Mod. Phys. (1960)

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no core shell model:

- Solution is exact ✓
- V_{eff} can be fundamental ✓

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- Solution is exact ✓
- V_{eff} can be fundamental ✓

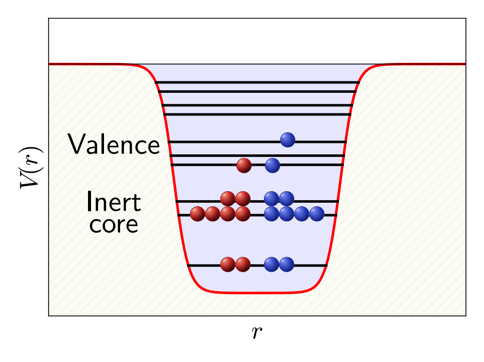
shell model:

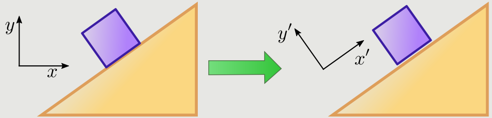
- If V_{eff} comes from fundamental theory, then solution is not exact ✗
- If V_{eff} is (empirically) adjusted to account for missing configurations, then it's not fundamental ✗
- If V_{eff} is derived from fundamental theory *and* accounts for missing configurations *and* operators are treated consistently ✓

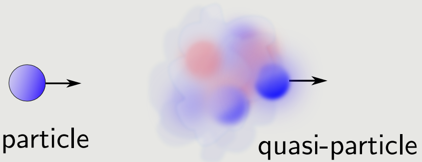
Allen and Karo, Rev. Mod. Phys. (1960)

How?

- A fundamental Hamiltonian will induce excitations out of the valence space
- Postulate: there exists some basis (d.o.f.) with identical quantum numbers, in which solution in the valence space reproduces the full solution
- Change of basis corresponds to a unitary transformation $\tilde{H} = UHU^{\dagger}$





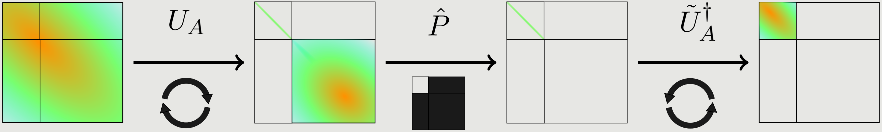


The methods on the market

Okubo-Lee-Suzuki	Many-body perturbation theory	In-medium SRG
• Solve the problem exactly • Obtain a valence space interaction which reproduces exact solution • Valence cluster expansion?	• Treat excitations out of valence space perturbatively • Q-box, resum select diagrams • Does the series converge?	• Series of unitary transformations • Renormalization group flow to desired form • Induced many-body forces?

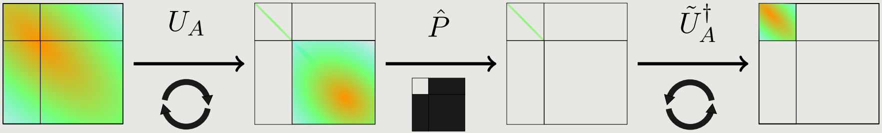
Coupled cluster may join in soon.

Okubo-Lee-Suzuki



- Not unitary (excluded-space information is lost)
- Small-space interaction *guaranteed* to reproduce eigenvalues of large space
- But we already know those!
- Calculate other nuclei w/ **valence cluster expansion**
- Hope higher-body terms are negligible, justification is *a posteriori*

Okubo-Lee-Suzuki



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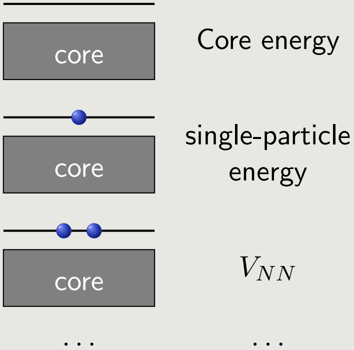
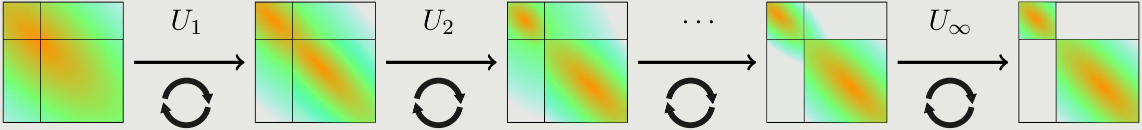
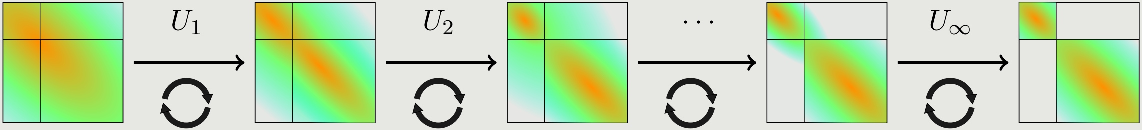




- Unitary (in principle): $\tilde{H} = e^{\Omega} H e^{-\Omega}$
- No need to solve the large-space problem first – work directly with H
- Induced 3-,4-. . .,A-body forces
- No guarantee that neglected higher-body terms will be unimportant, but. . .

In-medium SRG



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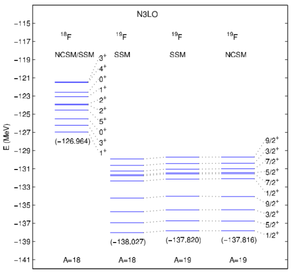
$$e^{\Omega} H e^{-\Omega} = H + [\Omega, H] + \frac{1}{2}[\Omega, [\Omega, H]] + \ldots$$

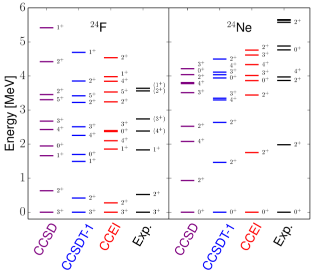
$$[\Omega, H] \leq 2 \; \|\Omega\| \; \|H\|$$

If $\|\Omega\| \lesssim \frac{1}{2}$, then the largest source of error is likely $[\Omega_{2b}, H_{2b}]_{3b}$, and we can treat this perturbatively.

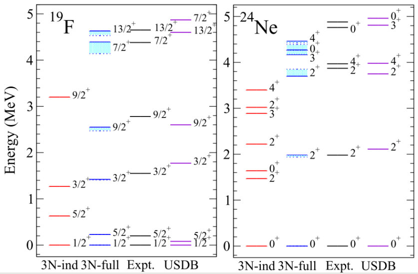
no core shell model + OLS



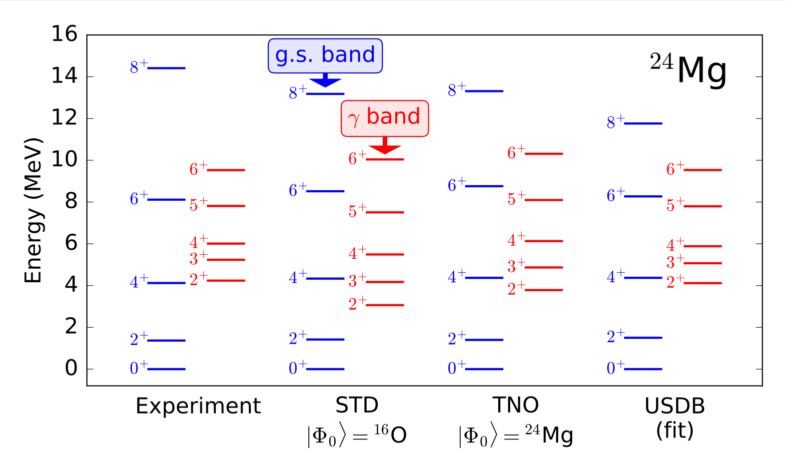
coupled cluster + OLS

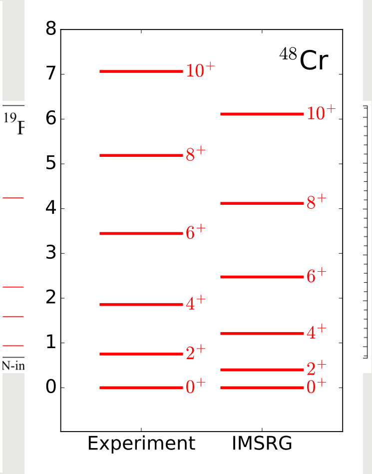


in-medium SRG



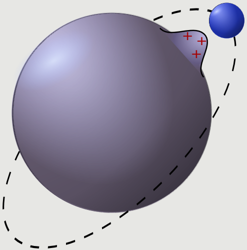
Dikmen et al. PRC (2015), Jansen et al. PRC(R) (2016), Stroberg et al. PRC(R) (2016)

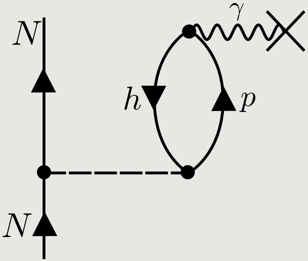




Dikmen et al. PRC (2015), Jansen et al. PRC(R) (2016), Stroberg et al. PRC(R) (2016)

Effective charges for electric quadrupole operators



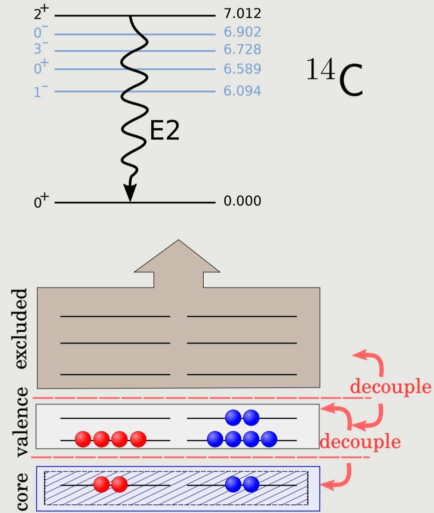


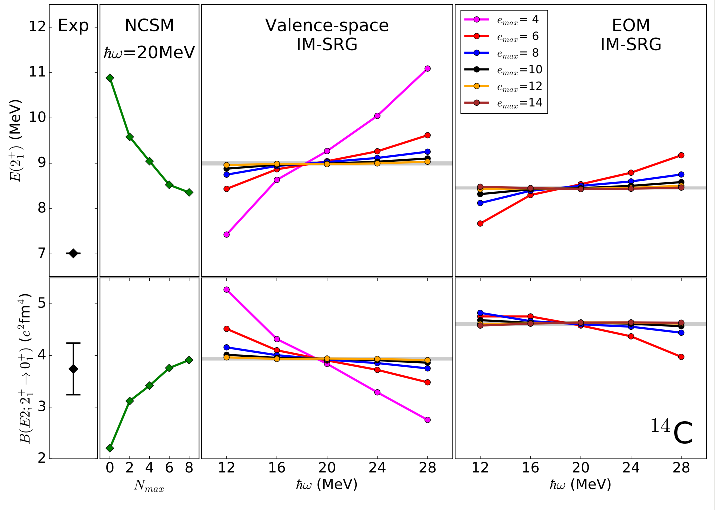
$$\mathcal{O}(E2) = \sum_i e_i r_i^2 Y^{(2)}(\theta_i)$$

$$e_p \approx 1.5, \; e_n \approx 0.5$$

Can we do without them?

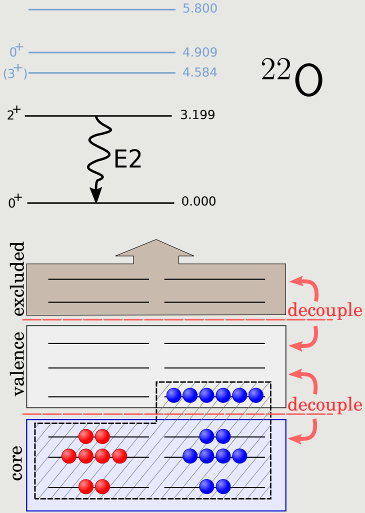
Electric quadrupole transitions

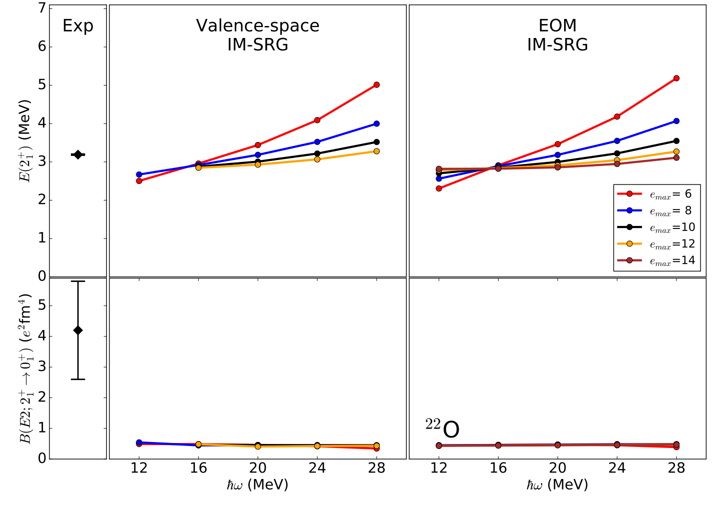




NCSM results from Petr Navrátil, EOM results from Nathan Parzuchowski

Electric quadrupole transitions

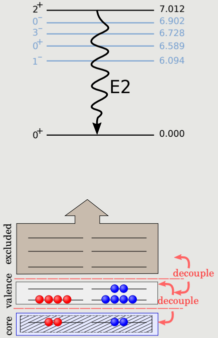


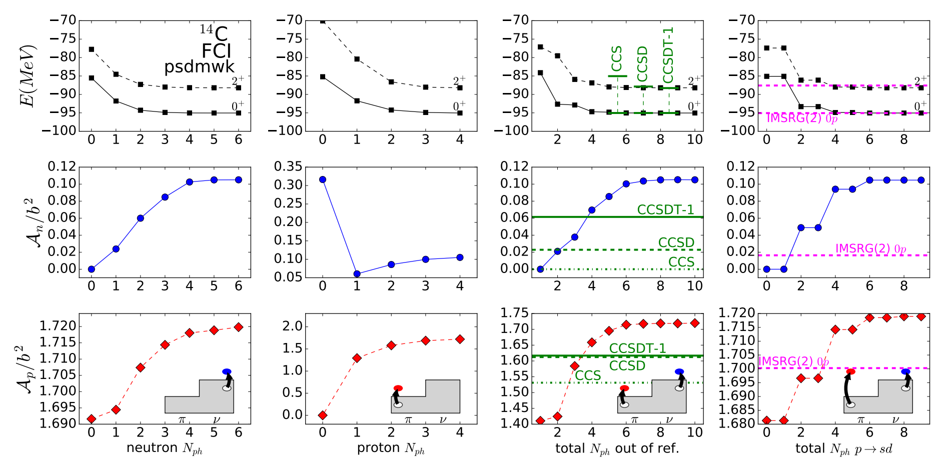


EOM results from Nathan Parzuchowski

Why???

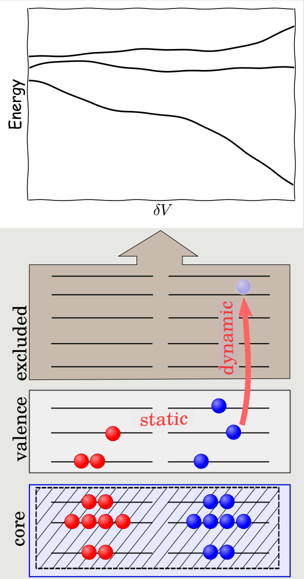
^{14}C in psd shell, compare CC, IM-SRG w/ FCI:





How should we think about the shell model?

- The shell model, as typically understood, is a **model** (but it's a pretty successful model)
- Fermi liquid theory: quasiparticles retain characteristics of the bare particles
- Quantum chemistry: separation into static and dynamic correlations
- An ab initio many-body method can be mapped onto the shell model → nonperturbative treatment of excitations near the Fermi surface.



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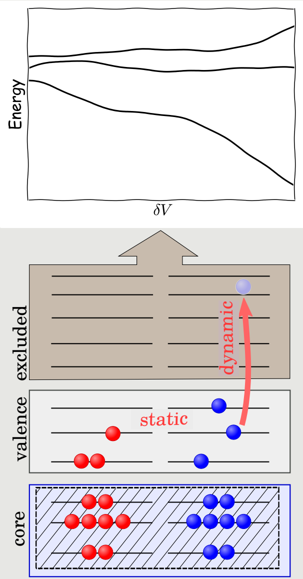
Paradigm:
If a model works well but isn't fundamental, and if the fundamental theory is hard to solve, then map the fundamental theory to the model through a unitary transformation (RG flow).



Can the shell model be formulated as an effective theory?

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VOLUME 84, NUMBER 24 PHYSICAL REVIEW LETTERS 12 JUNE 2000

Morphing the Shell Model into an Effective Theory

W. C. Haxton and C.-L. Song
Institute for Nuclear Theory, Box 351550, and Department of Physics, University of Washington, Seattle, Washington 98195
(Received 26 July 1999)

We describe a strategy for attacking the canonical nuclear structure problem—bound-state properties of a system of point nucleons interacting via a two-body potential—which involves an expansion in the number of particles scattering at high momenta, but is otherwise exact. The required self-consistent solutions of the Bloch-Horowitz equation for effective interactions and operators are obtained by an efficient Green's function method based on the Lanczos algorithm. We carry out this program for the simplest nuclei, *d* and ^{3}He, in order to explore the consequences of reformulating the shell model as a controlled effective theory.

PHYSICAL REVIEW C **93**, 044332 (2016)

Effective field theory in the harmonic oscillator basis

S. Binder, A. Ekström, G. Hagen, T. Papenbrock, and K. A. Wendt
*Department of Physics and Astronomy, University of Tennessee, Knoxville, Tennessee 37996, USA
and Physics Division, Oak Ridge National Laboratory, Oak Ridge, Tennessee 37831, USA*
(Received 11 December 2015; revised manuscript received 5 April 2016; published 25 April 2016)

We develop interactions from chiral effective field theory (EFT) that are tailored to the harmonic oscillator basis. As a consequence, ultraviolet convergence with respect to the model space is implemented by construction and infrared convergence can be achieved by enlarging the model space for the kinetic energy. In oscillator EFT, matrix elements of EFTs formulated for continuous momenta are evaluated at the discrete momenta that stem from the diagonalization of the kinetic energy in the finite oscillator space. By fitting to realistic phase shifts and deuteron data we construct an effective interaction from chiral EFT at next-to-leading order. Many-body coupled-cluster calculations of nuclei up to ^{132}Sn converge fast for the ground-state energies and radii in feasible model spaces.

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Physics Letters B 653 (2007) 358–362
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No-core shell model in an effective-field-theory framework

I. Stetcu [a,b,*], B.R. Barrett [a], U. van Kolck [a]
[a] *Department of Physics, University of Arizona, Tucson, AZ 85721, USA*
[b] *Theoretical Division, Los Alamos National Laboratory, Los Alamos, NM 87545, USA*

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Editor: W. Haxton

Abstract

We present a new approach to the construction of effective interactions suitable for many-body calculations by means of the no-core shell model (NCSM). We consider an effective field theory (EFT) with only nucleon fields directly in the NCSM model spaces. In leading order, we obtain the strengths of the three contact interactions from the condition that in each model space the experimental ground-state energies of ^{2}H, ^{3}H and ^{4}He be exactly reproduced. The first $(0^+;0)$ excited state of ^{4}He and the ground state of ^{6}Li are then obtained by means of NCSM calculations in several spaces and frequencies. After we remove the harmonic-oscillator frequency dependence, we predict for ^{4}He an energy level for the first $(0^+;0)$ excited state in remarkable agreement with the experimental value. The corresponding ^{6}Li binding energy is about 70% of the experimental value, consistent with the expansion parameter of the EFT.
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Institute for Nuclear Theory, Box 351550, and Department of Physics, University of Washington, Seattle, Washington 98195

(Received 26 July 1999)

We describe a strategy for attacking the canonical nuclear structure problem—bound-state properties of a system of point nucleons interacting via a two-body potential—which involves an expansion in the number of particles scattering at high momenta, but is otherwise exact. The required self-consistent solutions of the Bloch-Horowitz equation for effective interactions and operators are obtained by an efficient Green's function method based on the Lanczos algorithm. We carry out this program for the simplest nuclei, d and ^{3}He, in order to explore the consequences of reformulating the shell model as a controlled effective theory.

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Effective field theory in the harmonic oscillator basis

S. Binder, A. Ekström, G. Hagen, T. Papenbrock, and K. A. Wendt

Department of Physics and Astronomy, University of Tennessee, Knoxville, Tennessee 37996, USA
and Physics Division, Oak Ridge National Laboratory, Oak Ridge, Tennessee 37831, USA

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We develop interactions from chiral effective field theory (EFT) that are tailored to the harmonic oscillator basis. As a consequence, ultraviolet convergence with respect to the model space is implemented by construction and infrared convergence can be achieved by enlarging the model space for the kinetic energy. In oscillator EFT, matrix elements of EFTs formulated for continuous momenta are evaluated at the discrete momenta that stem from the diagonalization of the kinetic energy in the finite oscillator space. By fitting to realistic phase shifts and deuteron data we construct an effective interaction from chiral EFT at next-to-leading order. Many-body coupled-cluster calculations of nuclei up to ^{132}Sn converge fast for the ground-state energies and radii in feasible model spaces.

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No-core shell model in an effective-field-theory framework

I. Stetcu [a,b,*], B.R. Barrett [a], U. van Kolck [a]

[a] *Department of Physics, University of Arizona, Tucson, AZ 85721, USA*
[b] *Theoretical Division, Los Alamos National Laboratory, Los Alamos, NM 87545, USA*

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Abstract

We present a new approach to the construction of effective interactions suitable for many-body calculations by means of the no-core shell model (NCSM). We consider an effective field theory (EFT) with only nucleon fields directly in the NCSM model spaces. In leading order, we obtain the strengths of the three contact interactions from the condition that in each model space the experimental ground-state energies of ^{2}H, ^{3}H and ^{4}He be exactly reproduced. The first $(0^+;0)$ excited state of ^{4}He and the ground state of ^{6}Li are then obtained by means of NCSM calculations in several spaces and frequencies. After we remove the harmonic-oscillator frequency dependence, we predict for ^{4}He an energy level for the first $(0^+;0)$ excited state in remarkable agreement with the experimental value. The corresponding ^{6}Li binding energy is about 70% of the experimental value, consistent with the expansion parameter of the EFT.
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PACS: 21.30.-x; 21.60.Cs; 24.10.Cn; 45.50.Jf

All of these express chiral EFT in an oscillator basis and solve ≈exactly.

Can the shell model be formulated as an effective theory?

Answer: I don't know.

Can the shell model be formulated as an effective theory?

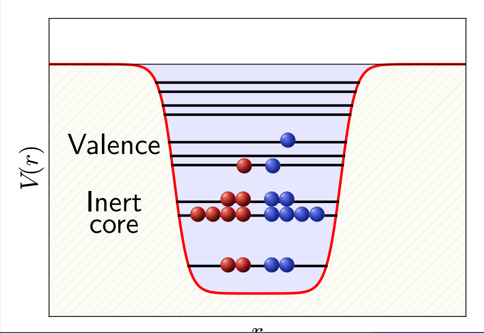
Answer: I don't know.

Why would we want to make it an effective theory?

- Shell model with uncertainty estimates
- No need to bother mapping chiral EFT to the shell model
- Systematic improvements, e.g. $3N$ interaction, 2-body operators

First steps

- Degrees of freedom: quasiparticles outside of core
- Breakdown scale: core excitation energy
- Symmetries: J,π,...
- Small scale: shell splitting?



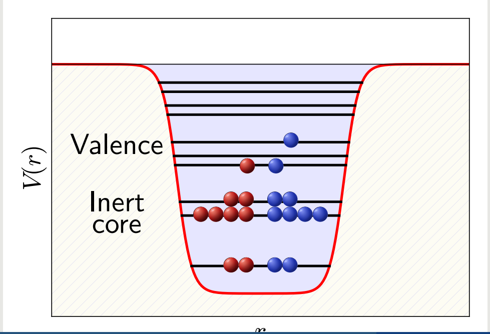
Shell model as an EFT

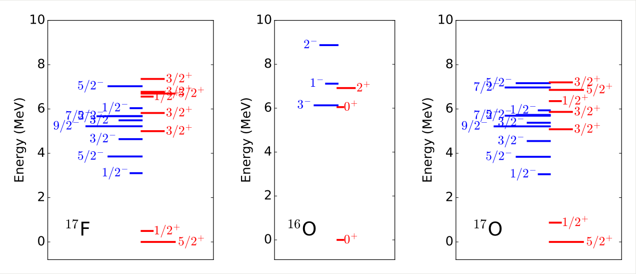
First steps

- Degrees of freedom: quasiparticles outside of core
- Breakdown scale: core excitation energy
- Symmetries: J, π, ...
- Small scale: shell splitting?

Challenges

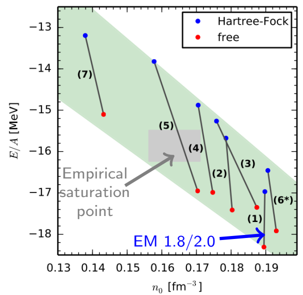
- Core shouldn't be a point-particle
- Is there any separation of scales?
- Which states to fit to?
- Origin of hierarchy of many-body forces?





One "magical" chiral (or chiral-inspired) interaction

	EM 500/400	EM 1.8/2.0
NN	N^3LO	same
	$\Lambda_{2N} = 500$ MeV	same
	non-local regulator	same
	fit to NN scattering, ^{2}H	same
	$\lambda_{SRG} = 1.88$ fm^{-1}	$\approx$ same
3N	N^2LO	same
	$\Lambda_{3N} = 400$ MeV	$\approx$ same
	local regulator	**non-local regulator**
	fit to ^{3}H BE, $t_{1/2}$	**fit to ^{3}H BE, ^{4}He r_{ch}**
	consistently SRG evolved	**no SRG for 3N**



Hebeler et al. PRC(R) (2011), Drischler et al. PRC (2016), Simonis et al. (in prep.)

One “magical” chiral (or chiral-inspired) interaction

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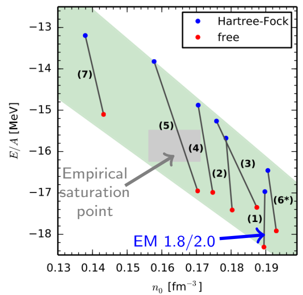
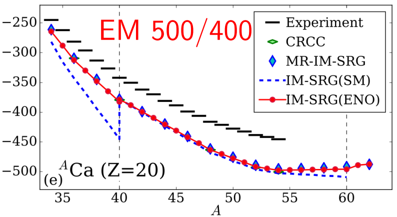
NN	N^{3}LO $\Lambda_{2N} = 500$ MeV non-local regulator fit to NN scattering, ^{2}H $\lambda_{SRG} = 1.88$ fm^{-1}	same same same same ≈ same
3N	N^{2}LO $\Lambda_{3N} = 400$ MeV **local regulator** **fit to ^{3}H BE, $t_{1/2}$** **consistently SRG evolved**	same ≈ same **non-local regulator** **fit to ^{3}H BE, ^{4}He r_{ch}** **no SRG for 3N**





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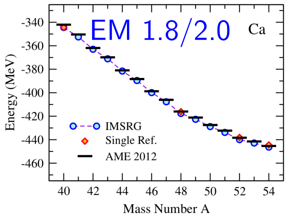

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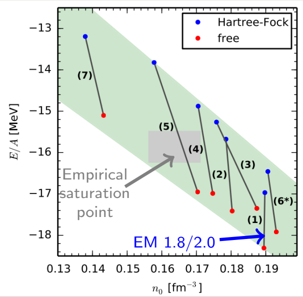
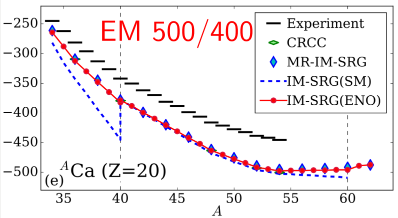
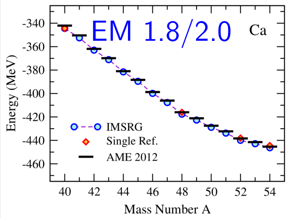




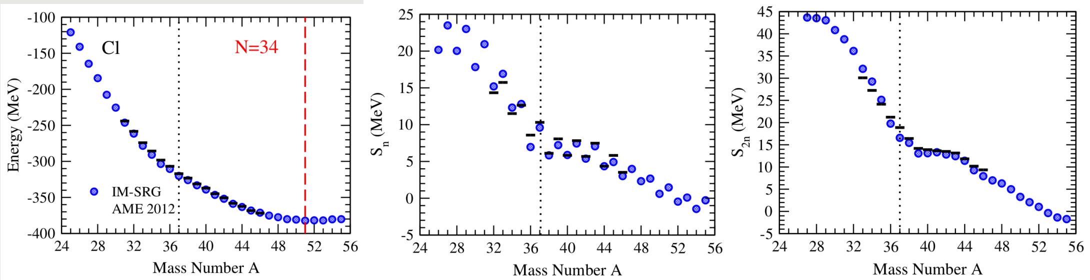


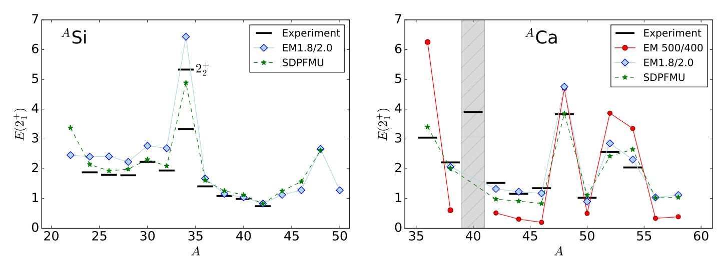
- Neither interaction is fully consistent

  however...
- Saturation properties appear important for finite nuclei

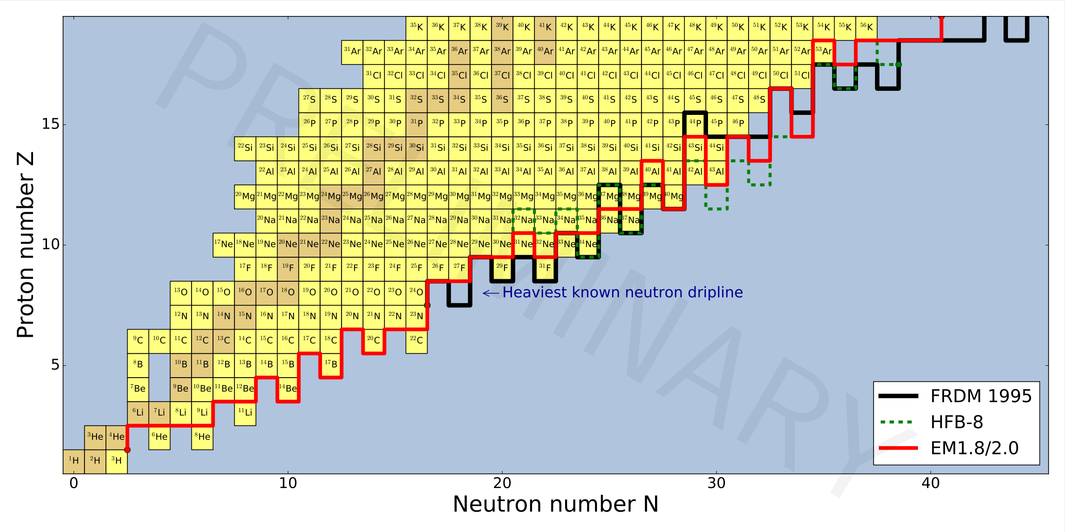
Hebeler et al. PRC(R) (2011), Drischler et al. PRC (2016), Simonis et al. (in prep.)

EM 1.8/2.0 interaction



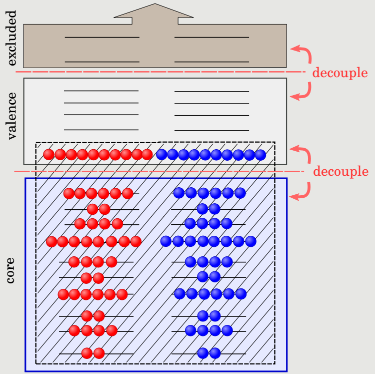


The neutron dripline

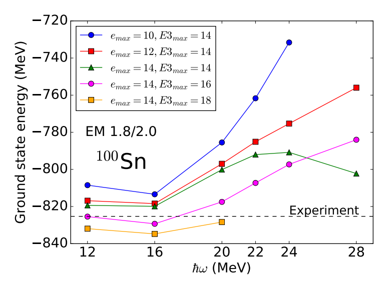


Baumann et al. Nature (2007), Möller et al. (1995), Samyn et al. (2004), Holt et al. (in prep.)

The tin isotopes ($Z = 50$)

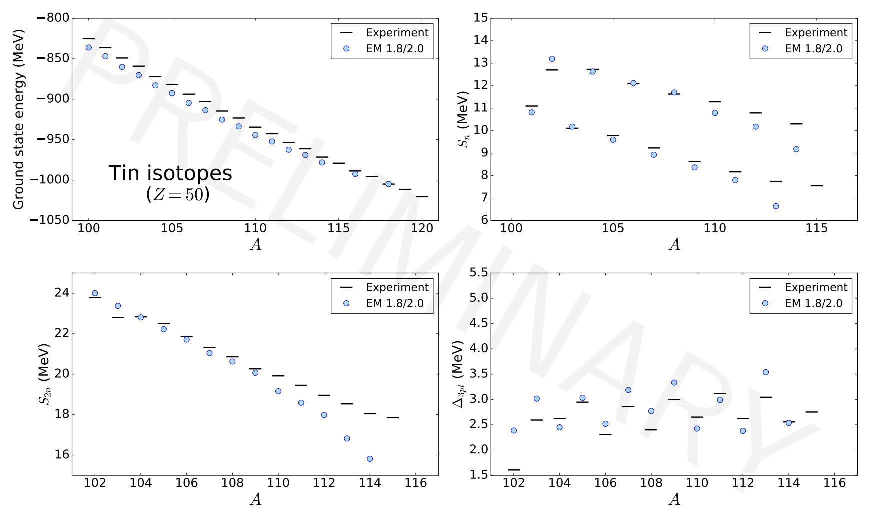


- ^{100}Sn: 50 protons, 50 neutrons
- Open shell valence space: full gds shell
- m-scheme dimension $\sim 10^{12}$
- Need importance truncation to diagonalize!



Simonis et al. (in prep.), Stumpf et al. PRC(R) (2016)

Isotopic chain with $\hbar\omega = 16$, $e_{max} = 14$, $E3_{max} = 16$



Collaborators

- The shell model can be derived ab initio
- The SM can be seen as an efficient separation of degrees of freedom
- Attempts at ab initio effective charges aren't yet successful
- Formulating the SM as an effective theory appears fraught with difficulties
- EM 1.8/2.0 interaction suggests that once you get NN scattering and saturation, things fall into place

Collaborators:

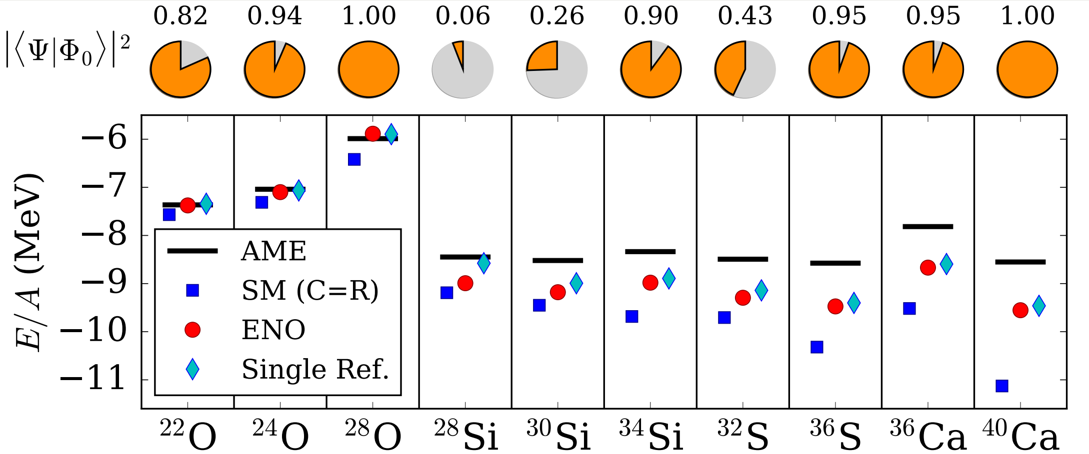
TRIUMF A. Calci, J. Holt, J. Kozaczuk, D. Morrissey, P. Navrátil

NSCL/MSU S. Bogner, H. Hergert, N. Parzuchowski

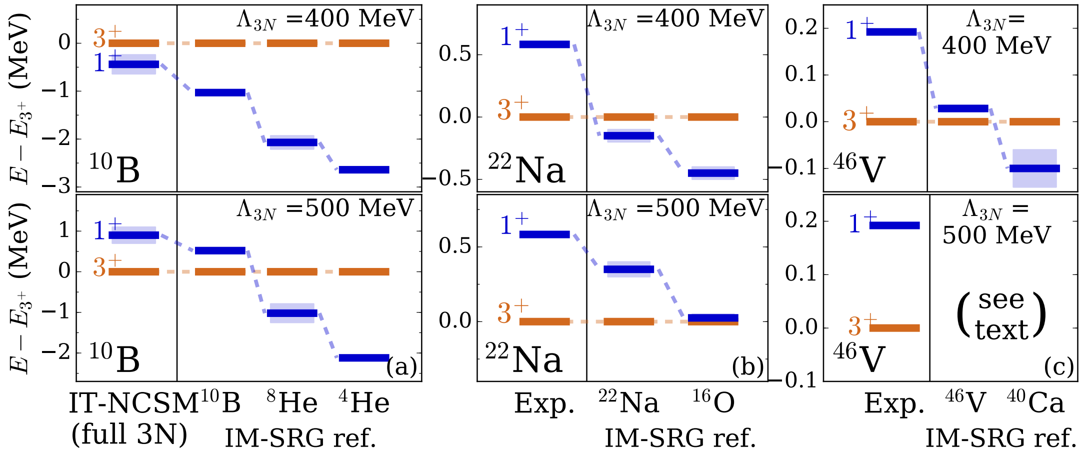
TU Darmstadt R. Roth, A. Schwenk, J. Simonis

ORNL/UT G. Hagen, T. Morris

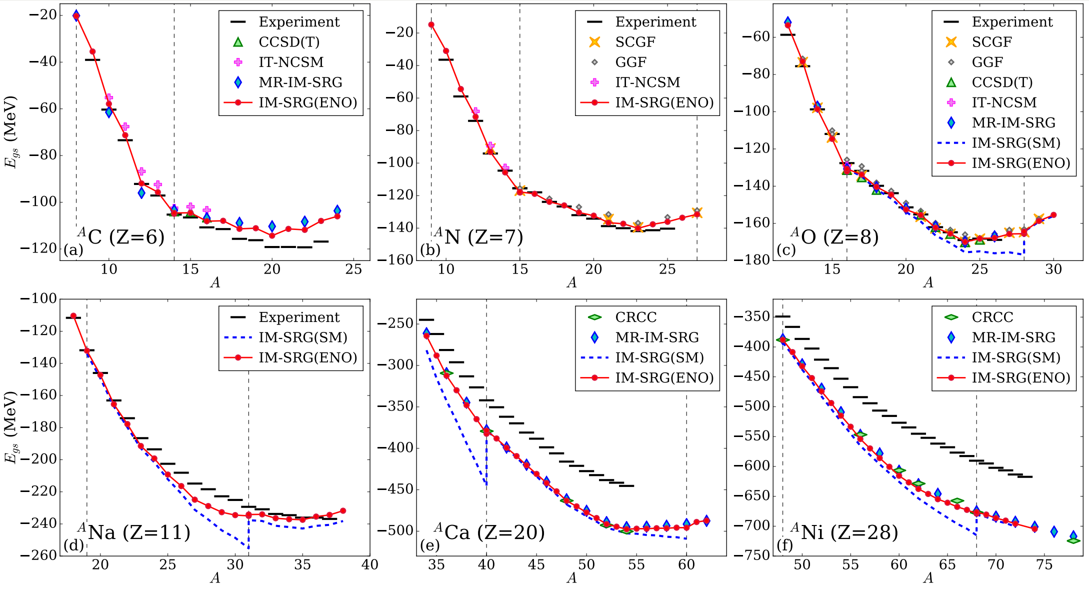
Backup slides



$|\langle\Psi|\Phi_0\rangle|^2$
0.82 0.94 1.00 0.06 0.26 0.90 0.43 0.95 0.95 1.00
E/A (MeV)
−6
−7
−8
−9
−10
−11
AME
SM (C=R)
ENO
Single Ref.
^{22}O ^{24}O ^{28}O ^{28}Si ^{30}Si ^{34}Si ^{32}S ^{36}S ^{36}Ca ^{40}Ca



Λ_{3N} =400 MeV
Λ_{3N} =500 MeV
$E - E_{3^+}$ (MeV)
^{10}B
^{22}Na
^{46}V
3^+
1^+
(see text)
(a)
(b)
(c)
IT-NCSM (full 3N)
^{10}B ^{8}He ^{4}He
IM-SRG ref.
Exp. ^{22}Na ^{16}O
IM-SRG ref.
Exp. ^{46}V ^{40}Ca
IM-SRG ref.


(a) ^{A}C (Z=6)
Experiment
CCSD(T)
IT-NCSM
MR-IM-SRG
IM-SRG(ENO)
(b) ^{A}N (Z=7)
Experiment
SCGF
GGF
IT-NCSM
IM-SRG(ENO)
(c) ^{A}O (Z=8)
Experiment
SCGF
GGF
CCSD(T)
IT-NCSM
MR-IM-SRG
IM-SRG(SM)
IM-SRG(ENO)
(d) ^{A}Na (Z=11)
Experiment
IM-SRG(SM)
IM-SRG(ENO)
(e) ^{A}Ca (Z=20)
CRCC
MR-IM-SRG
IM-SRG(SM)
IM-SRG(ENO)
(f) ^{A}Ni (Z=28)
CRCC
MR-IM-SRG
IM-SRG(SM)
IM-SRG(ENO)
E_{gs} (MeV)
A