Effective Interactions for Nuclear Structure Calculations: The No Core Shell Model and Beyond

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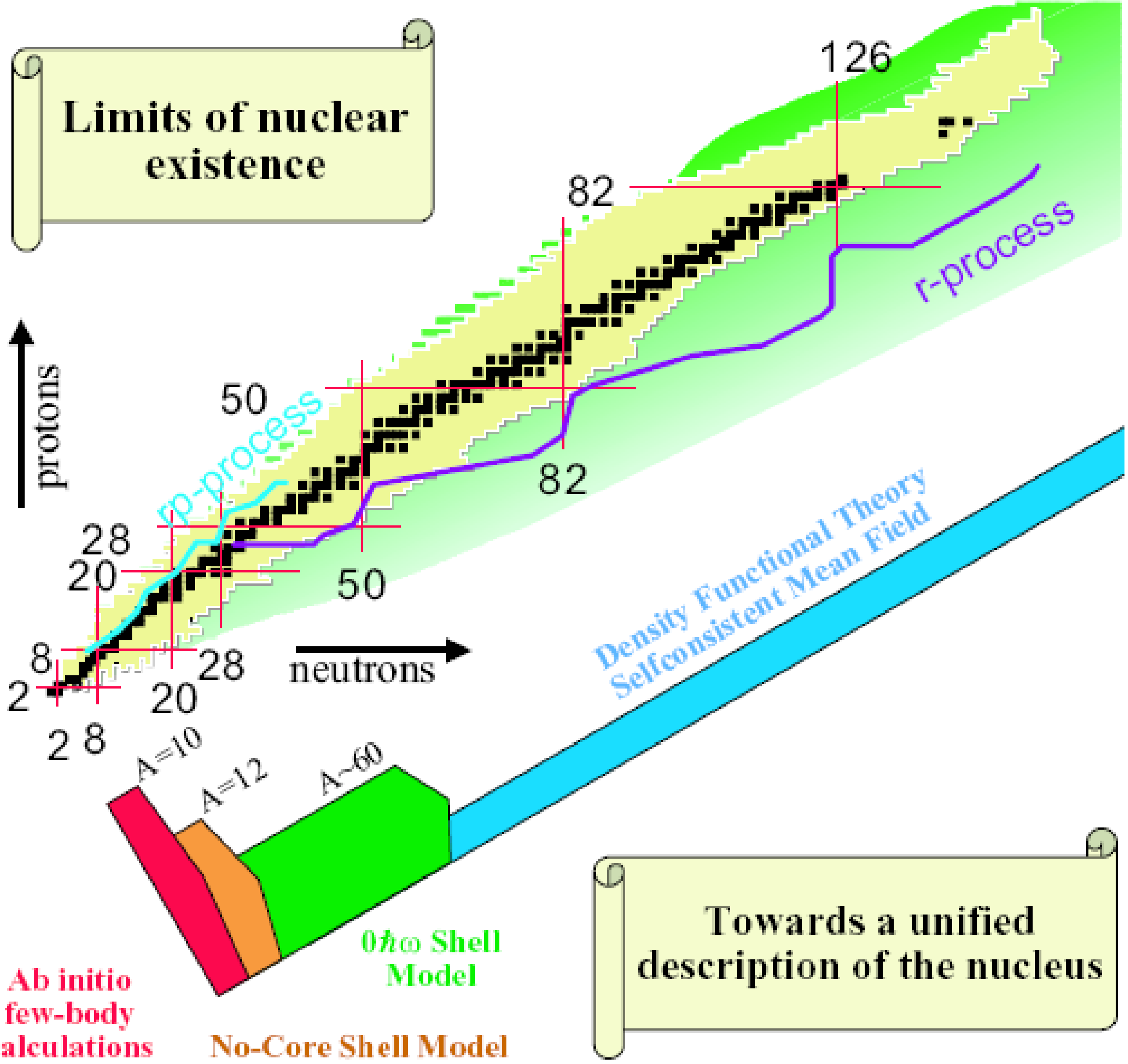
THE UNIVERSITY OF ARIZONA.
Arizona's First University.

Ab initio Nuclear Density Functional Theory

ESNT Workshop, CEA/Saclay April 11, 2012


Limits of nuclear existence
protons
neutrons
126
82
50
28
20
8
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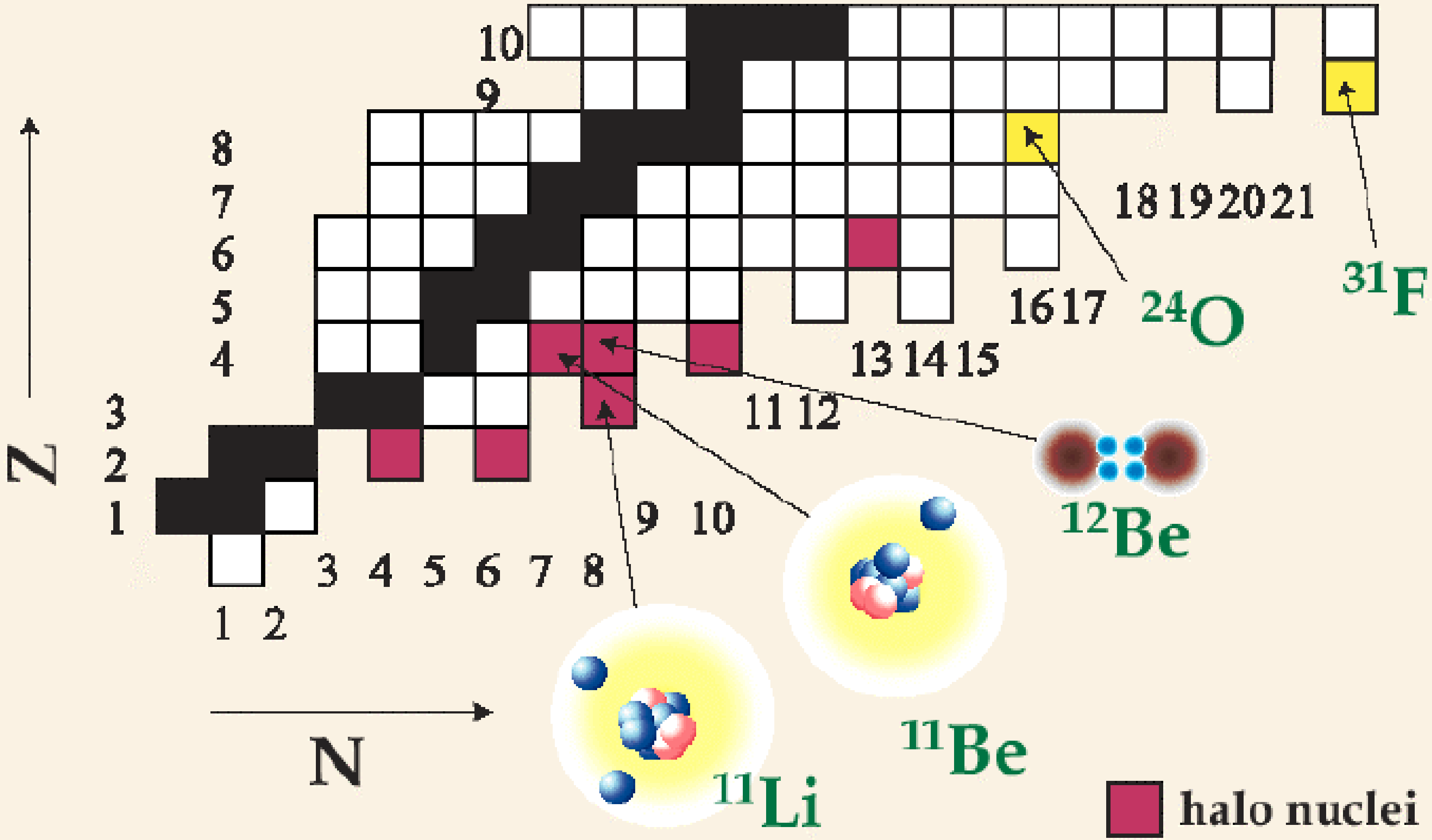
82
rp-process
r-process
Density Functional Theory
Selfconsistent Mean Field
A=10
A=12
A~60
Ab initio few-body calculations
No-Core Shell Model
0ħω Shell Model
Towards a unified description of the nucleus

Light drip line nuclei



MICROSCOPIC NUCLEAR-STRUCTURE THEORY

1. Start with the bare interactions among the nucleons

2. Calculate nuclear properties using nuclear many-body theory

Strong-Interaction Theory

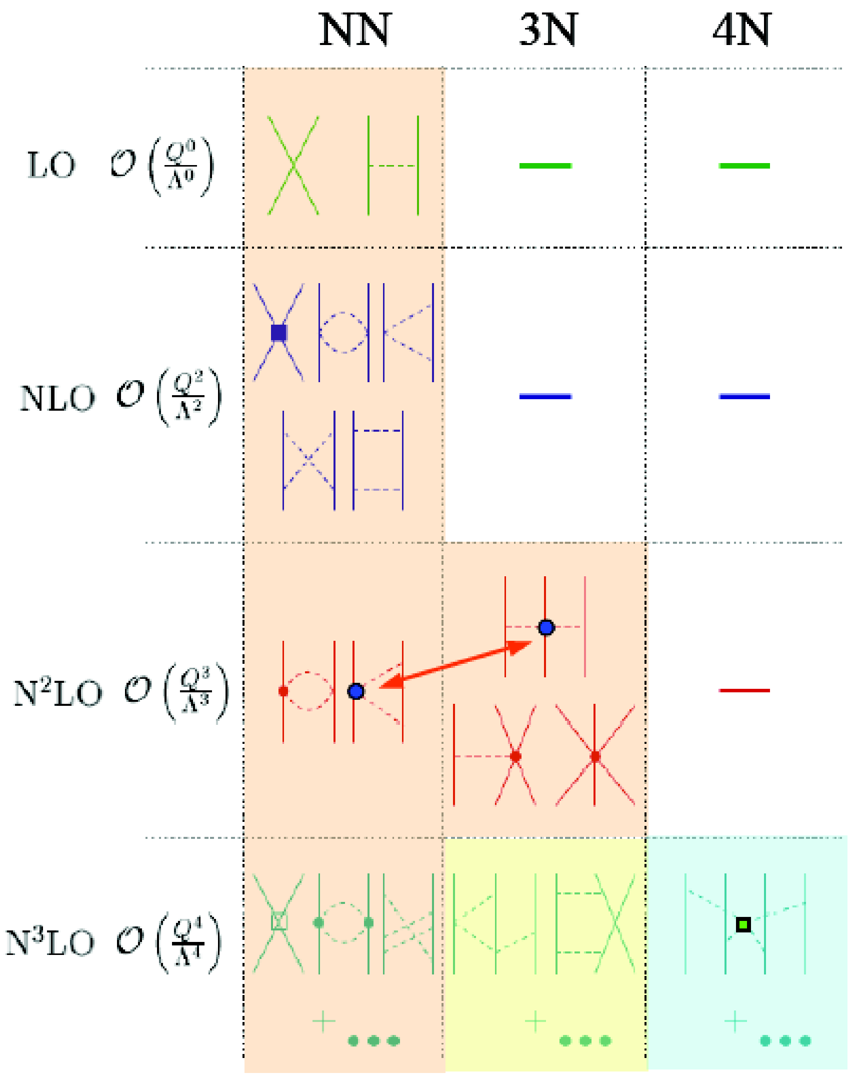
1. Strong Interaction ----> Standard Model

2. Standard Model -------> Quarks exchanging gluons

However, at the energy level of low-energy nuclear physics the quark degrees of freedom are frozen out in favor of nucleon and meson degrees of freedom.

Chiral effective field theory (EFT) for nuclear forces

Separation of scales: low momenta $\frac{1}{\lambda} = Q \ll \Lambda_b$ breakdown scale Λ_b

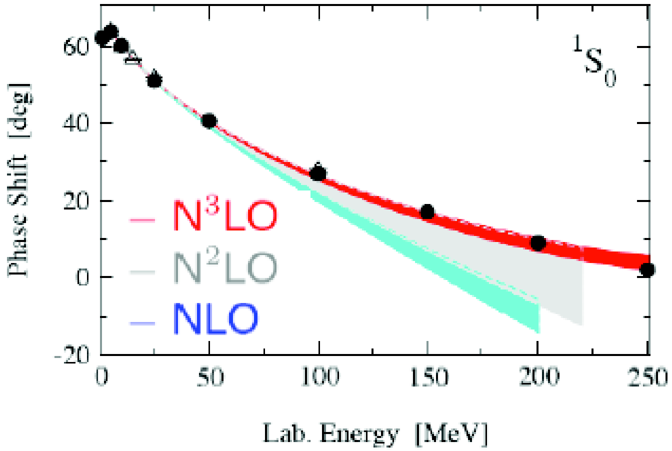


explains pheno hierarchy:
NN > 3N > 4N > …

NN-3N, πN, ππ, electro-weak,…
consistency

3N,4N: 2 new couplings to N³LO!

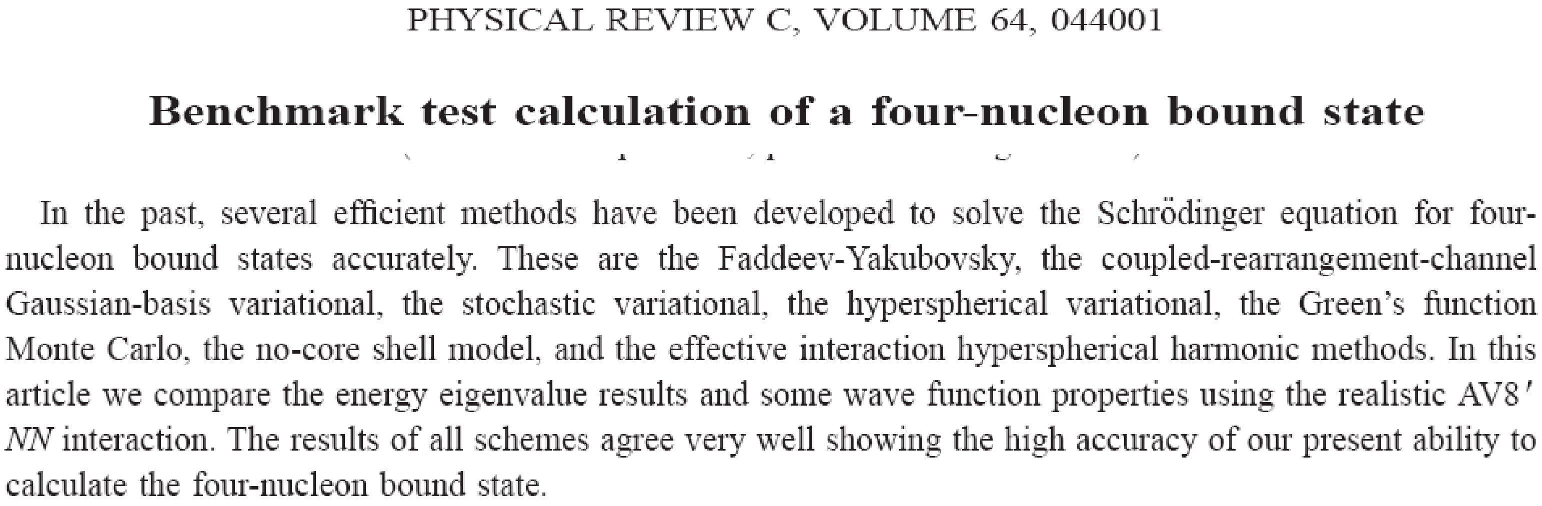
theoretical error estimates



Weinberg, van Kolck, Kaplan, Savage, Wise, Epelbaum, Meissner, Nogga, Machleidt,…

A. Schwenk

H. Kamada, *et al.*, Phys. Rev. C 64, 044001 (2001)



PHYSICAL REVIEW C, VOLUME 64, 044001

Benchmark test calculation of a four-nucleon bound state

In the past, several efficient methods have been developed to solve the Schrödinger equation for four-nucleon bound states accurately. These are the Faddeev-Yakubovsky, the coupled-rearrangement-channel Gaussian-basis variational, the stochastic variational, the hyperspherical variational, the Green's function Monte Carlo, the no-core shell model, and the effective interaction hyperspherical harmonic methods. In this article we compare the energy eigenvalue results and some wave function properties using the realistic AV8′ *NN* interaction. The results of all schemes agree very well showing the high accuracy of our present ability to calculate the four-nucleon bound state.

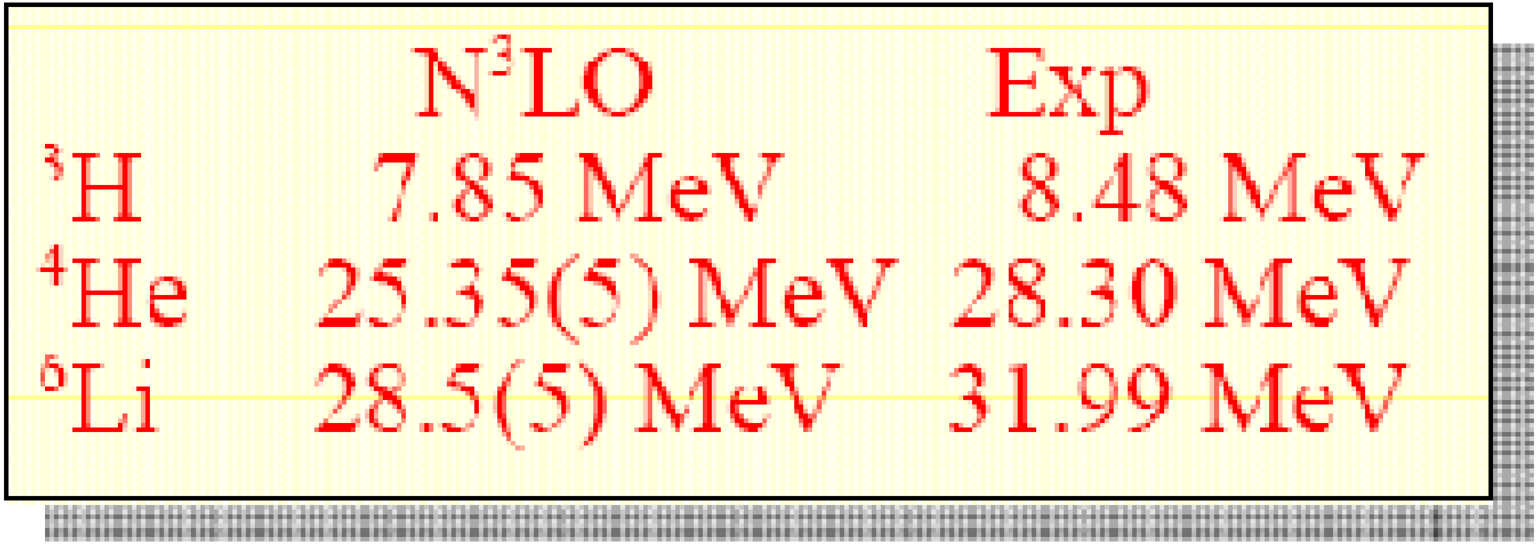
$BE_{th} \approx 25.91$ MeV

$BE_{exp} \approx 28.296$ MeV

I. Forces among nucleons

1. QCD ---> EFT ---> CPT --> Self-consistent nucleon interactions

2. Need NN and NNN and perhaps NNNN interactions



	N^3LO	Exp
^3H	7.85 MeV	8.48 MeV
^4He	25.35(5) MeV	28.30 MeV
^6Li	28.5(5) MeV	31.99 MeV

P. Navratil and E. Caurier, Phys. Rev. C 69, 014311 (2004)

MICROSCOPIC NUCLEAR-STRUCTURE THEORY

1. Start with the bare interactions among the nucleons
2. Calculate nuclear properties using nuclear many-body theory

Towards a unified description of the nucleus

The goal of nuclear structure theory:

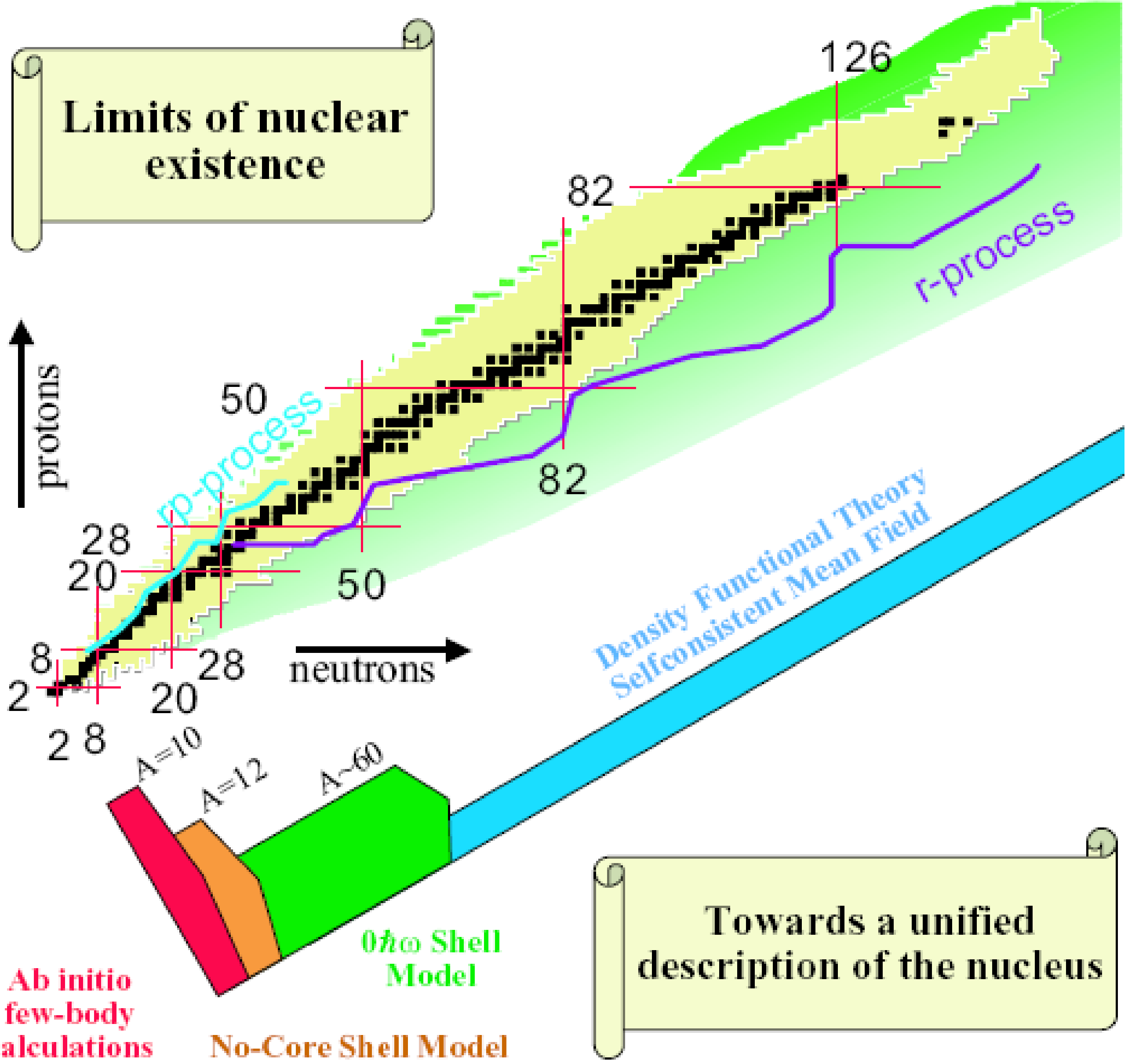
exact treatment of nuclei based on NN, NNN,... interactions

⇨ need to build a bridge between:

ab initio few-body & light nuclei calculations: $A \lesssim 24$

$0\hbar\Omega$ Shell Model calculations: $16 \leq A \leq 60$

Density Functional Theory calculations: $A \geq 60$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Many-Body Techniques for Solving the A-Nucleon Problem

1. Light Nuclei: *ab initio* approaches: s- and p-shell nuclei

Green's Function Monte Carlo (GFMC) (J. Carlson, et al.),
No-Core Shell Model (NCSM), Faddeev-Yakubovsky,
UCOM, V_low-k, SRG, Coupled Cluster (CC), ...

2. sd- and pf-shell nuclei:

NCSM, extended NCSM, Standard Shell Model (SSM), Coupled Cluster,
UCOM, Shell Model Monte Carlo (SMMC) (sign problem defeated?),
Monte Carlo Shell Model (MCSM) (Otsuka, et al.) ...

3. Heavier Nuclei:

Density Functional Theory (DFT) (SciDAC project: UNEDF); CC; Monte Carlo approaches, ...

$$H \Psi = E \Psi$$

We cannot, in general, solve the full problem in the complete Hilbert space, so we must truncate to a finite model space

$\Rightarrow$ We must use effective interactions and operators!

Effective Interactions

Except for approaches, such as GFMC, one usually needs to renormalize the NN interaction:

1. for the strong short-range correlations in the NN interaction

and

2. for the truncation of the Hilbert space.

There are two basic approaches to obtaining effective interactions:

1. Phenomenological

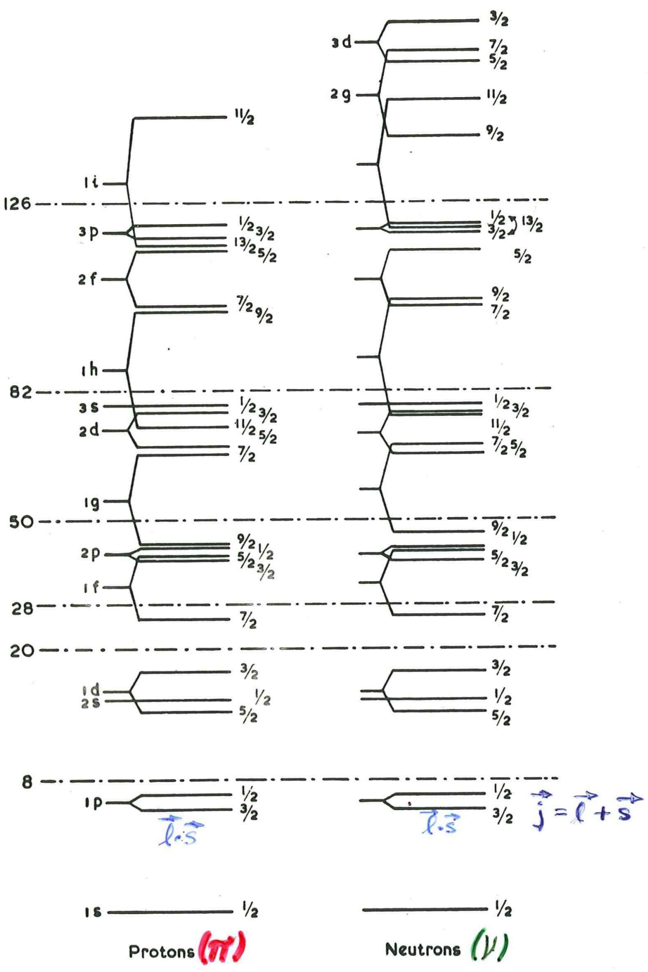
and

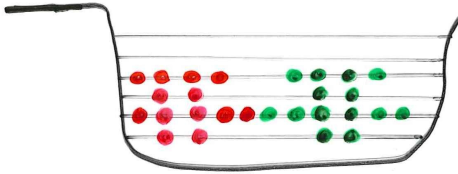
2. Microscopic

Standard Shell Model

Maria Goeppert-Mayer
J. Hans D. Jensen (1949)

Nobel Prize for Physics 1963





Mean Field

$$H=\sum_{i=1}^{A} t_i+\sum_{i<j}^{A} v_{ij}$$
$$= T + V$$
$$=(T+U^{sp})+(V-U^{sp})$$
$$= H_0^{sp}+\overline{V}\text{(residual interaction)}$$

Some current shell-model references

1. E. Caurier, G. Martinez-Pinedo, F. Nowacki, A. Poves, and A. P. Zuker, “The Shell Model as a Unified View of Nuclear Structure,” *Reviews of Modern Physics* **77**, 427 (2005)

2. B. A. Brown, “The Nuclear Shell Model towards the Drip Lines,” *Progress in Particle and Nuclear Physics* **47**, 517 (2001)

3. I. Talmi, “Fifty Years of the Shell Model-The Quest for the Effective Interaction,” *Advances in Nuclear Physics*, Vol. **27**, ed. J. W. Negele and E. Vogt (Plenum, NY, 2003)

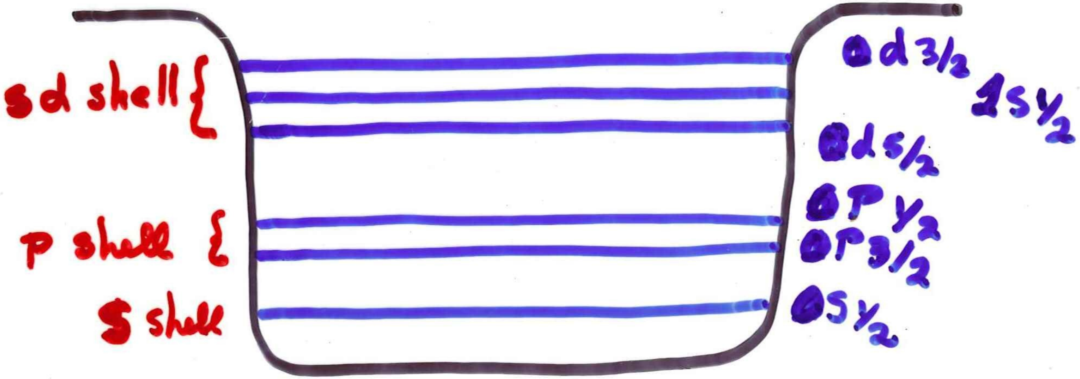
4. B. R. B., “Effective Operators in Shell-Model Calculations,” 10th Indian Summer School of Nuclear Physics:Theory of Many-Fermion Systems, *Czechoslovak Journal of Physics* **49**, 1 (1999)

PHENOMENOLOGICAL EFFECTIVE INTERACTIONS

1. Usually constructed for a single major shell
2. Take experimental single-particle energies
3. Determine two-body matrix elements

$$\langle (j_1 j_2) J T | V | (j_3 j_4) J T \rangle$$

by a least-squares fit to some subset of the experimental data



No Core Shell Model

"*Ab Initio*" approach to microscopic nuclear structure calculations, in which all A nucleons are treated as being active.

Want to solve the A-body Schrödinger equation

$$H_A \Psi^A = E_A \Psi^A$$

No Core Shell Model (NCSM)

Selected References:

1. Topical Review: P. Navratil, S. Quaglioni, I. Stetcu, and BRB, J. Phys. G: Nucl. Part. Phys. **36**, 083101 (2009)

2. P. Navratil, J.P. Vary and BRB, Phys. Rev. C **62**, 054311 (2000) and Phys. Rev. Lett. 88, 152502 (2000)

3. P. Navratil and BRB, Phys. Rev. C **54**, 2986 (1996) and Phys. Rev. C 57, 562 (1998)

4. BRB, P. Navratil and J.P. Vary, Nuclear Physics News International, **21**, No. **2**, 5 (2011). Review article.

From few-body to many-body

Ab initio
No Core Shell Model

Realistic NN & NNN forces

Effective interactions in cluster approximation

Diagonalization of many- body Hamiltonian

Many-body experimental data

No-Core Shell-Model Approach

Start with the purely intrinsic Hamiltonian

$$H_A = T_{rel} + \mathcal{V} = \frac{1}{A}\sum_{i<j=1}^{A}\frac{(\vec{p}_i - \vec{p}_j)^2}{2m} + \sum_{i<j=1}^{A} V_{NN} \left(+ \sum_{i<j<k}^{A} V_{ijk}^{3b} \right)$$

Note: There are no phenomenological s.p. energies!

Can use any NN potentials

Coordinate space: Argonne V8’, AV18
Nijmegen I, II

Momentum space: CD Bonn, EFT Idaho

No-Core Shell-Model Approach

Next, add CM harmonic-oscillator Hamiltonian

$$H_{CM}^{HO} = \frac{\vec{P}^{\,2}}{2Am} + \frac{1}{2}Am\Omega^2\vec{R}^{\,2}\,; \quad \vec{R} = \frac{1}{A}\sum_{i=1}^{A}\vec{r}_i\,, \quad \vec{P} = Am\dot{\vec{R}}$$

To H$_A$, yielding

$$H_A^{\Omega} = \sum_{i=1}^{A}\left[\frac{\vec{p}_i^{\,2}}{2m} + \frac{1}{2}m\Omega^2\vec{r}_i^{\,2}\right] + \underbrace{\sum_{i<j=1}^{A}\left[V_{NN}(\vec{r}_i - \vec{r}_j) - \frac{m\Omega^2}{2A}(\vec{r}_i - \vec{r}_j)^2\right]}_{V_{ij}}$$

Defines a basis (*i.e.* HO) for evaluating V_{ij}

$$H\Psi = E\Psi$$

We cannot, in general, solve the full problem in the complete Hilbert space, so we must truncate to a finite model space

⇒ We must use effective interactions and operators!

Effective Interaction

Must truncate to a finite model space V_{ij} --> $V_{ij}^{effective}$

In general, V_{ij}^{eff} is an *A*-body interaction

We want to make an *a*-body cluster approximation

$$\mathcal{H} = \mathcal{H}^{(1)} + \mathcal{H}^{(A)} \quad \underset{a < A}{\gtrapprox} \quad \mathcal{H}^{(1)} + \mathcal{H}^{(a)}$$

$H\Psi_\alpha = E_\alpha\Psi_\alpha$ where $H = \sum_{i=1}^{A} t_i + \sum_{i\leq j}^{A} v_{ij}.$

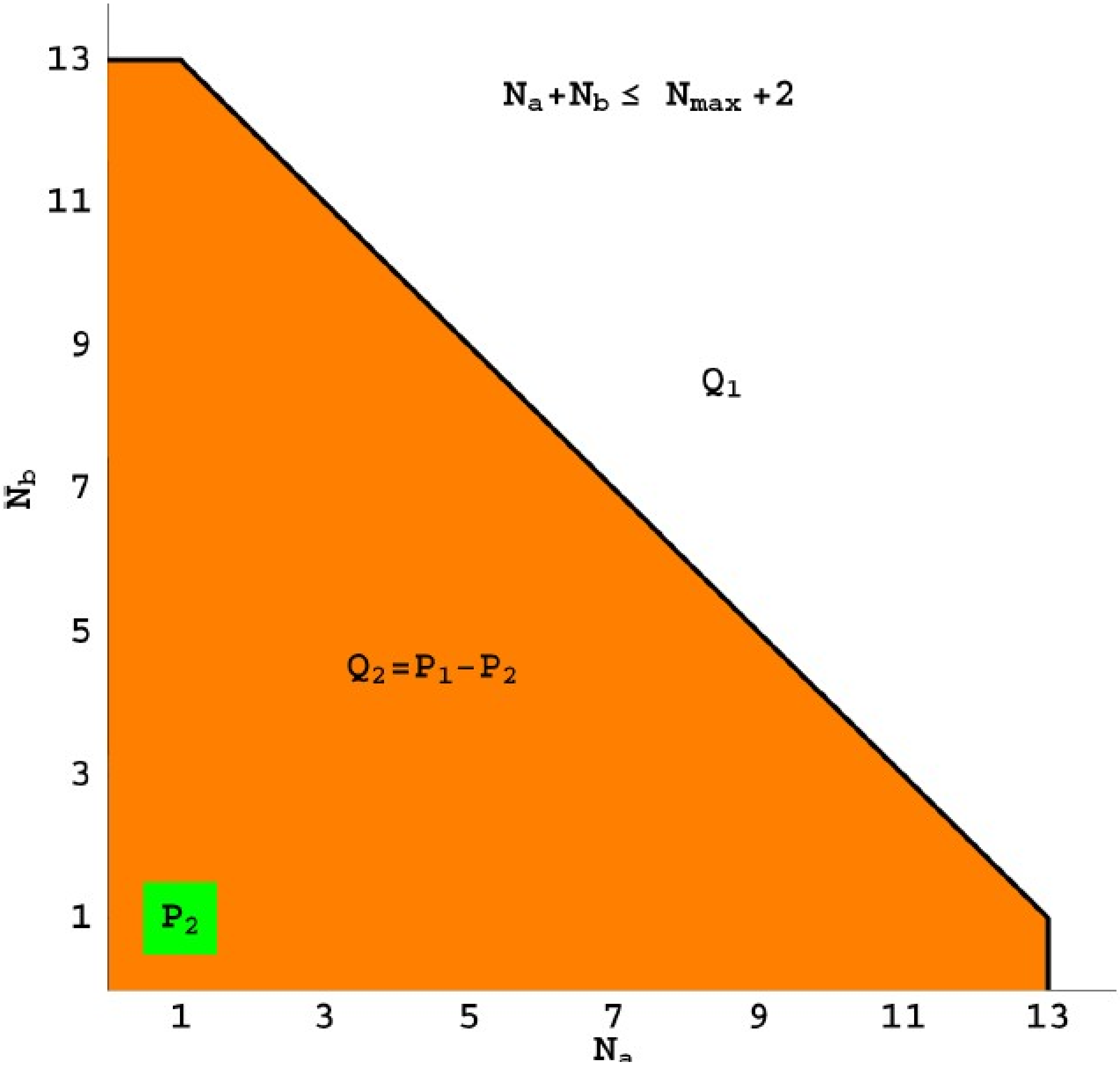
$$\mathcal{H}\Phi_\beta = E_\beta\Phi_\beta$$

$$\Phi_\beta = P\Psi_\beta$$

P is a projection operator from S into $\mathcal{S}$

$$< \tilde{\Phi}_\gamma|\Phi_\beta >= \delta_{\gamma\beta}$$

$$\mathcal{H} = \sum_{\beta\epsilon\mathcal{S}} |\Phi_\beta > E_\beta < \tilde{\Phi}_\beta|$$


$N_a + N_b \leq N_{max} + 2$
Q_1
$Q_2 = P_1 - P_2$
P_2
N_b
N_a
1
3
5
7
9
11
13
1
3
5
7
9
11
13

Effective Hamiltonian for NCSM

Solving $\boxed{H^{\Omega}_{A,\,a=2}\Psi_{a=2} = E^{\Omega}_{A,\,a=2}\Psi_{a=2}}$ in “infinite space” 2n+l = 450
relative coordinates

P + Q = 1; P – model space; Q – excluded space;

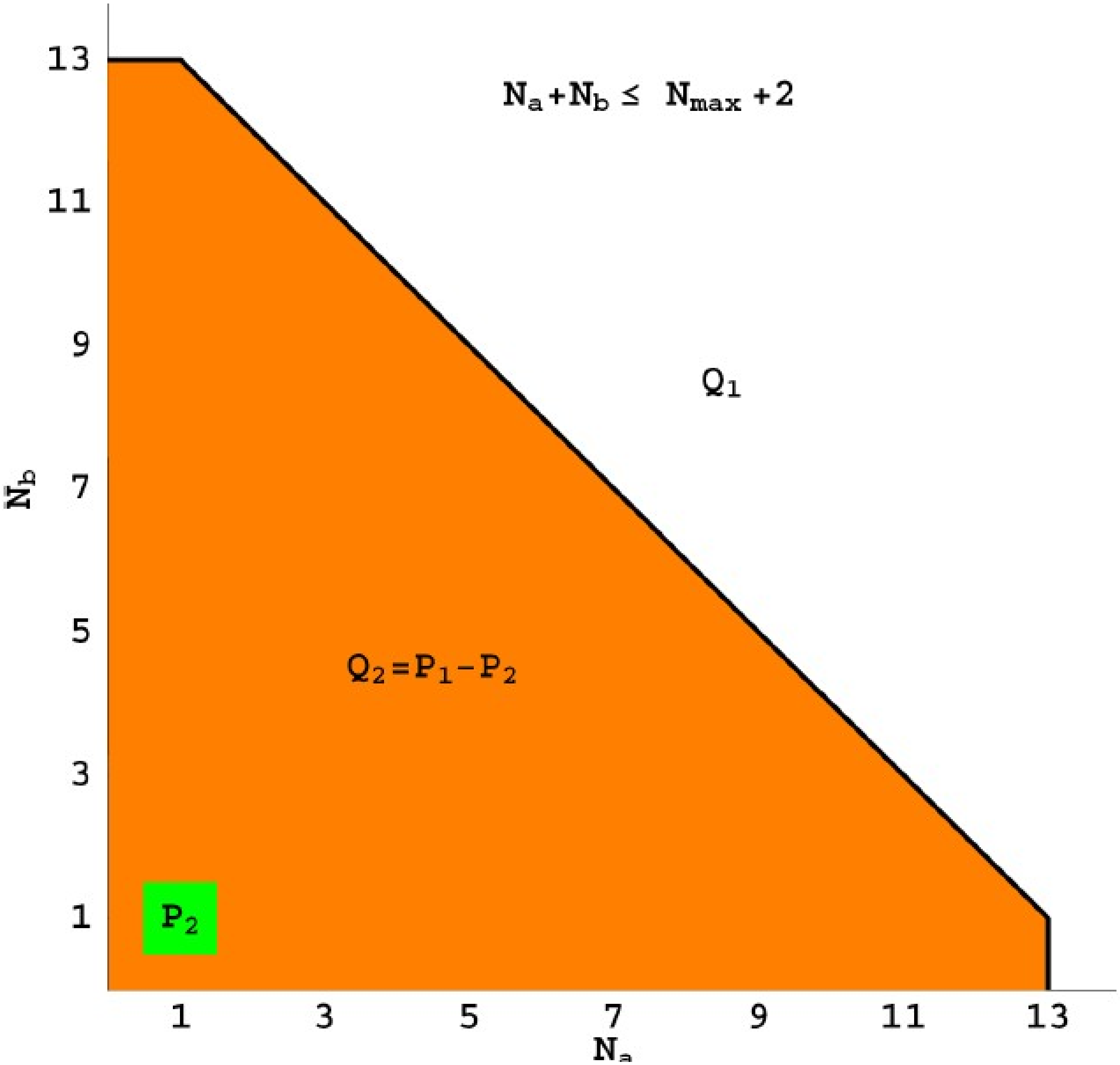
$$\boxed{E^{\Omega}_{A,2} = U_2 H^{\Omega}_{A,2} U_2^{\dagger}} \qquad U_2 = \begin{pmatrix} \boxed{U_{2,P}} & U_{2,PQ} \\ U_{2,QP} & U_{2,Q} \end{pmatrix} \qquad E^{\Omega}_{A,2} = \begin{pmatrix} \boxed{E^{\Omega}_{A,2,P}} & 0 \\ 0 & E^{\Omega}_{A,2,Q} \end{pmatrix}$$

$$\boxed{H^{N_{\max},\Omega,\mathrm{eff}}_{A,2} = \frac{U^{\dagger}_{2,P}}{\sqrt{U^{\dagger}_{2,P}U_{2,P}}} E^{\Omega}_{A,2,P} \frac{U_{2,P}}{\sqrt{U^{\dagger}_{2,P}U_{2,P}}}}$$

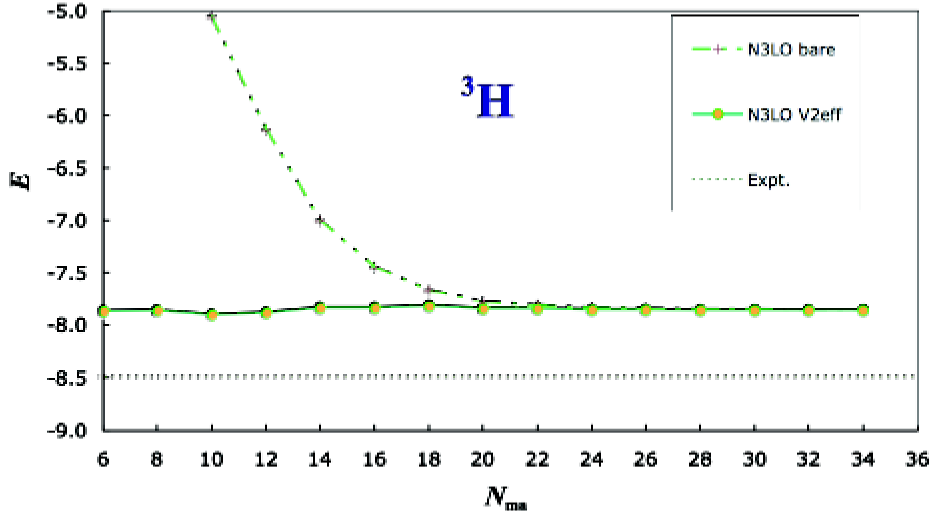
Two ways of convergence:

1) For P → 1 and fixed a: $H^{\mathrm{eff}}_{A,a=2} \rightarrow H_A$

2) For a → A and fixed P: $H^{\mathrm{eff}}_{A,a} \rightarrow H_A$

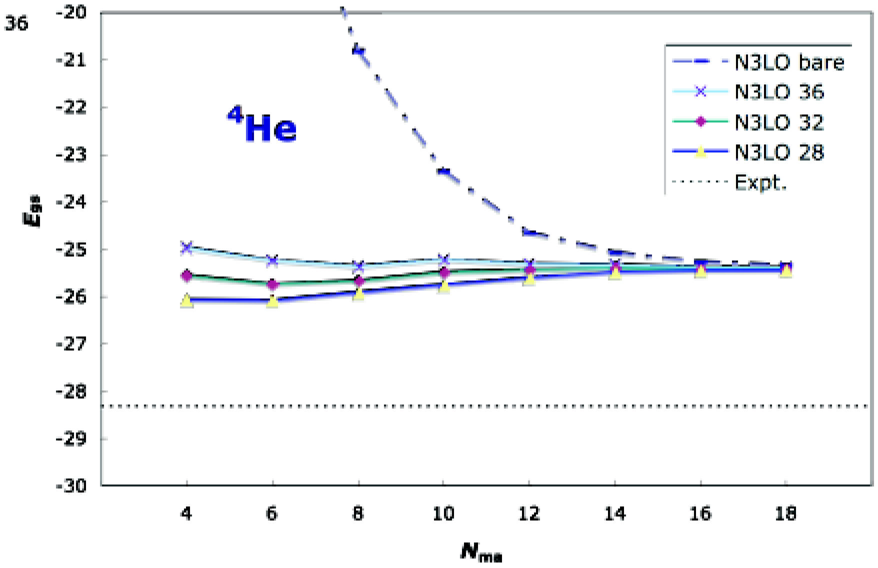

$N_a+N_b \leq N_{max}+2$
Q_1
$Q_2=P_1-P_2$
P_2
13
11
9
7
5
3
1
N_b
1
3
5
7
9
11
13
N_a

- NCSM convergence test
  - Comparison to other methods

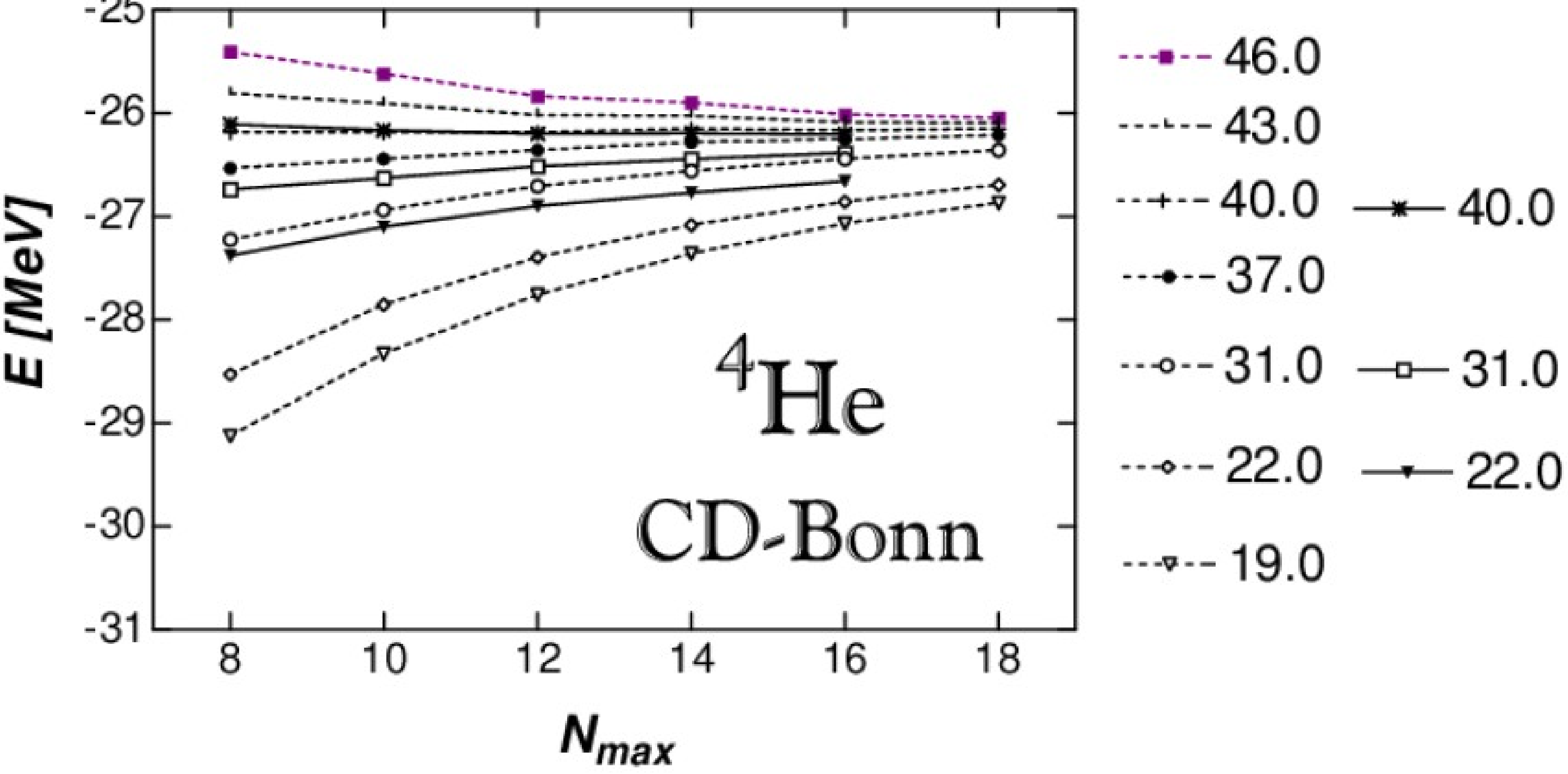


N³LO NN	NCSM	FY	HH
³H	7.852(5)	7.854	7.854
⁴He	25.39(1)	25.37	25.38

- ➢Short-range correlations ⇒ effective interaction
- ➢Medium-range correlations ⇒ multi-$h\Omega$ model space
- ➢Dependence on
  - ▪size of the model space (N_{max})
  - ▪HO frequency ($h\Omega$)
- ➢Not a variational calculation
- ➢Convergence OK
- ➢NN interaction insufficient to reproduce experiment



P. Navratil, INT Seminar, November 13, 2007, online


-25
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E [MeV]
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N_max
^{4}He
CD-Bonn
46.0
43.0
40.0
40.0
37.0
31.0
31.0
22.0
22.0
19.0

H. Kamada, *et al.*, Phys. Rev. C 64, 044011 (2001)

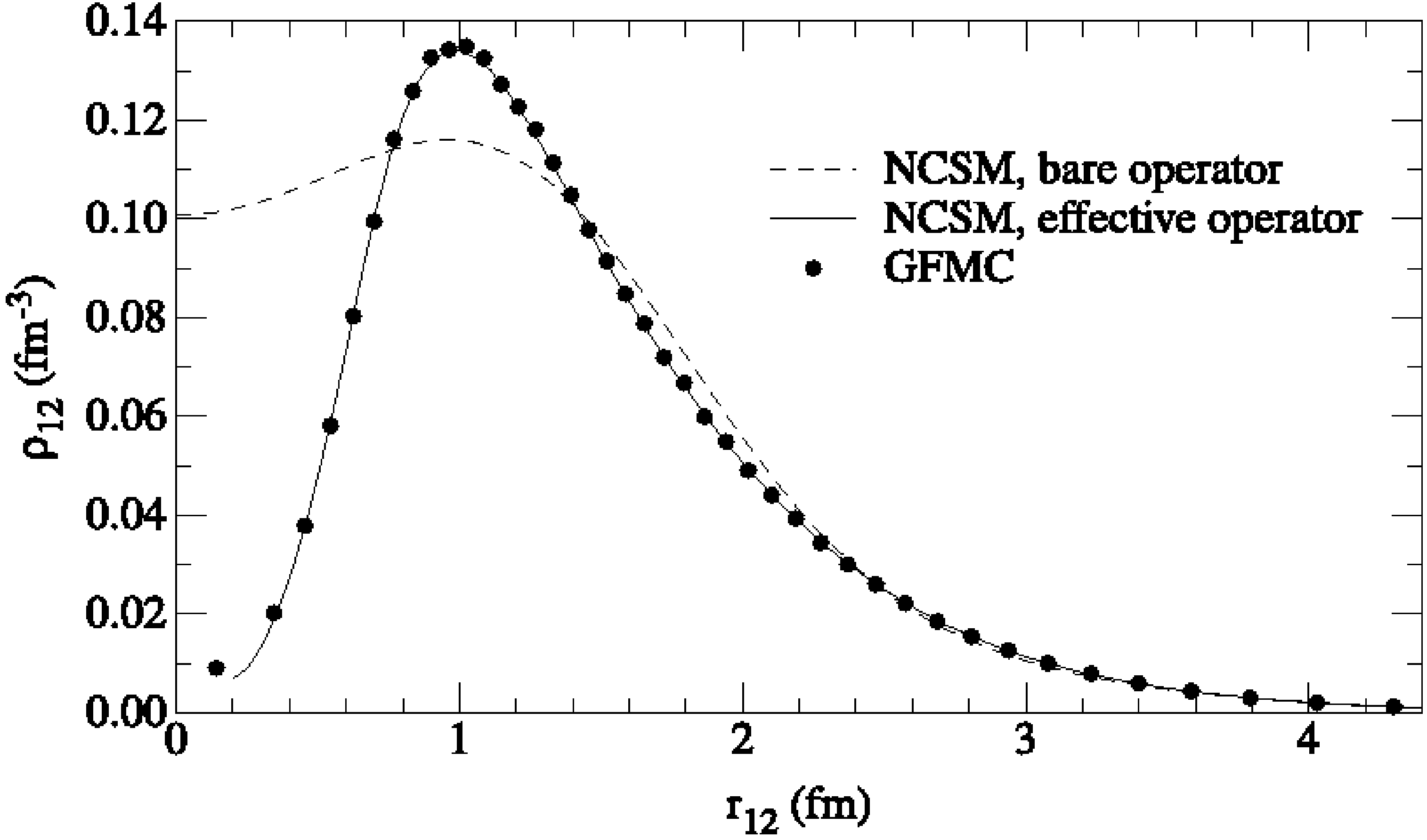
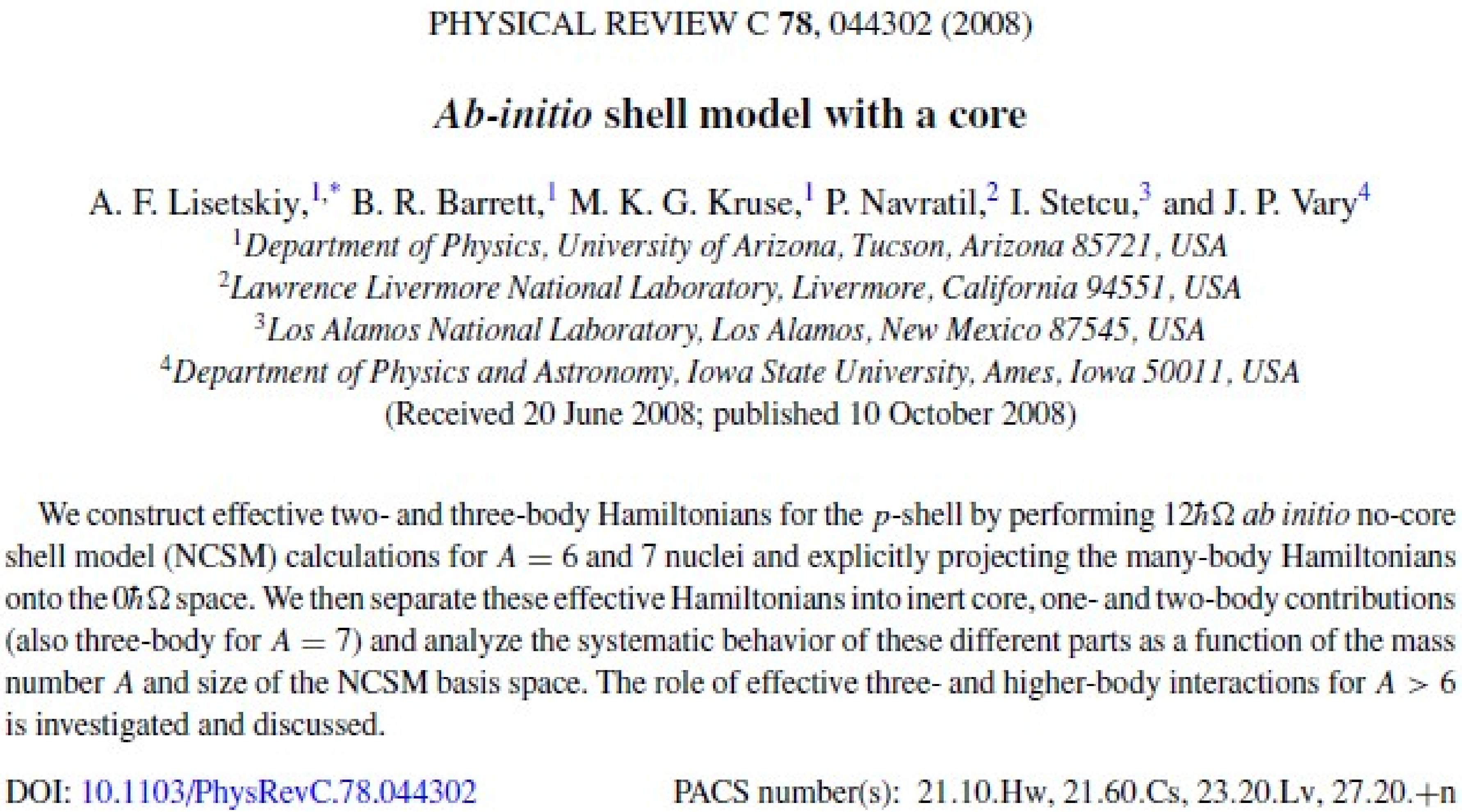


Figure 2. *NCSM and GFMC NN pair density in ^{4}He.*



PHYSICAL REVIEW C **78**, 044302 (2008)

Ab-initio shell model with a core

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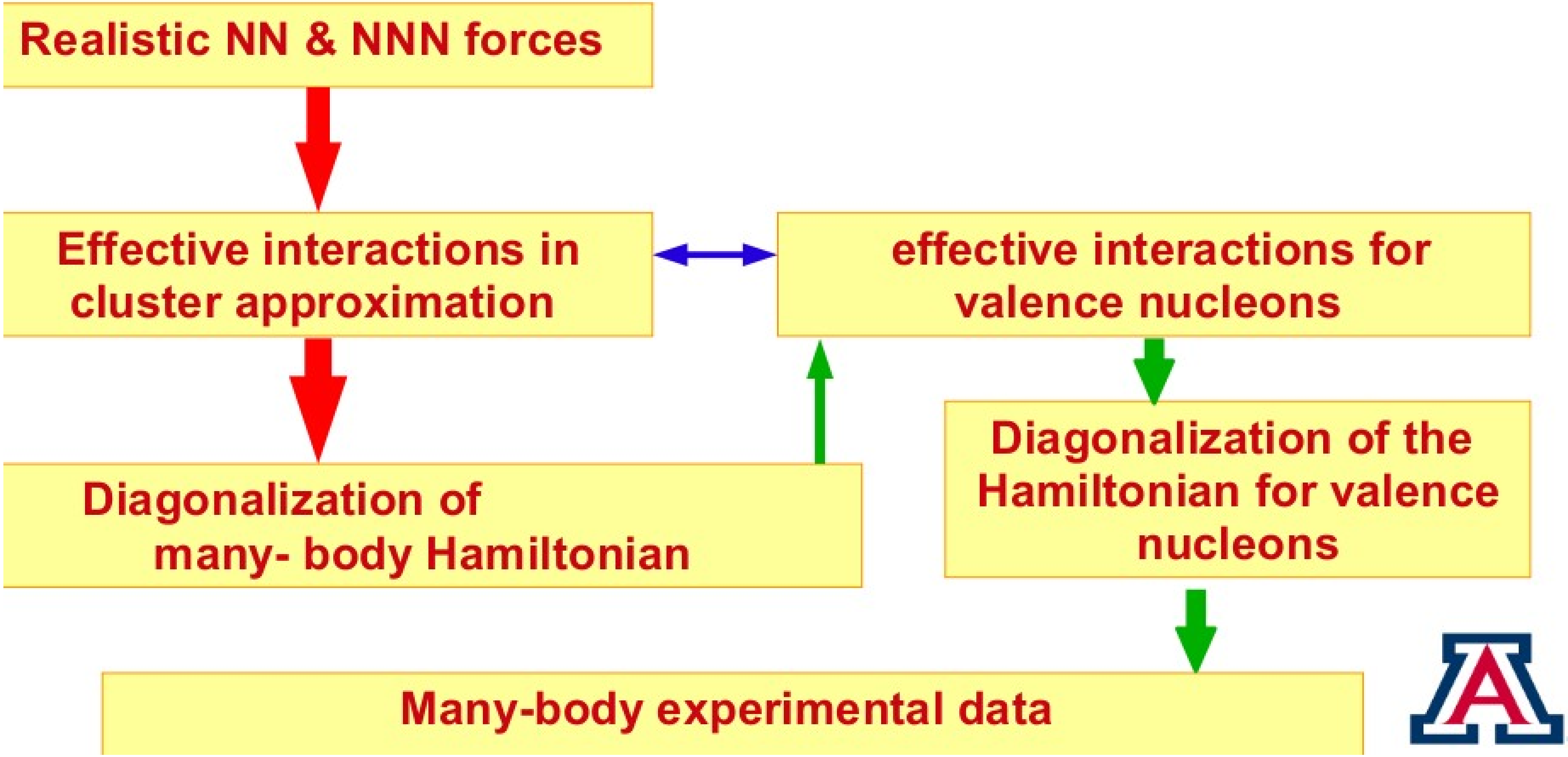
We construct effective two- and three-body Hamiltonians for the p-shell by performing $12\hbar\Omega$ *ab initio* no-core shell model (NCSM) calculations for $A = 6$ and 7 nuclei and explicitly projecting the many-body Hamiltonians onto the $0\hbar\Omega$ space. We then separate these effective Hamiltonians into inert core, one- and two-body contributions (also three-body for $A = 7$) and analyze the systematic behavior of these different parts as a function of the mass number A and size of the NCSM basis space. The role of effective three- and higher-body interactions for $A > 6$ is investigated and discussed.

DOI: 10.1103/PhysRevC.78.044302 PACS number(s): 21.10.Hw, 21.60.Cs, 23.20.Lv, 27.20.+n

From few-body to many-body

Ab initio
No Core Shell Model

Core Shell Model



Realistic NN & NNN forces

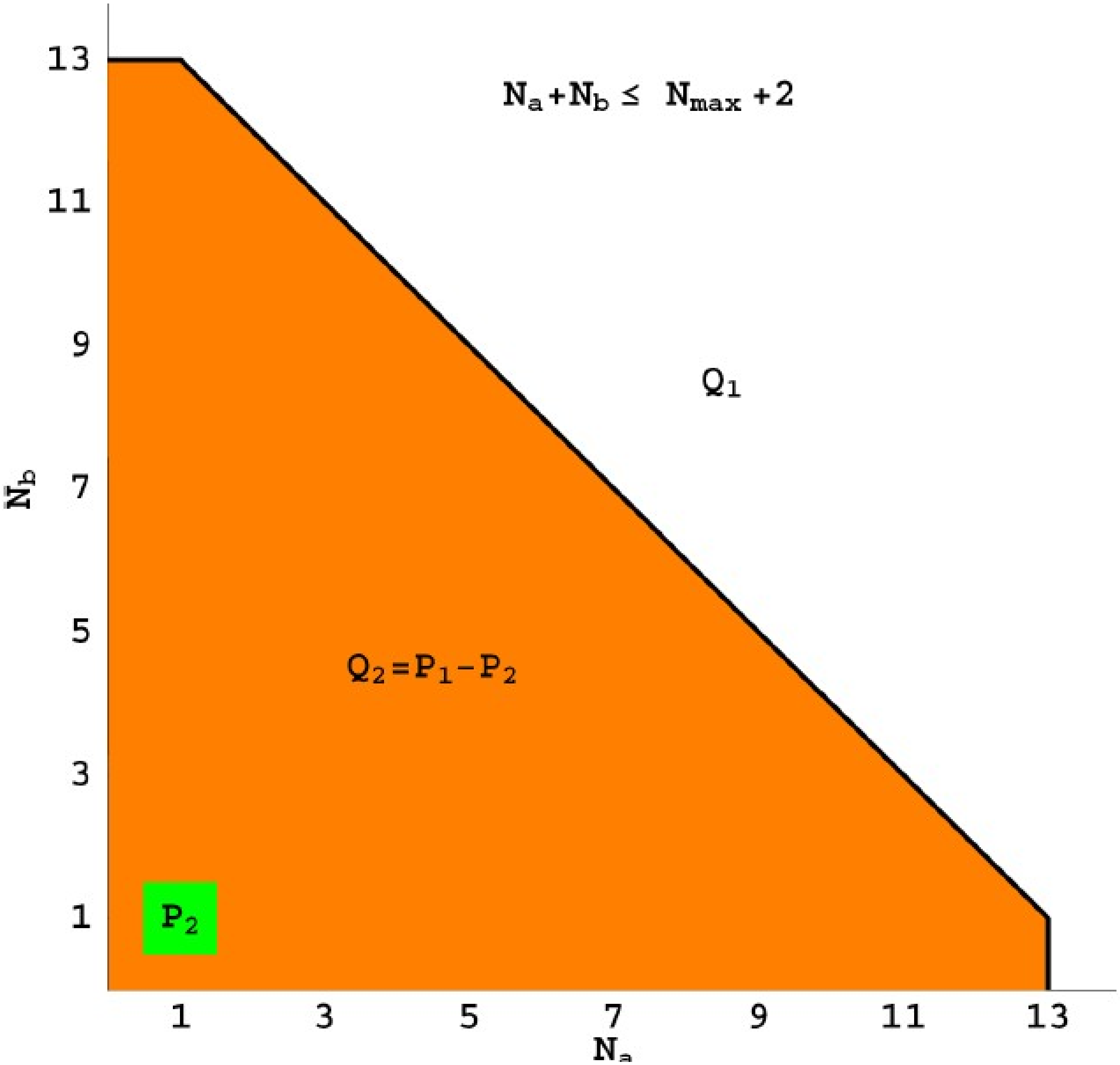
Effective interactions in cluster approximation

effective interactions for valence nucleons

Diagonalization of many- body Hamiltonian

Diagonalization of the Hamiltonian for valence nucleons

Many-body experimental data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N_a
$N_a+N_b \leq N_{max}+2$
Q_1
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P_2

No Core Shell Model (NCSM):

Advantages:

1. Applies to all nuclei using any NN (+NNN) potential
2. Obtain wave functions and all excited states/low-lying states are stable
3. Obtain detailed spectroscopic information
4. Exact treatment of the spurious center of mass motion

Limitations: some fundamental/some computational

1. Difficult to go beyond A=20 due to rapid growth of computational space
2. Questions related to size extensivity if wave functions are truncated
3. Long range operators more difficult to handle than short range operators

Some other methods for producing effective NN interactions

1. Methods for making bare NN interactions “softer”:

   a.) V_low-k NN interactions

   b.) Similarity Renormalization Group (SRG)

2. NCSM in an Effective Field Theory Framework

A. Schwenk

Tjon line

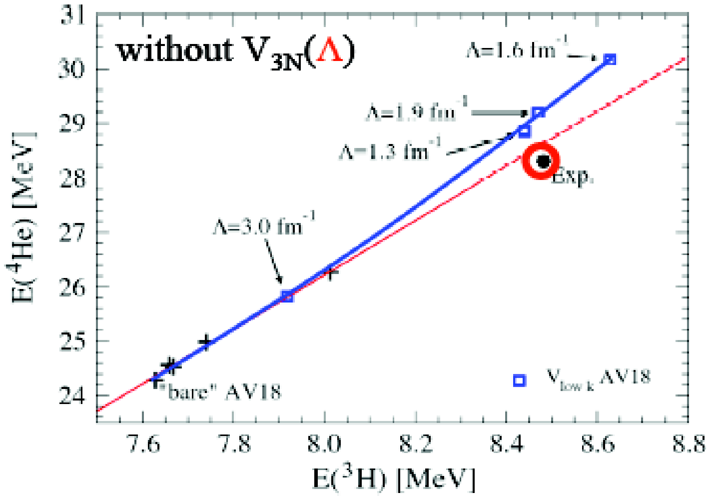
$V_{\mathrm{low}\,k}(\Lambda)$ defines class of NN interactions with cutoff-independent low-energy NN observables

cutoff variation estimates errors due to neglected parts in $H(\Lambda)$

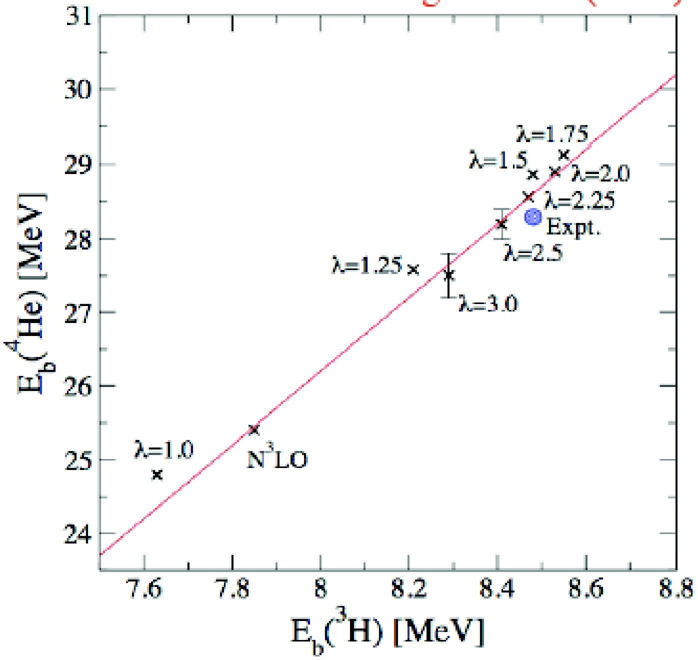
Cutoff dependence explains Tjon line, 3N required by renormalization

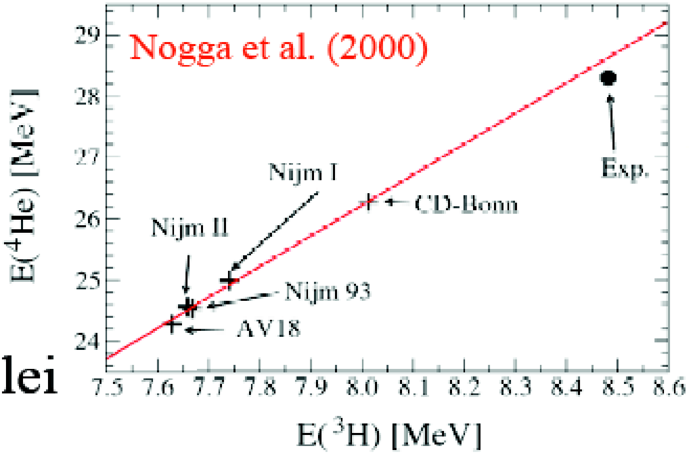
Experiment breaks from line ⇒ 3N

Nogga, Bogner, AS (2004)



SRG interactions: Bogner et al. (2007)





Tjon lines in p-shell nuclei

Bogner et al. (2007)

SIMILARITY RENORMALIZATION GROUP (SRG)

The SRG is a nonperturbative approach that performs a continuous sequence of unitary transformations on a Hamiltonian H

$$H_s = U(s) H U^\dagger(s)$$

yielding the generating class of equations,

$$\frac{d}{ds} H_s = [\eta_s, H_s] = [[C, H_s], H_s]$$

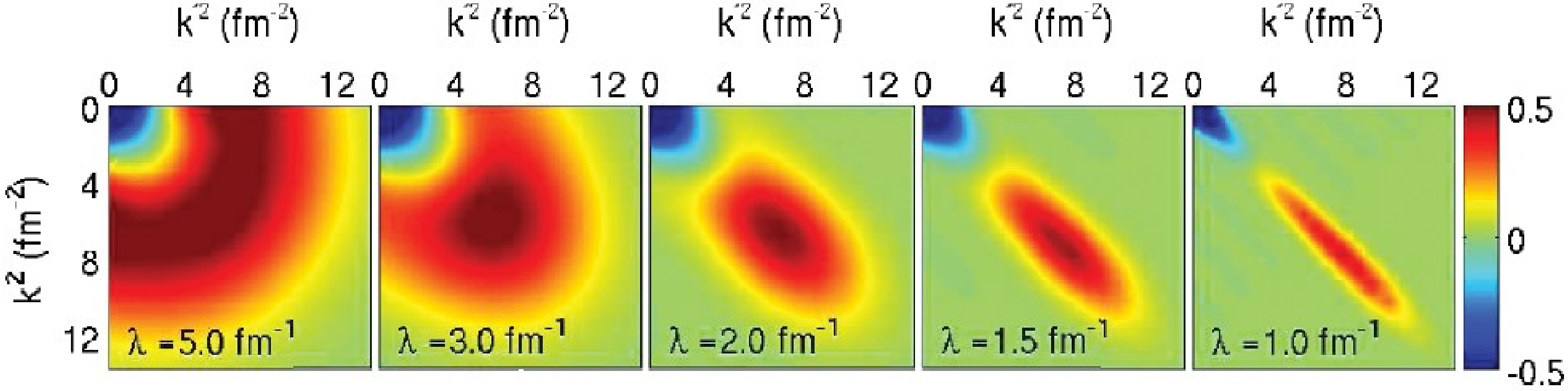
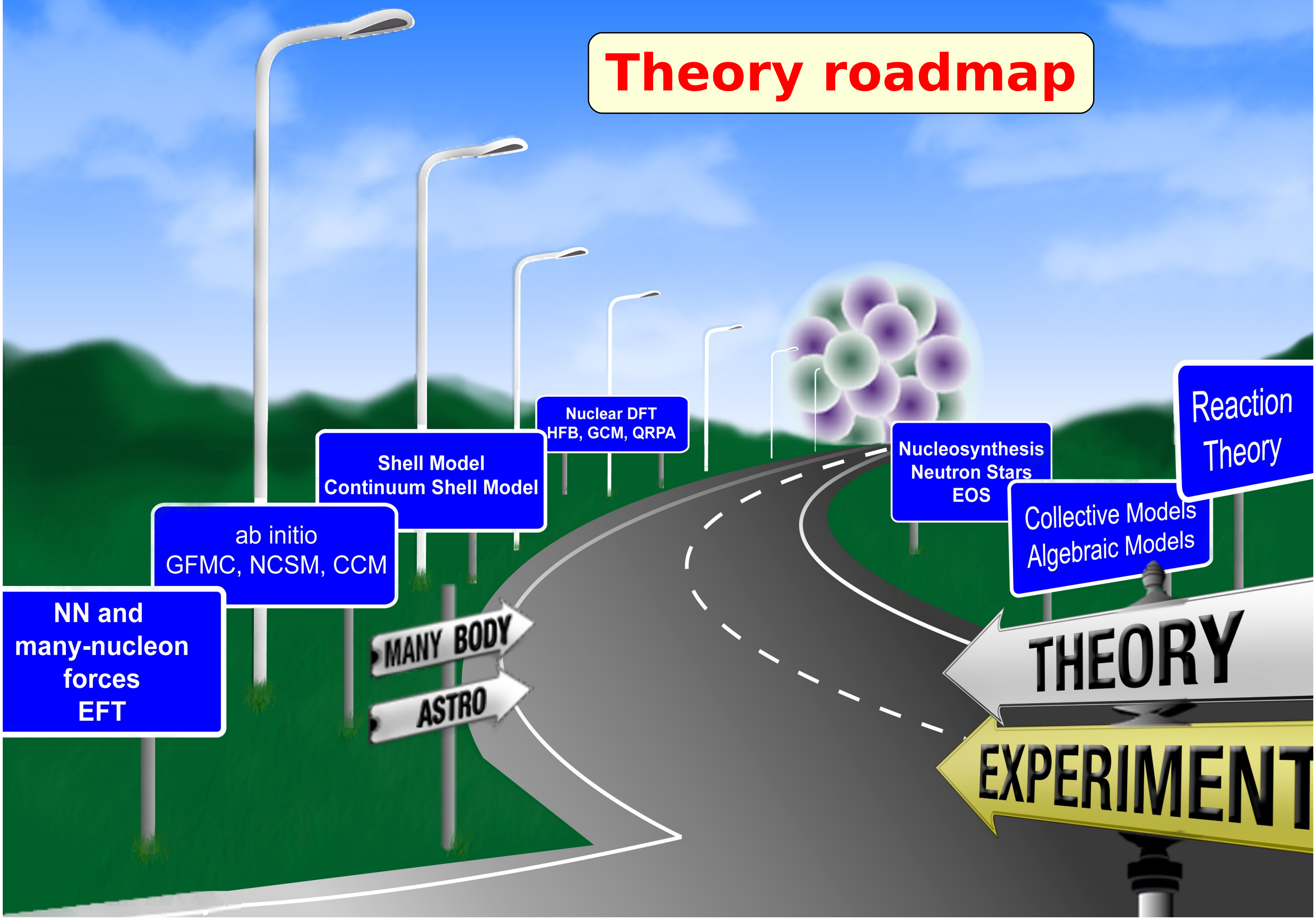


Figure 2. *Illustration of how the SRG procedure [15] weakens the strong off-diagonal couplings of an NN potential in momentum space as the flow proceeds to smaller values of λ (left to right panels).*

SOME REMAINING CHALLENGES

1. Understanding the fundamental interactions among the nucleons in terms of QCD, e.g., NN, NNN, ...
2. Determination of the mean field (the monopole effect).
3. Microscopic calculations of medium- to heavy-mass nuclei:
   - a.) How to use the advances for light nuclei to develop techniques for heavier nuclei.
   - b.) Building in more correlations among the nucleons in small model spaces, e.g., effective interactions for heavier nuclei.
4. Extensions of these microscopic advances for nuclear structure to nuclear reactions.

Theory roadmap



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PROCEEDINGS
OF THE
INTERNATIONAL CONFERENCE
ON
NUCLEAR STRUCTURE

KINGSTON, CANADA

AUGUST 29 - SEPTEMBER 3
1960

EDITED BY

D.A. BROMLEY
E.W. VOGT

UNIVERSITY OF TORONTO PRESS: TORONTO
NORTH HOLLAND PUBLISHING COMPANY: AMSTERDAM

1960

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how matter came about, and they add a great deal of significance and importance to nuclear physics and to certain experiments in nuclear physics which would have only little importance to the problems we have discussed here. Perhaps in the next conference we should have a session where we discuss these things; it is not enough just to go to Mr. Cameron or Mr. Fowler and ask him what shall we measure, we ought to know why we do it.

The second and last point I would like to raise is this. To round up the conference I come back to the first remark of Peierls, when he opened up the conference and asked the question, why are we interested in nuclear structure. May I add my own little verse to this. I have heard many people say that Nuclear Structure is not a fundamental problem, the real thing is high energy physics; the object of nuclear structure is after all nothing else but solving a Schroedinger equation for A particles. I strongly disagree with this point of view. The discovery and the understanding of phenomena hidden in a many-body problem can be a task of fundamental importance, if the object itself is of central interest.

Physics inquires into the nature of things. The nucleus, our nucleus, is an essential part of nature, it is the centre of the atom. It is not just a little phenomenon, it is the most prominent constituent of matter. The understanding of the phenomena occurring in this nucleus is therefore of paramount importance. Hence Nuclear Physics is an essential part of physics. I found out that some theorists, both in the east and in the west, consider the only thing worth doing is elementary particle physics. Experimentalists usually don't say so because they work with real matter and hence they know that the nucleus is an important thing. These theorists, however, worship the theory of elementary particles, a theory which in fact doesn't even exist. They knock their heads daily against a wall of dispersion-relations, Mandelstam representations and the like. Let them do it. After all the proton and the meson are also an important part of nature. In fact we should give them all the moral support they need. They are a brave lot who fight a very difficult fight and some day they will find the theory. But don't let yourself be talked into believing that the nucleus is not interesting. It is so small and it has so few parts and still it shows a tremendous variety of phenomena. Its investigation requires the whole arsenal of presently available experimental techniques and its understanding makes use of almost all branches of theoretical physics. What a marvellous invention! It is worth devoting a lifetime to it.