The No Core Gamow Shell Model: Including the Continuum in the NCSM

Bruce R. Barrett
University of Arizona, Tucson

THE UNIVERSITY OF ARIZONA.
Arizona's First University.

COLLABORATORS

Christian Forssen, Chalmers U. of Tech., Goteborg, Sweden

Nicolas Michel, NSCL, Michigan State University

George Papadimitriou, Lawrence Livermore National Lab

Marek Ploszajczak, GANIL, Caen, France

Jimmy Rotureau, NSCL, Michigan State University

OUTLINE

I. Introduction: NCSM to the NCGSM

II. NCGSM Formalism

III. NCGSM: Applications to Light Nuclei

IV. Summary and Outlook

I. Introduction: NCSM to the NCGSM

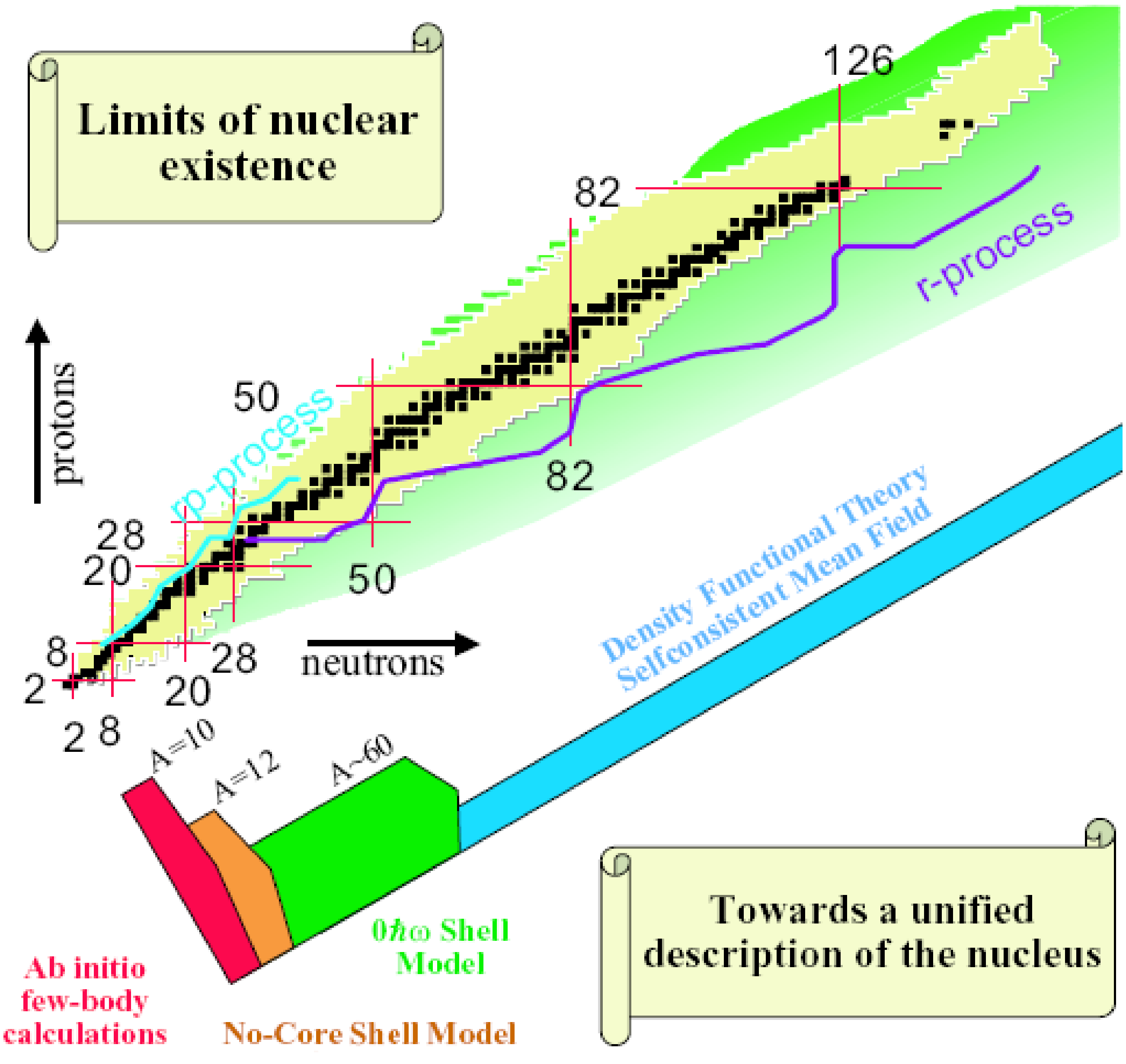
No Core Shell Model

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

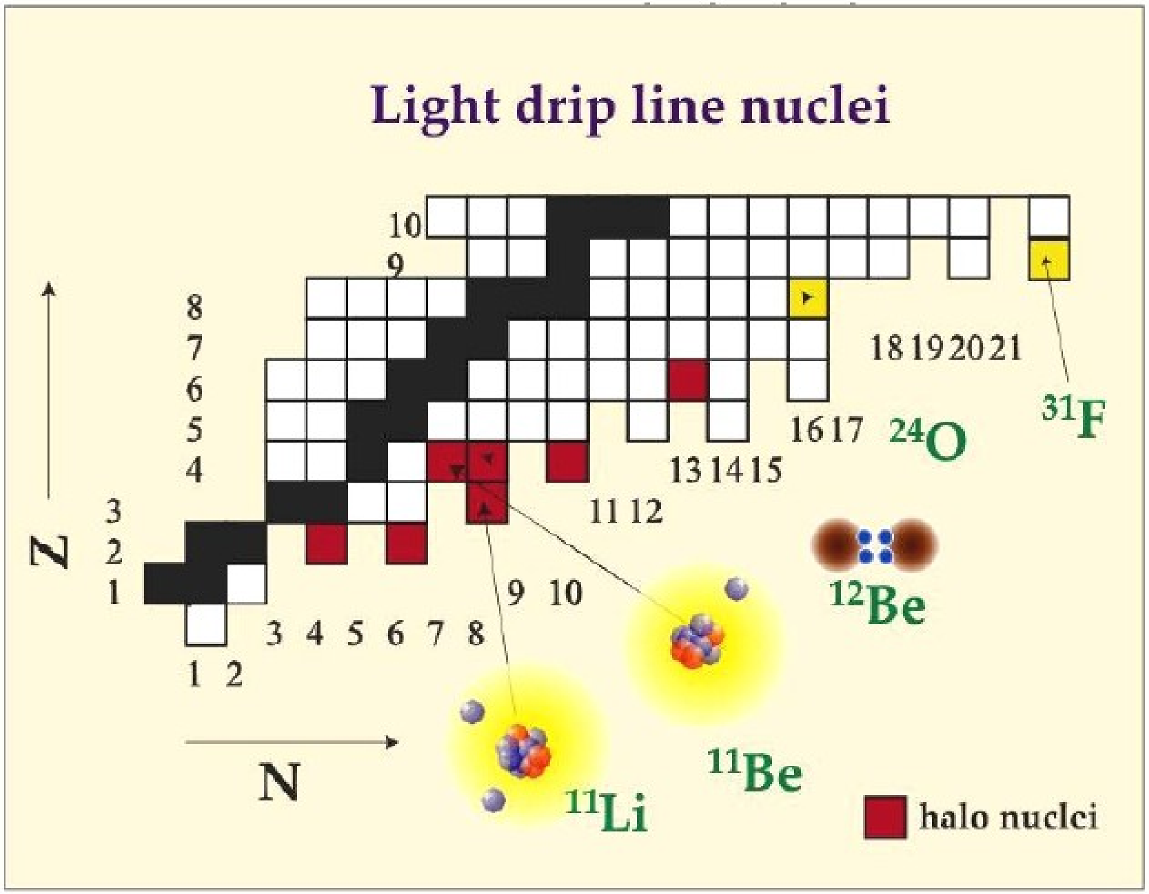
Want to solve the A-body Schrödinger equation

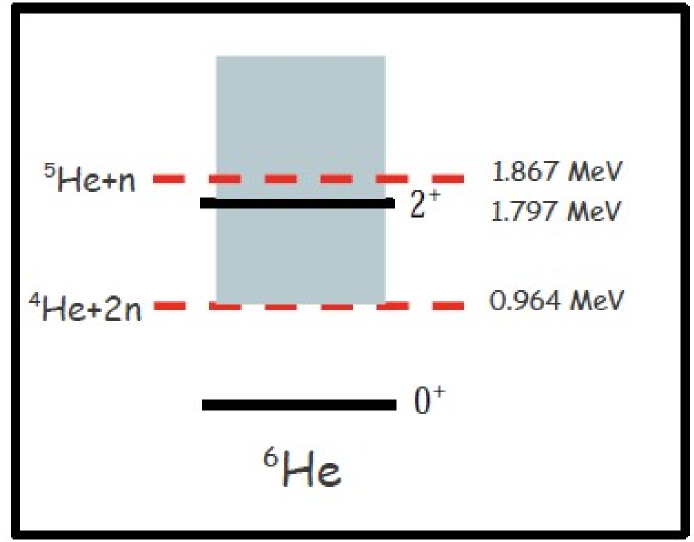
$$H_A \Psi^A = E_A \Psi^A$$

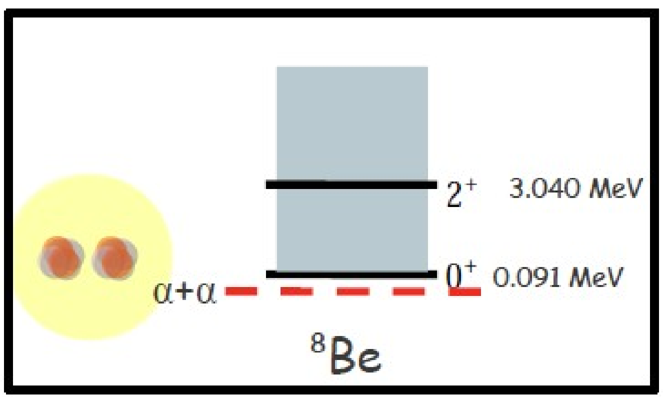
R P. Navrátil, J.P. Vary, B.R.B., PRC 62, 054311 (2000)
P. Navratil, et al., J.Phys. G: Nucl. Part. Phys. 36, 083101 (2009)
B.R.B., P. Navratil and J.P. Vary, PPNP 69, 131 (2013)

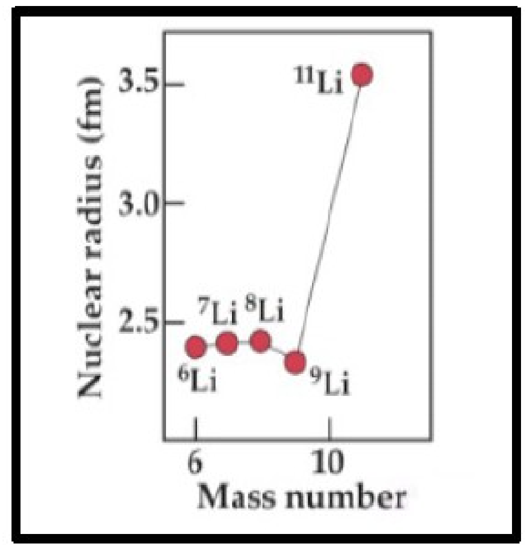


Limits of nuclear existence
126
82
50
28
20
8
2
2 8
20
28
50
82
protons
neutrons
rp-process
r-process
Density Functional Theory
Selfconsistent Mean Field
A=10
A=12
A~60
Ab initio few-body calculations
No-Core Shell Model
$0\hbar\omega$ Shell Model
Towards a unified description of the nucleus

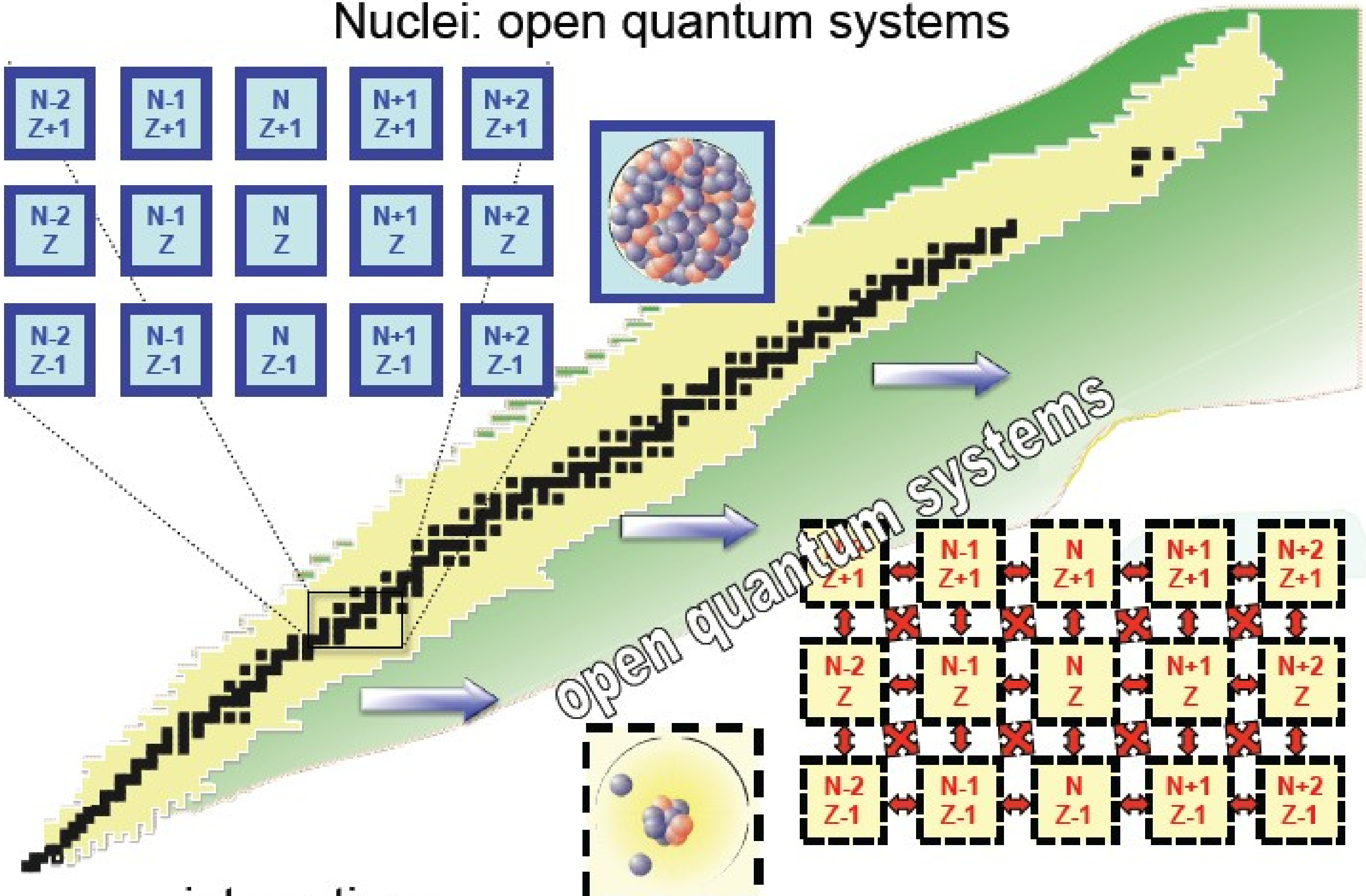

Light drip line nuclei
Z
N
1 2 3 4 5 6 7 8 9 10
1 2 3 4 5 6 7 8 9 10 11 12 13 14 15 16 17 18 19 20 21
11Li
11Be
12Be
24O
31F
halo nuclei


5He+n
1.867 MeV
2+
1.797 MeV
4He+2n
0.964 MeV
0+
6He


2+
3.040 MeV
0+
0.091 MeV
α+α
8Be


Nuclear radius (fm)
3.5
3.0
2.5
6
10
Mass number
6Li
7Li
8Li
9Li
11Li

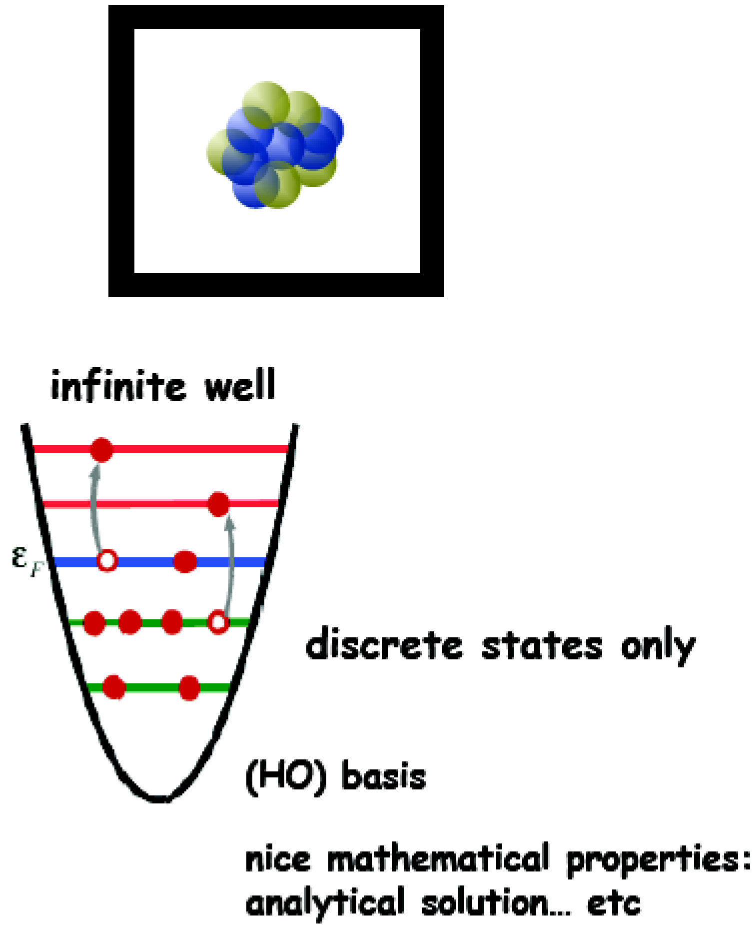
Nuclei: open quantum systems



interactions
correlations
many-body techniques

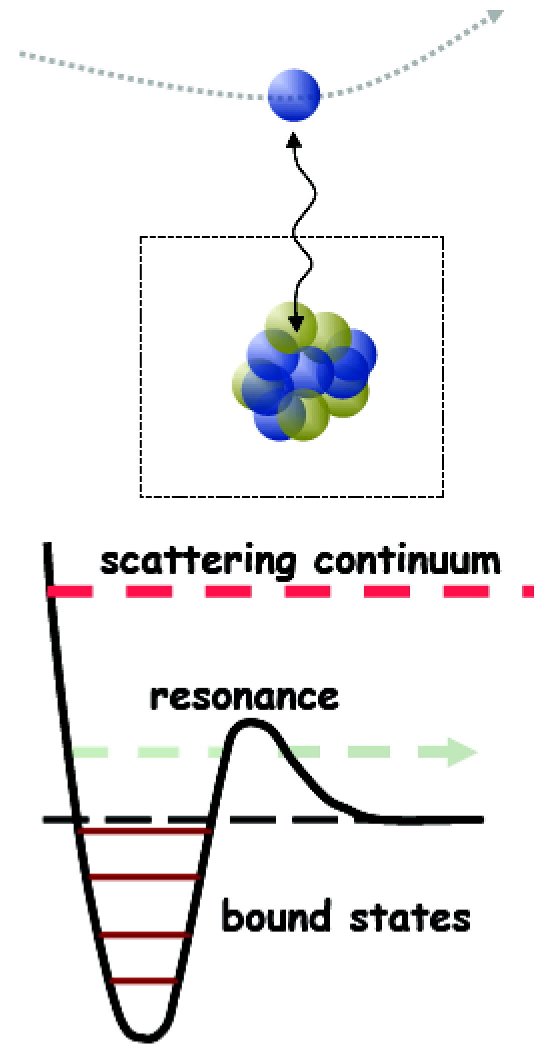
Closed Quantum System

(low lying states near the valley of stability)



Open quantum system

(weakly bound nuclei far away from stability)



II. NCGSM Formalism

Theories that incorporate the continuum, selected references

Real Energy Continuum Shell Model

- U.Fano, Phys.Rev.124, 1866 (1961)
- A.Volya and V.Zelevinsky PRC 74, 064314 (2006)

Shell Model Embedded in Continuum (SMEC)

- J. Okolowicz.,*et al*, PR 374, 271 (2003)
- J. Rotureau *et al*, PRL 95 042503 (2005)

Complex Energy Gamow Shell Model

- N. Michel *et al*., Phys. Rev. C67, 054311 (2003)
- G. Hagen *et al*, Phys. Rev. C71, 044314 (2005)
- J.Rotureau *et al* PRL 97 110603 (2006)
- N. Michel *et al*, J.Phys. G: Nucl.Part.Phys 36, 013101 (2009)
- G.P et al PRC(R) 84, 051304 (2011)

Selected References (continued):

NCSM/Resonating Group Method

S. Quaglioni and P. Navratil, Phys. Rev. C 79, 044606 (2009)

S. Baroni, P. Navratil, and S. Quaglioni, Phys. Rev. Lett. 110, 022505; Phys. Rev. C 87, 034326 (2013).

Coupled Cluster approach/Berggren basis

G. Hagen, et al., Phys. Lett. B 656, 169 (2007)

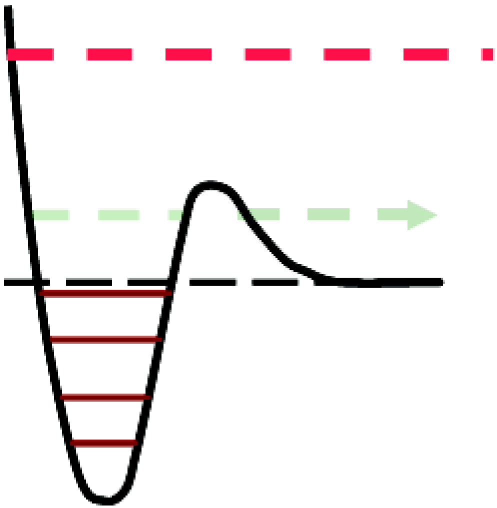
G. Hagen, T. Papenbrock, and M. Hjorth-Jensen, Phys. Rev. Lett. 104, 182501 (2013)

Green's Function Monte Carlo approach

K. M. Nollett, et al., Phys. Rev. Lett. 99, 022502 (2007)

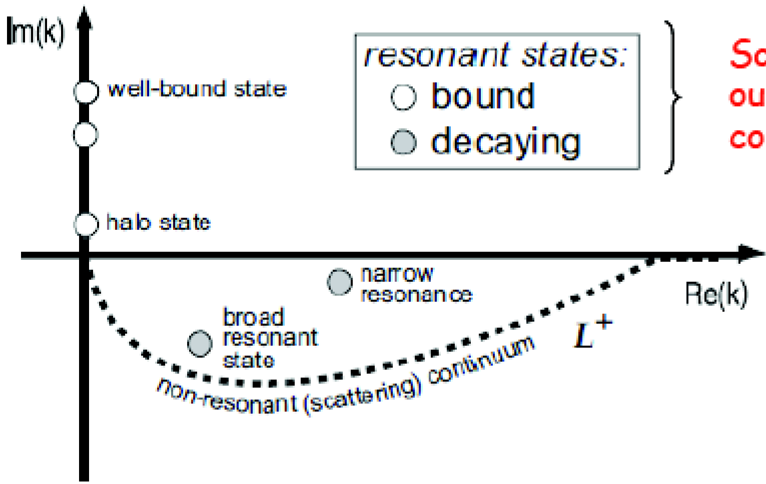
K. M. Nollett, Phys. Rev. C 86, 044330 (2012)

Resonant and non-resonant states (how do they appear?)



$$\left(-\frac{d^2}{dr^2}+v(r)+\frac{l(l+1)}{r^2}-k^2\right)u_l(k,r)=0$$

$$k=\sqrt{\frac{2mE}{\hbar^2}}$$



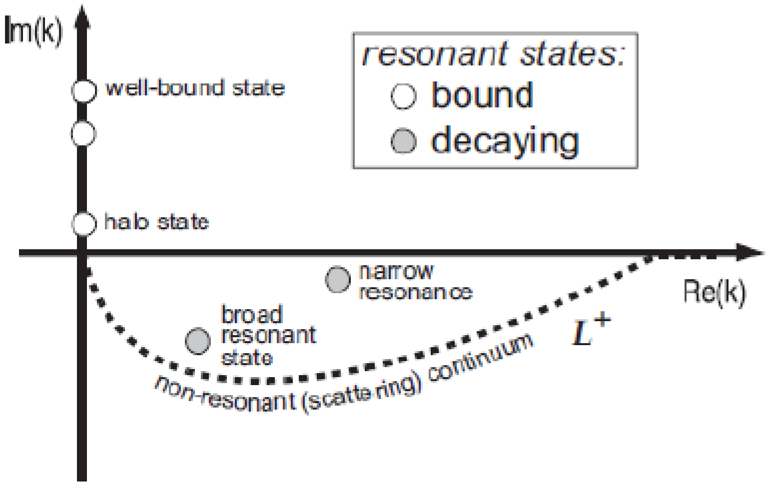
Solutions with outgoing boundary conditions

Solution of
the one-body Schrödinger equation with outgoing boundary conditions and a finite depth potential

$$u_l(k,r)\sim C_+H_l^+(k,r)\,,r\to\infty \quad bound\ \ states,\ resonances$$

$$u_l(k,r)\sim C_+H_l^+(k,r)+C\_H_l^-(k,r)\,,r\to\infty \quad scattering\ \ states$$

The Berggren basis (cont'd)



T.Berggren (1968)
NP A109, 265

The eigenstates of the 1b Shrödinger equation form a complete basis, **IF**:

we also consider the L_+ scattering states

$$\sum |u_{res}\rangle\langle u_{res}| + \int_{L^+} dk |u_k\rangle\langle u_k| = 1$$

$|u_k\rangle$ are complex continuum states along the L^+ contour (they satisfy scattering b.c)

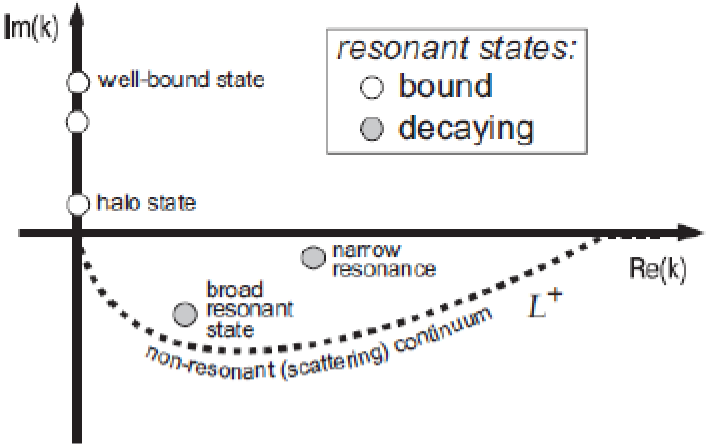
The shape of the contour is arbitrary, but it has to be below the resonance(s) position(s) (proof by T. Berggren)

In practice the continuum is discretized via a quadrature rule (e.g Gauss-Legendre):

$$\sum |u_{res}\rangle\langle u_{res}| + \sum_i |u_{ki}\rangle\langle u_{ki}| \simeq 1 \qquad \text{with} \qquad |u_k\rangle = \sqrt{\omega_i}|u_{ki}\rangle$$

Berggren's Completeness relation and Gamow Shell Model

N.Michel *et.al* 2002
PRL 89 042502



$$\sum |u_{res}\rangle\langle u_{res}| + \int_{L^+} dk|u_k\rangle\langle u_k| = 1$$

resonant states (bound, resonances...)

Non-resonant Continuum along the contour

$$\sum |u_{res}\rangle\langle u_{res}| + \sum_i |u_{ki}\rangle\langle u_{ki}| \simeq 1$$

$$|SD_i\rangle = |u_{i1} \ldots\ldots u_{iA}\rangle$$

The GSM in 4 steps

Hermitian Hamiltonian

Many-body $|SD_i\rangle$ basis

Hamiltonian matrix is built (complex symmetric):

$$\langle SD|H|SD\rangle$$

Hamiltonian diagonalized

$$|\Psi\rangle = \sum_n c_n|SD_n\rangle$$

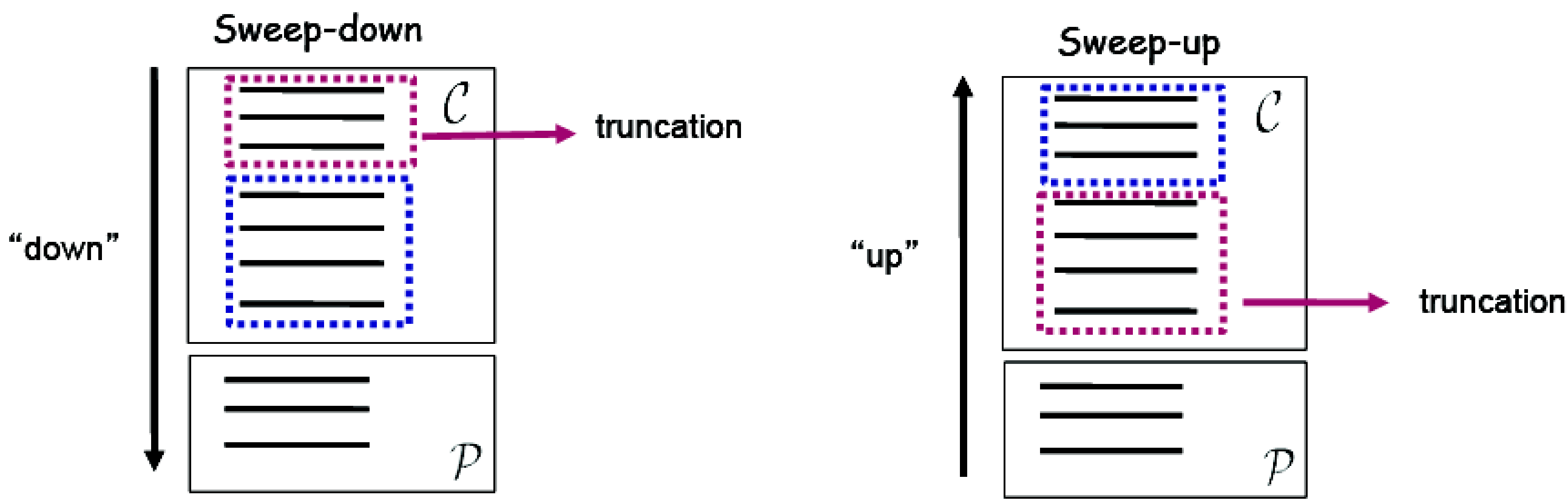
Many body correlations and coupling to continuum are taken into account simultaneously

- truncation with the density matrix :

$$\rho^{J_c}_{c,c'} = \sum_p \Psi_{pc} \Psi_{pc'}$$

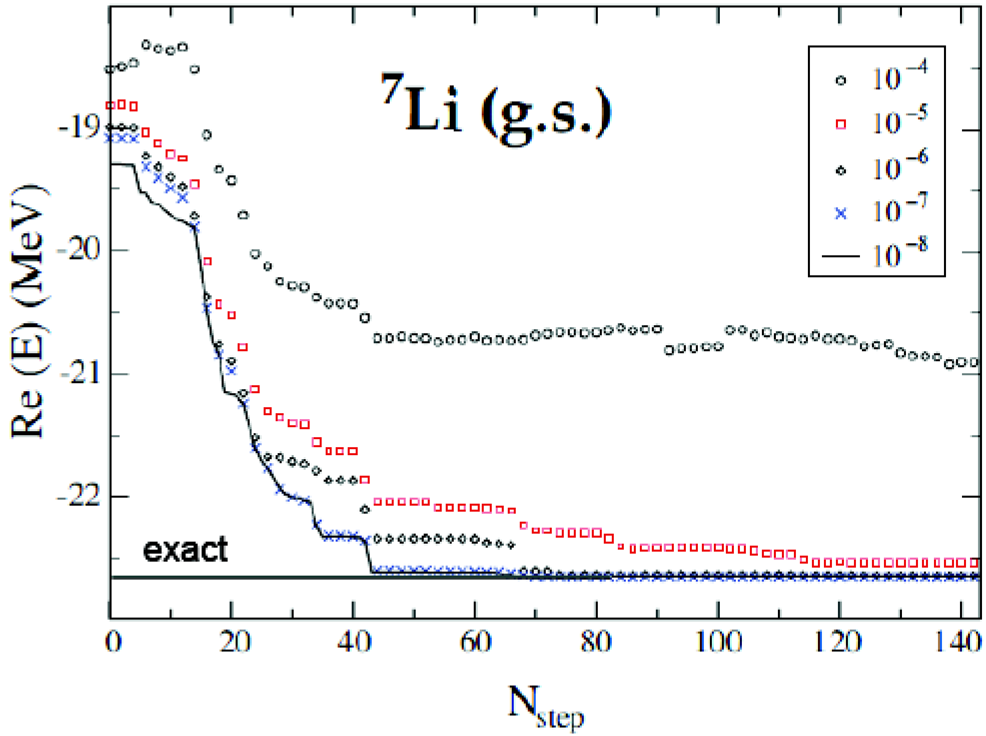
→ N_{opt} states that correspond to the largest eigenvalues of the density matrix are kept

- The process is reversed…
- In each step (shell added) the Hamiltonian is diagonalized and N_{opt} states are kept.
- Iterative method to take into account all the degrees of freedom in an effective manner.
- In the end of the process the result is the same with the one obtained by "brute" force diagonalization of H.



Density Matrix Renormalization Group – Examples – (GSM with a ^{4}He core)

J.Rotureau et al PRC 79 (2009) 014304



^{7}Li: 3 nucleons outside ^{4}He.
Max dim in DMRG: ~1400
19% of the full space space

$$\left| 1 - \mathcal{R}e\left(\sum_{i=1}^{N_\rho} w_i \right) \right| < e$$

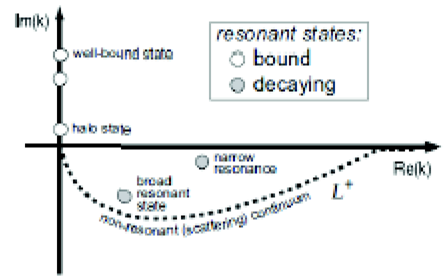
Small ε → more states of ρ are kept in each step

$$\sum_\alpha w_\alpha = 1$$

Gamow Shell Model in an ab-initio framework

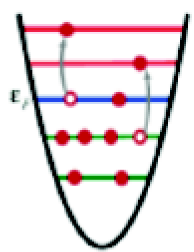
$$H = \frac{1}{A}\sum_{i<j}^{A}\frac{(\vec{p}_i-\vec{p}_j)^2}{2m} + V_{NN,ij} + \ldots \quad (1)$$

- Only NN forces at present
  → Argonne V18, (Wiringa, Stoks, Schiavilla PRC 51, 38, 1995)
  → N^3LO (D.R.Entem and R. Machleidt PRC(R) 68, 041001, 2003)
  → V_{lowk} technique used to decouple high/low momentum nodes. $\Lambda_{Vlowk} = 1.9\ fm^{-1}$
  (S. Bogner et al, Phys. Rep. 386, 1, 2003)



- Basis states
  → s- and p- states generated by the HF potential

  → l > 1 H.O states



- Diagonalization of (1) → Applications to ^3H, ^4He, ^5He

III. NCGSM: Applications to Light Nuclei

The Density Matrix Renormalization Group (DMRG)

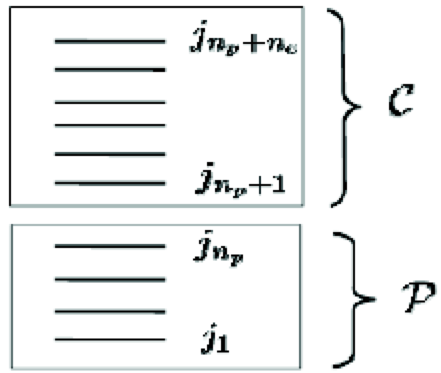
S.R White PRL 69 (1992) 2863
T.Papenbrock and D.Dean J.Phys.G 31 (2005) S1377
S.Pittel et al PRC 73 (2006) 014301
J.Rotureau et al PRC 79 (2009) 014304
J. Rotureau et al PRL 97 (2006) 110603

✓ **Truncation Method** applied to lattice models, spin chains, atomic nuclei….

GSM+DMRG

$$|\Psi\rangle^J = \sum_{p,c} \Psi_{pc} \left[|p\rangle^{J_p} |c\rangle^{J_c} \right]^J$$

DMRG ⟶ truncation in $\mathcal{C}$

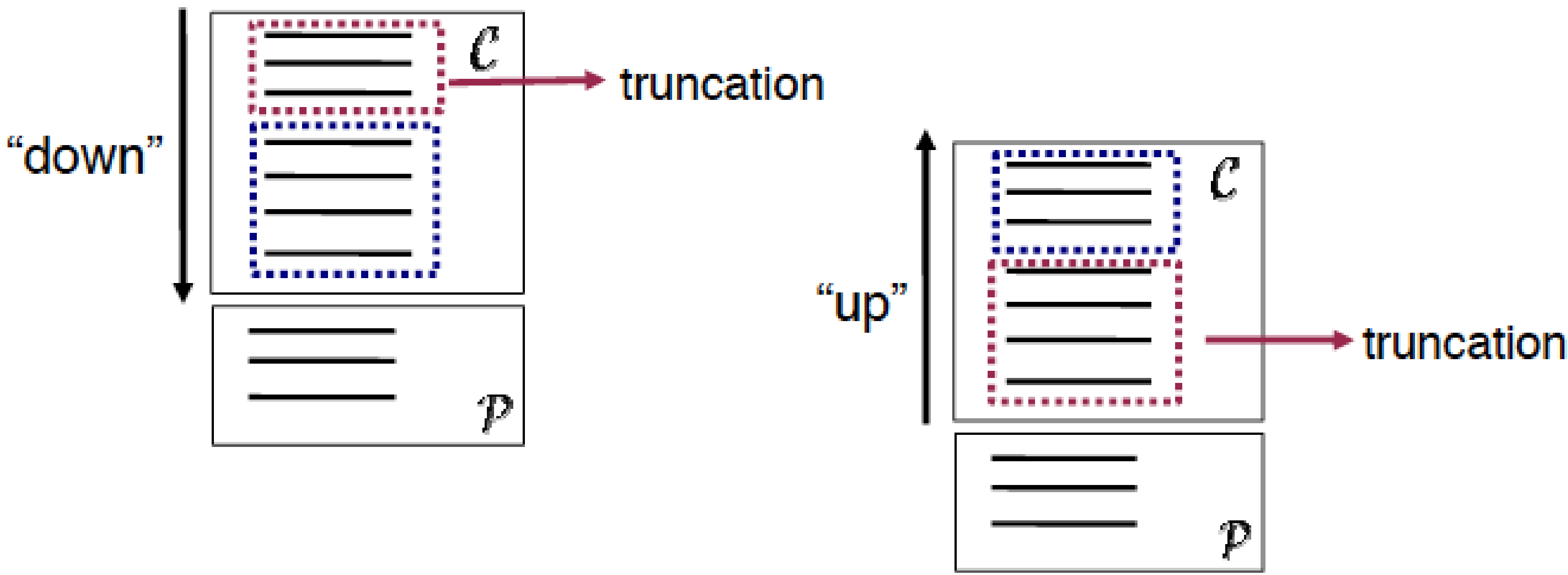


P: poles
C: Continua

✓ Iterative method: In each step (N_{step}) a scattering shell is added from C.
→ Hamiltonian is diagonalized and density matrix is constructed:

$$\rho^{J_c}_{c,c'} = \sum_p \Psi_{pc} \Psi_{pc'}$$

sweeping phase

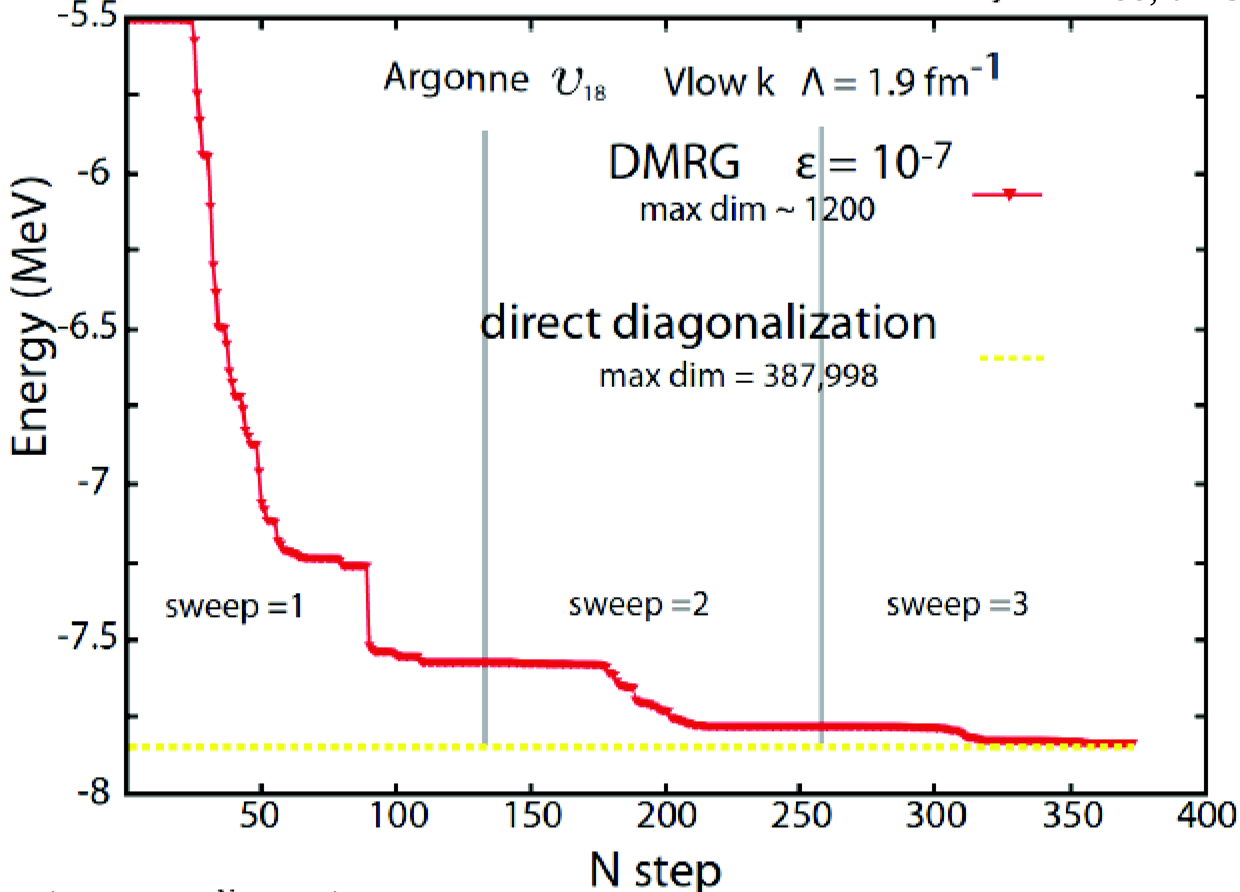


sweeping until convergence is reached ....

Very good scaling with number of shells

Results: Triton

G.Papadimitriou, J.Rotureau, B. Barrett, N. Michel, M.Ploszajczak arXiv:1301.7140
Submitted at Phys.Rev.C 88, 044318 (2013)



- 2 neutrons
- 1 proton
- Pole space A:0s1/2 (p/n)
- Continuum space B:
  - p3/2,p1/2,s1/2 real energy continua
  - d5/2-d3/2 H.O states
- 130 s.p. states total

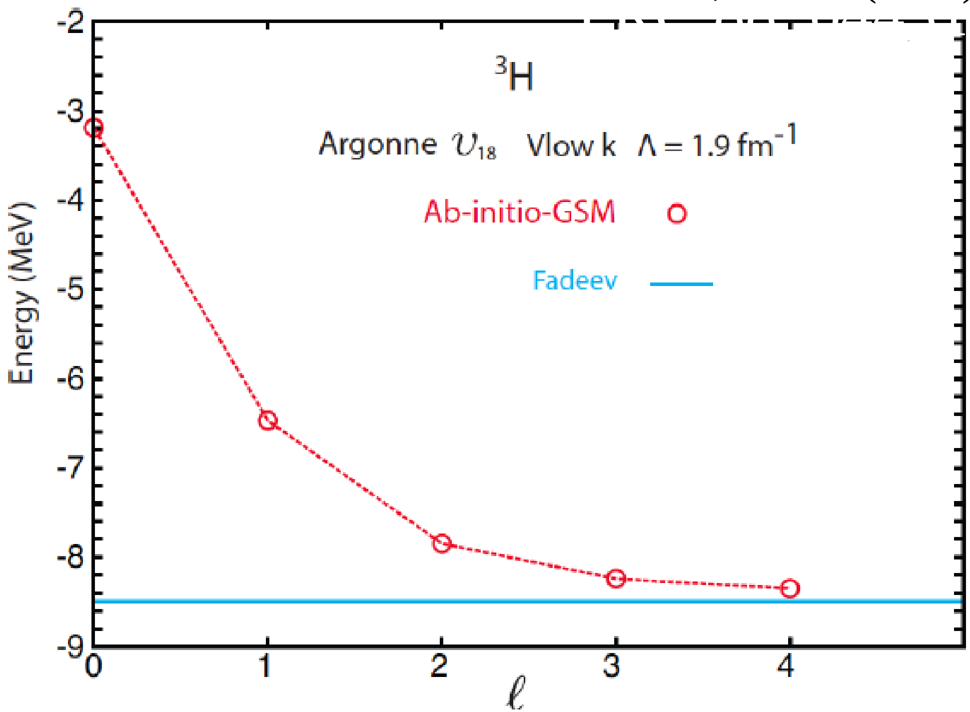
$$\left| 1 - \mathcal{R}e\left(\sum_{i=1}^{N_\rho} w_i\right)\right| < e$$

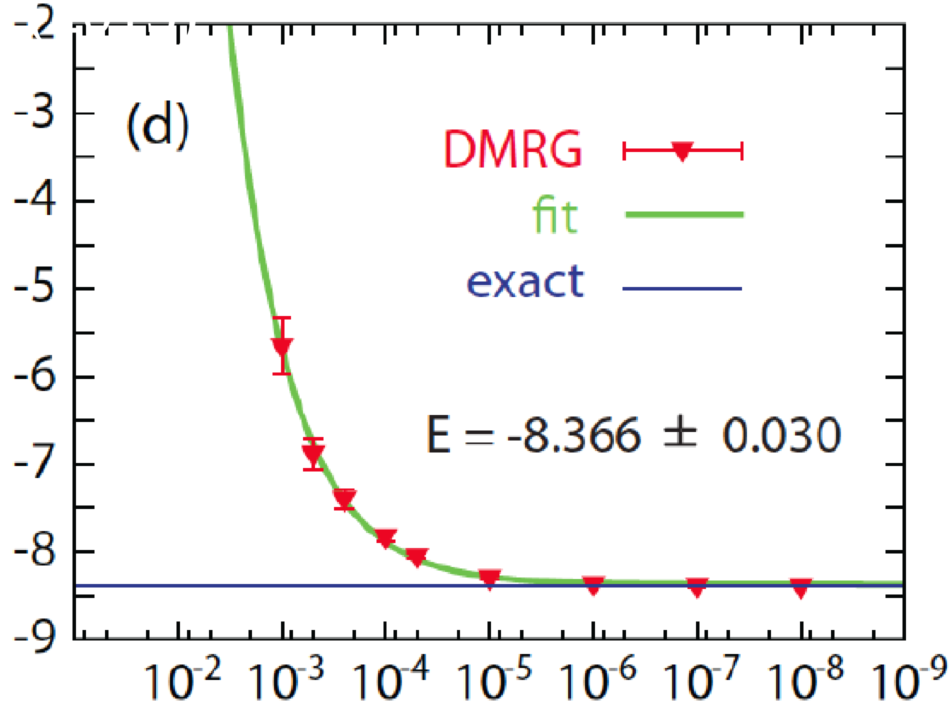
$$\sum_\alpha w_\alpha = 1$$

E_{exact} = -7,840 MeV
$E_{DMRG\ (\varepsilon = 10^{-7})}$ = -7,832 MeV
$E_{DMRG\ (\varepsilon = 10^{-6})}$ = -7,820 MeV

Results: Triton

G.P., J.Rotureau, N. Michel, M.Ploszajczak, B. Barrett arXiv:1301.7140
PRC 88,044318 (2013)





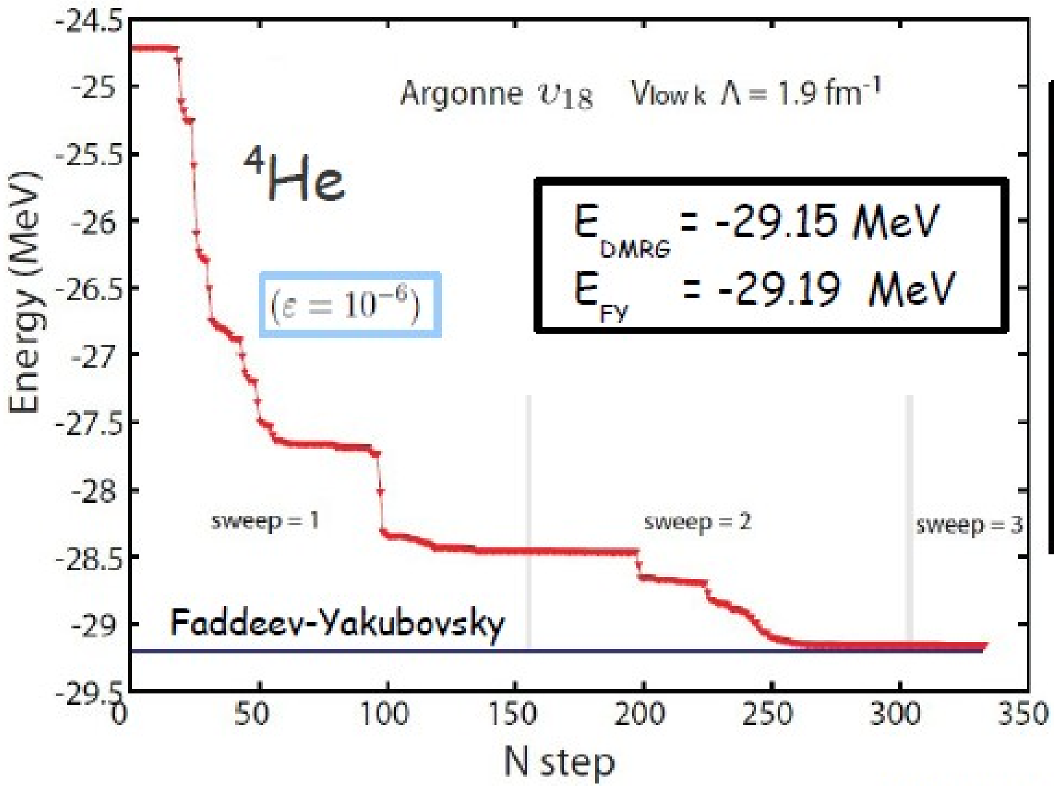
E_{Fadeev} = -8.47 MeV

$E_{ab-initio}$ = -8.39 MeV (exact diagonalization)

Truncation error decreases
Very fast with increasing the
number of states kept

Dim in DMRG = 2,575
Dim in exact = 890,021

Faddeev result from (Nogga, Bogner, Schwenk, PRC 70,061002, 2004)



i) $s_{1/2}$ $p_{3/2}$ $p_{1/2}$ real-energy HF states

ii) dfg H.O states

* $0s_{1/2}$(p) : E= -24.453 MeV
* $0s_{1/2}$(n) : E= -26.290 MeV

156 Shells

G. Papadimitriou *et al*, arXiv:1301.7140

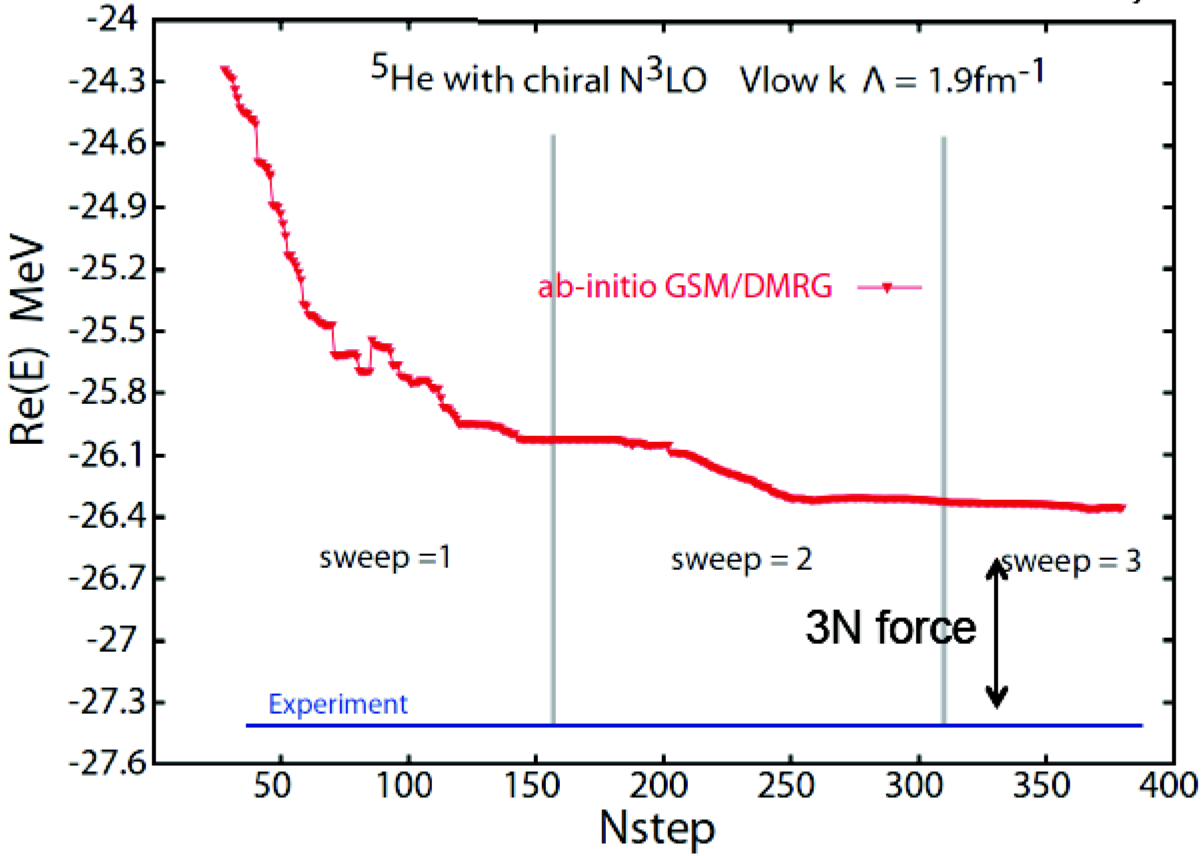
J-scheme dimension

* Full NCGSM space: 6,230,512
* DMRG ~ 6000

(FY result from Nogga et al, PRC 70 (2004))

Results: ^{5}He with chiral N^3LO (real part)

G.Papadimitriou, J.Rotureau, B. Barrett, N. Michel, M.Ploszajczak arXiv:1301.7140
Submitted at Phys.Rev.C



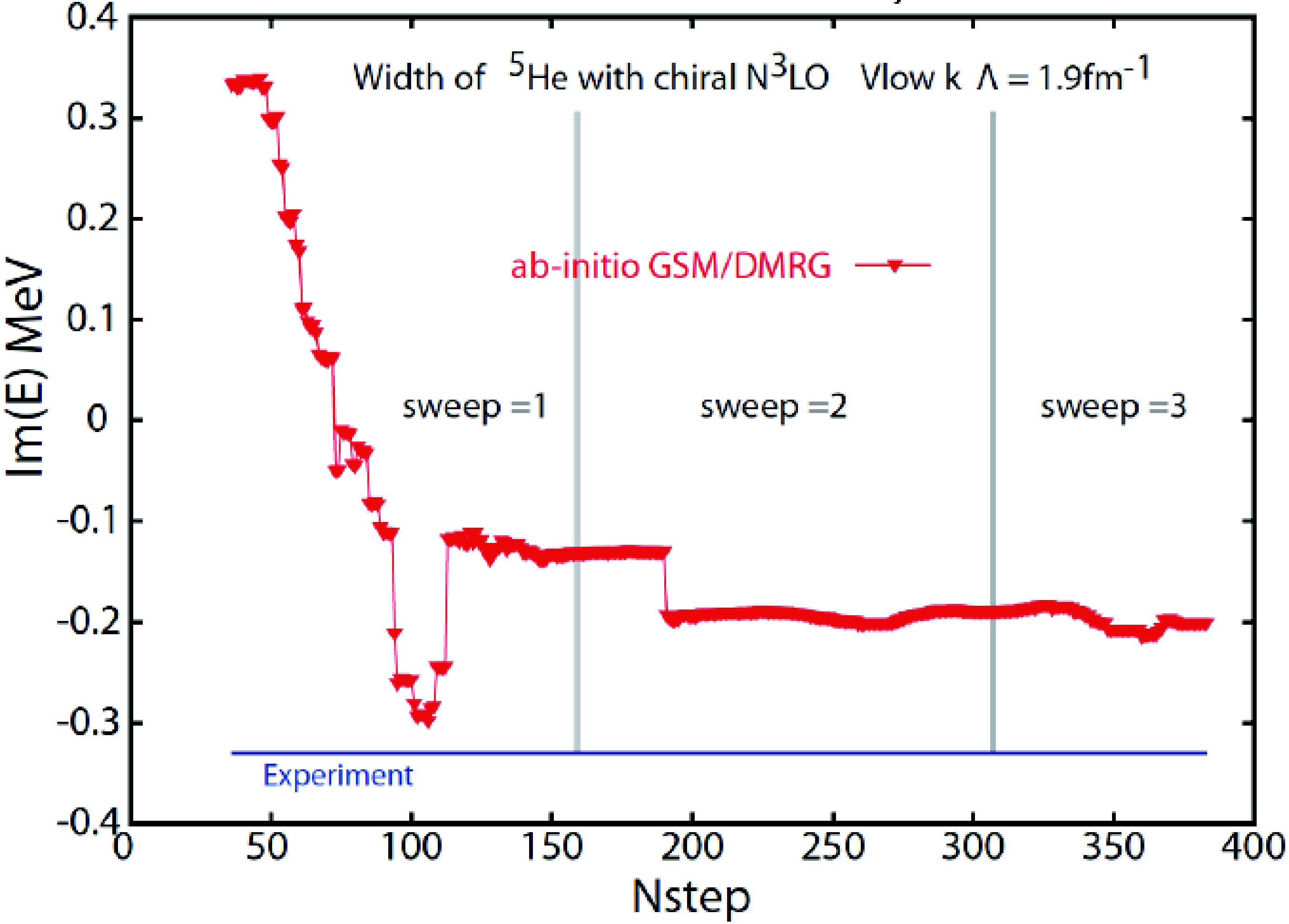
- 3 neutrons
- 2 protons
- Pole space A:0s1/2 (p/n) + 0p3/2 n resonant state
- Continuum space B:
  - p3/2 complex continuum
  - p1/2-s1/2 real continua
  - d5/2-d3/2, f5/2-f7/2, g7/2-g9/2 } H.O states
- 157 s.p. states total

Dim for direct diagon: $3*10^9$

DMRG dim ~ 10^5

Results: ^5He imaginary part (width) with chiral N^3LO

G.Papadimitriou, J.Rotureau, B. Barrett, N. Michel, M.Ploszajczak arXiv:1301.7140
Submitted at Phys.Rev.C



S_{1n} = -1.20 MeV

S_{1n} (exp) = -0.89 MeV

Unbound character of ^5He reproduced within an ab-initio framework

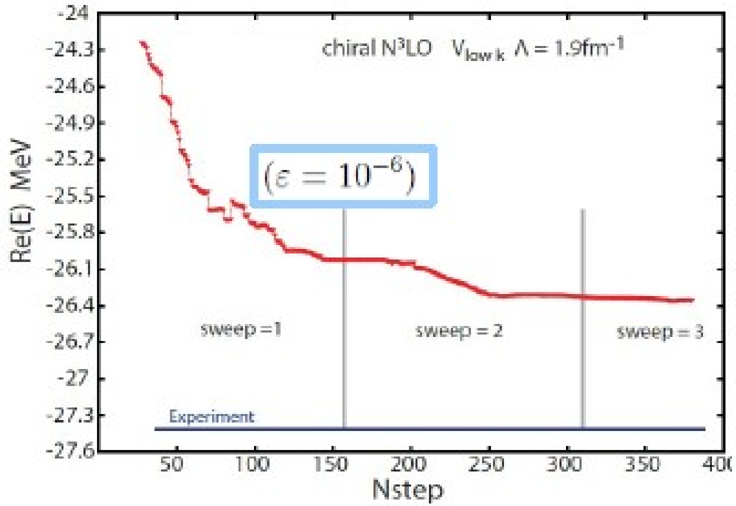
Satisfactory agreement of the **width** with experiment

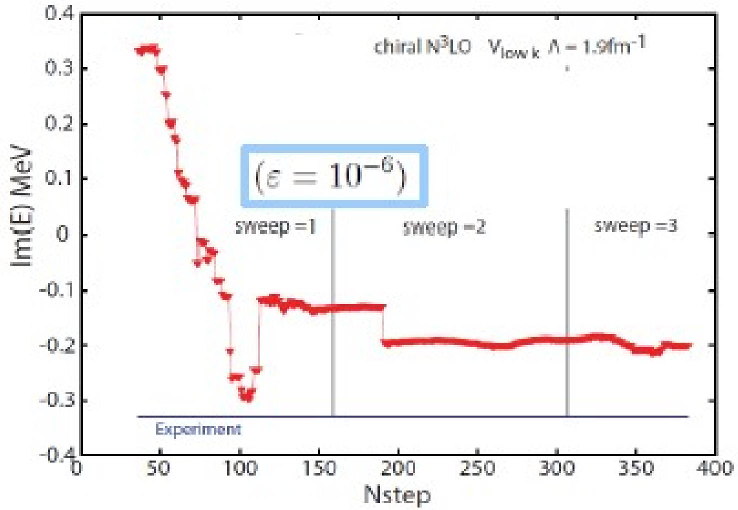
^{5}He

HF poles

* 0p3/2 (n): E= (1.194,-0.633) MeV
* 0s1/2(p) : E= -23.291 MeV
* 0s1/2(n) : E= -23.999 MeV

Inclusion of $p_{3/2}$ complex-continuum contour for neutron





157 Shells

J-scheme dimension

* Full NCGSM space: 1,379,196,439
* DMRG ~ 1.10[5]

DMRG $(\varepsilon = 10^{-6})$	Coupled Cluster (CCSD)
(-26.31,-0.20)	(-24.87,-0.16)

G. Hagen *et al*, PLB 656 (2007) 169.

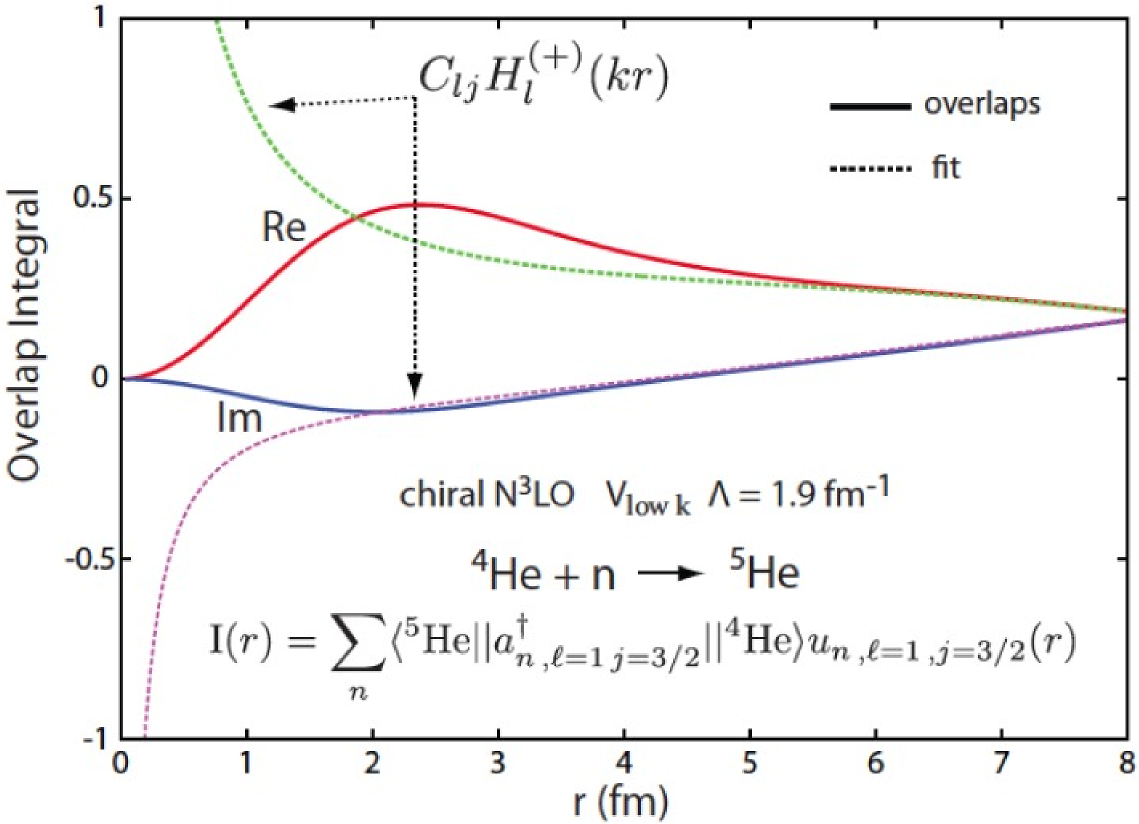
Comparison of Position and Width of the 5He Ground State: Theory and Experiment

Method	Energy (MeV)	Width (MeV)
NCGSM/DMRG:	1.17	0.400
"Extended" R-matrix*:	0.798	0.648
Conventional R-matrix*:	0.963	0.985

*D. R. Tilley, et al., Nucl. Phys. A 708, 3 (2002)

Results: Ab-initio overlaps in the NC-GSM

- Basic ingredients of the theory of direct reactions
- Useful measures of the configuration mixing in the many-body wavefunction



$$C = \sqrt{\frac{\Gamma\mu}{\hbar^2 \Re(k)}} \quad (1)$$

The ANC is extracted by fitting the tail of the overlap with a Hankel function

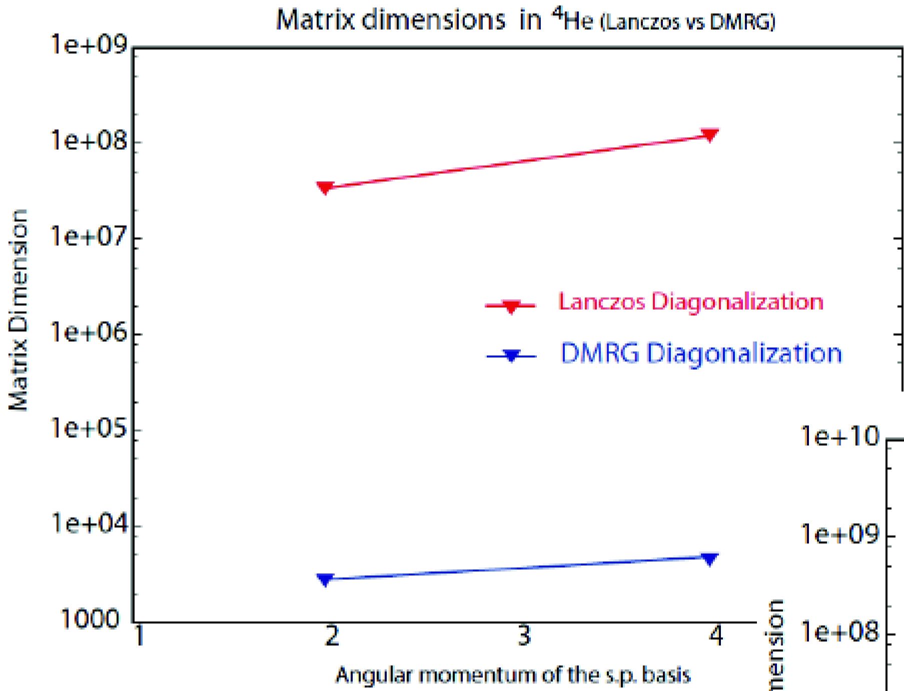
C = 0.197

and from (1)

Γ = 311 keV

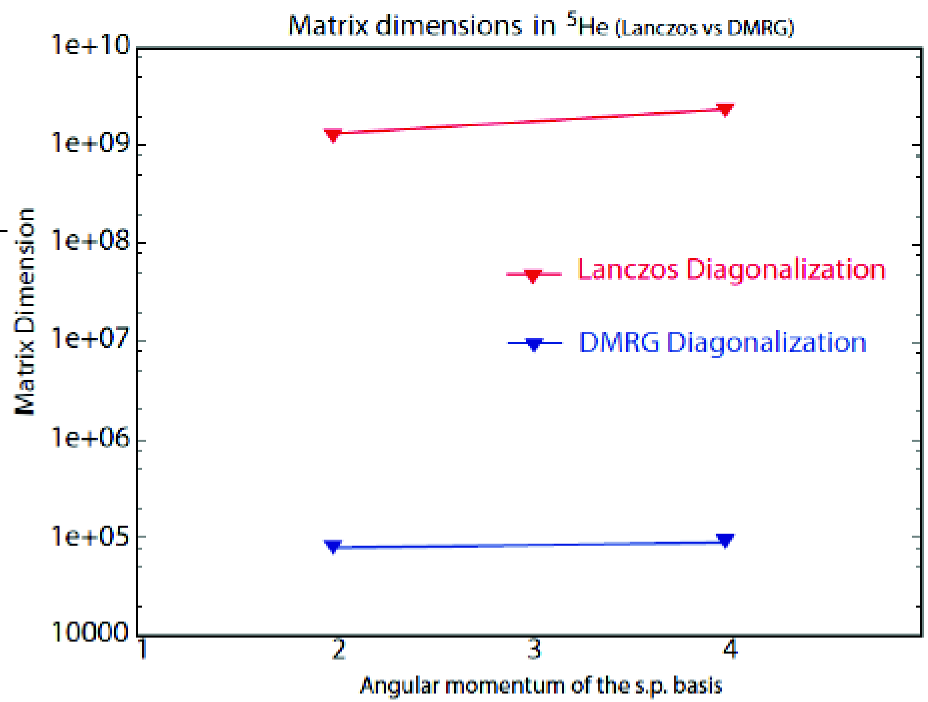
Two ways of calculating the width
a) many body diagonalization ⟶ Equivalent
b) from overlap function

Dimension comparison

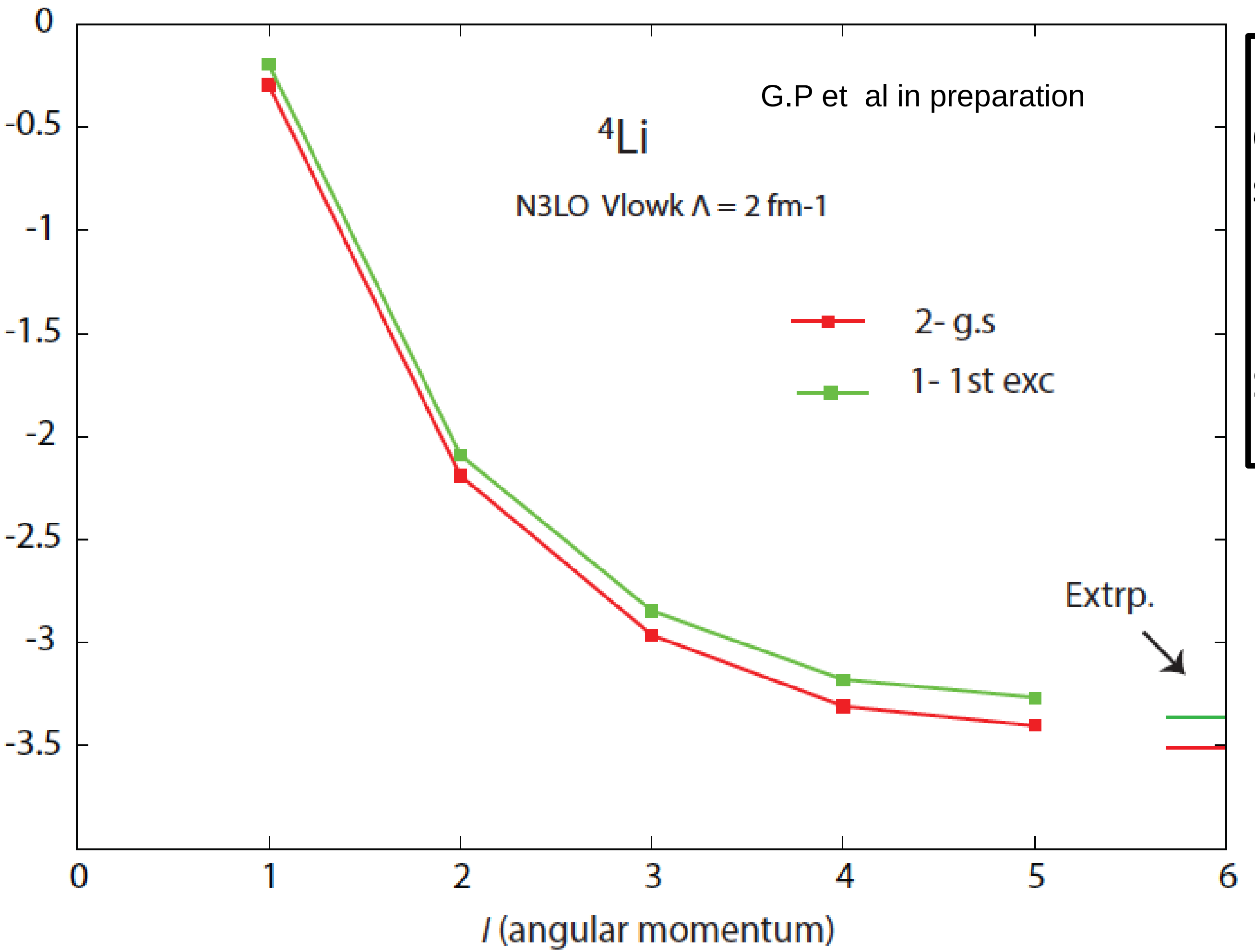


→ Lanczos: "brute" force diagon of H.

→ DMRG: Diagon of H in the space where only the most important degrees of "freedom" are considered

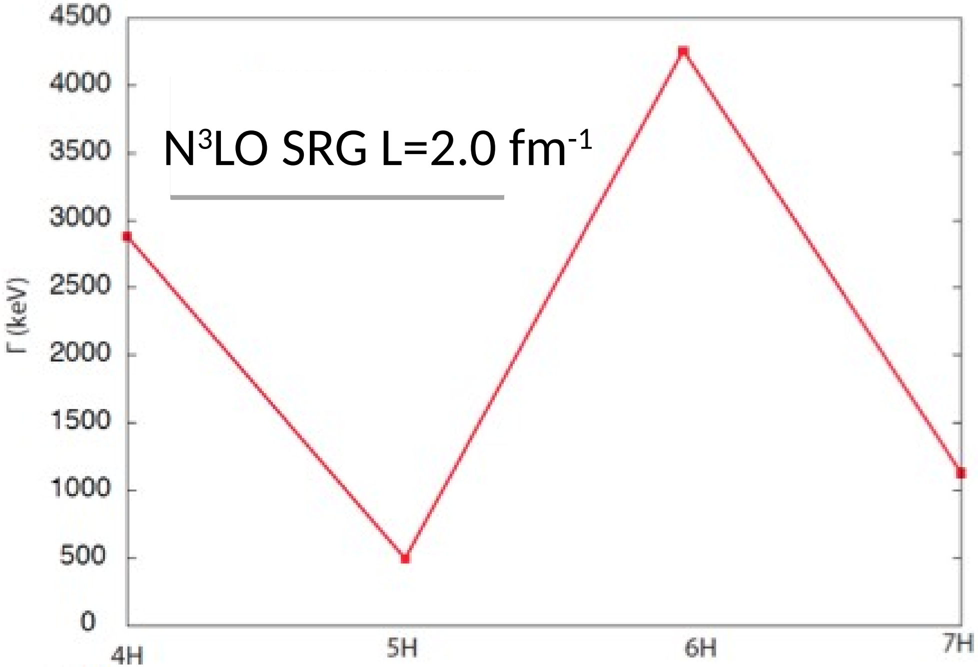


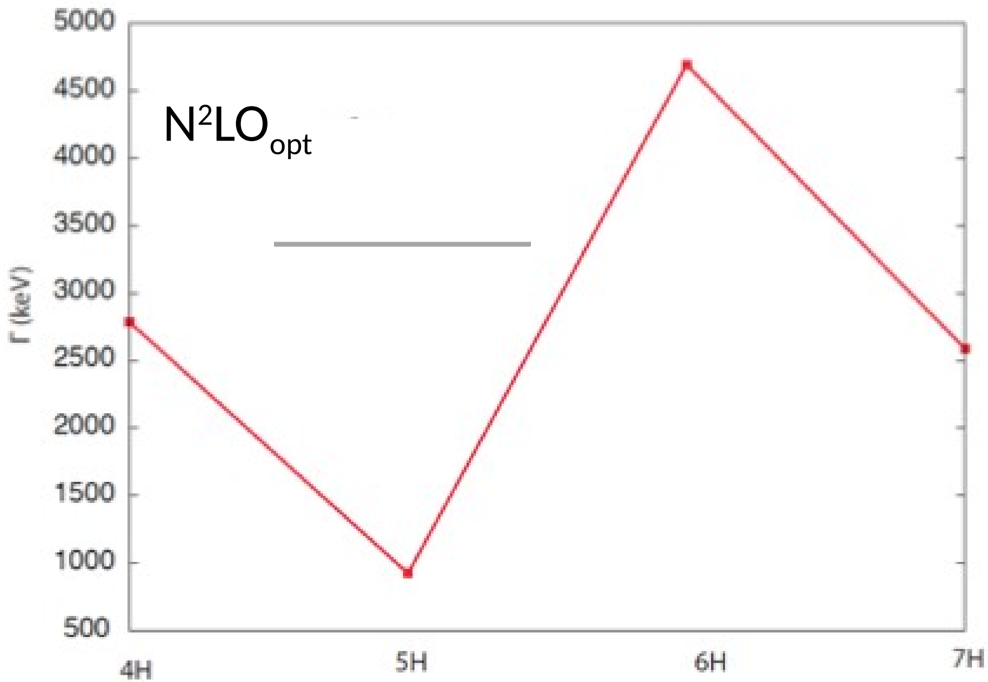
Preliminary Results



Basis:
Gamow p3/2 proton states
(0p3/2 s.p. res) +
20 scattering continua.
Rest up to h-waves are H.O
States of hw= 20 MeV

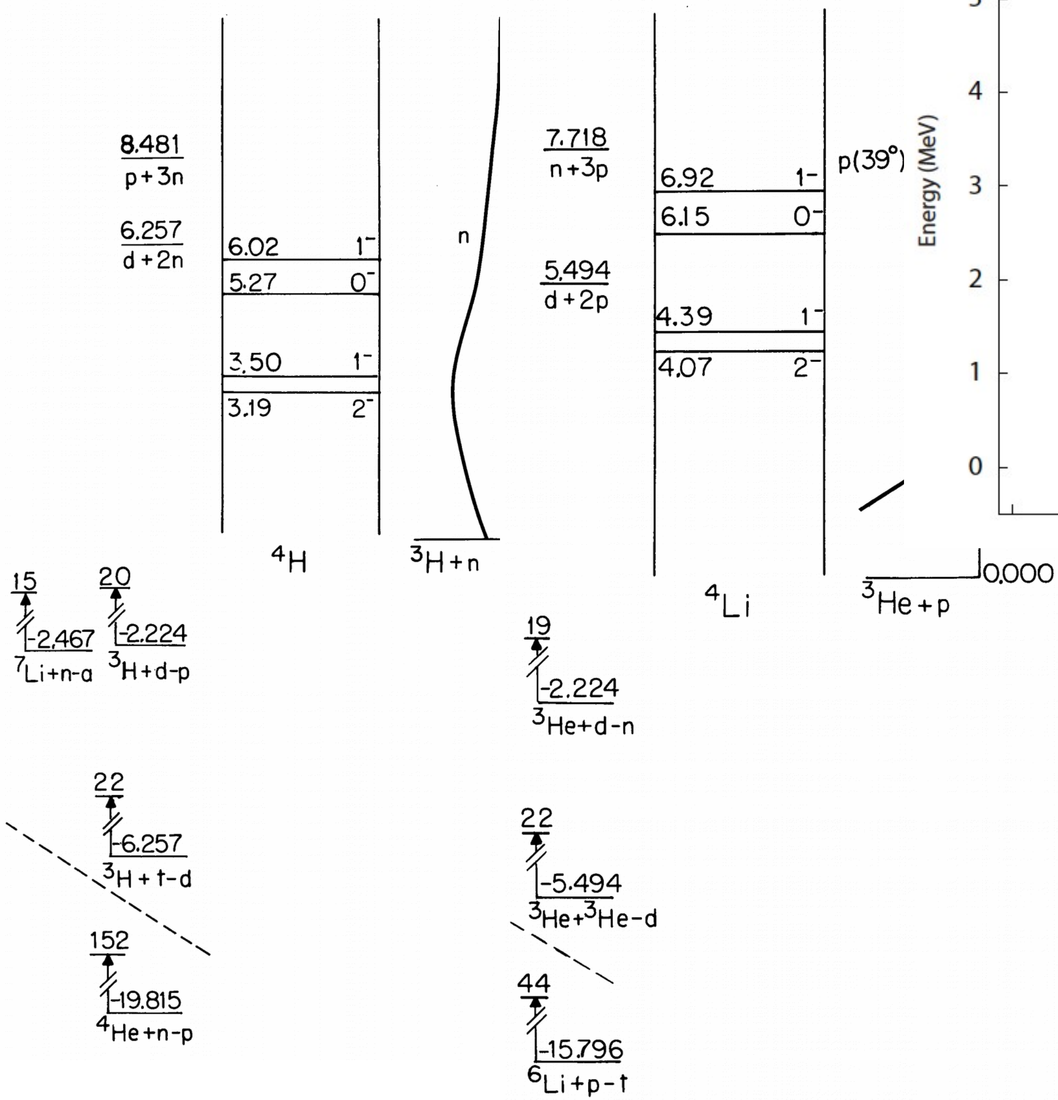
- Similar trend with 4H

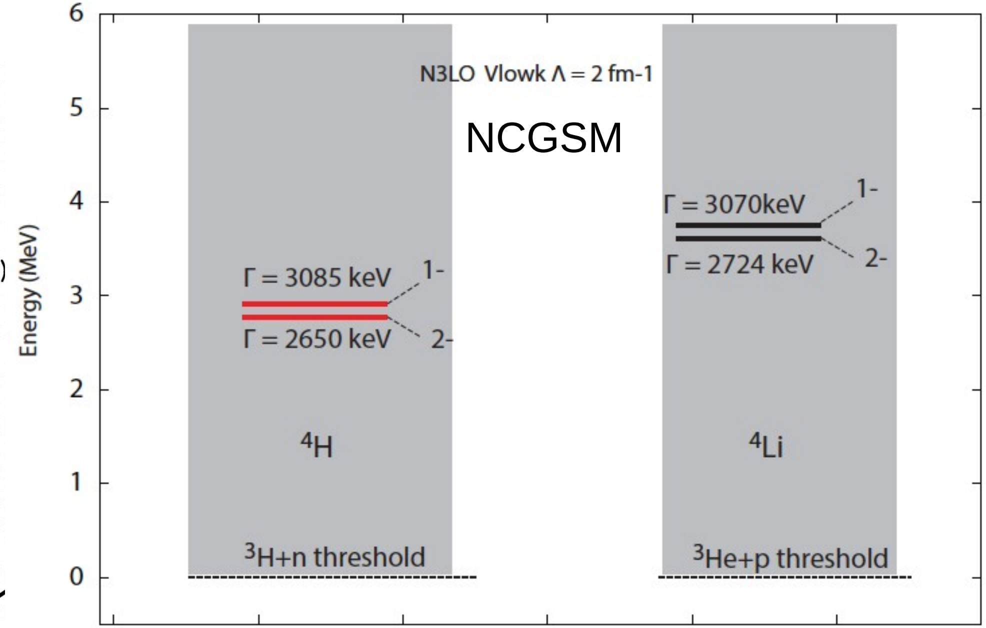

N3LO SRG L=2.0 fm-1
Γ (keV)
4500
4000
3500
3000
2500
2000
1500
1000
500
0
4H
5H
6H
7H


N2LOopt
Γ (keV)
5000
4500
4000
3500
3000
2500
2000
1500
1000
500
4H
5H
6H
7H

Results as compared to experiment

http://www.tunl.duke.edu/nucldata/chain/04.shtml





4H:
2- g.s: 2.775 MeV   Γ = 2650 keV
1- 1st 2.915 MeV   Γ = 3085 keV

4Li:
2- g.s: 3.613 MeV   Γ = 2724 keV
1- 1st   3.758 MeV   Γ = 3070 keV

3H: -7.92 MeV
3He: -7.12 MeV   (for the thresholds)

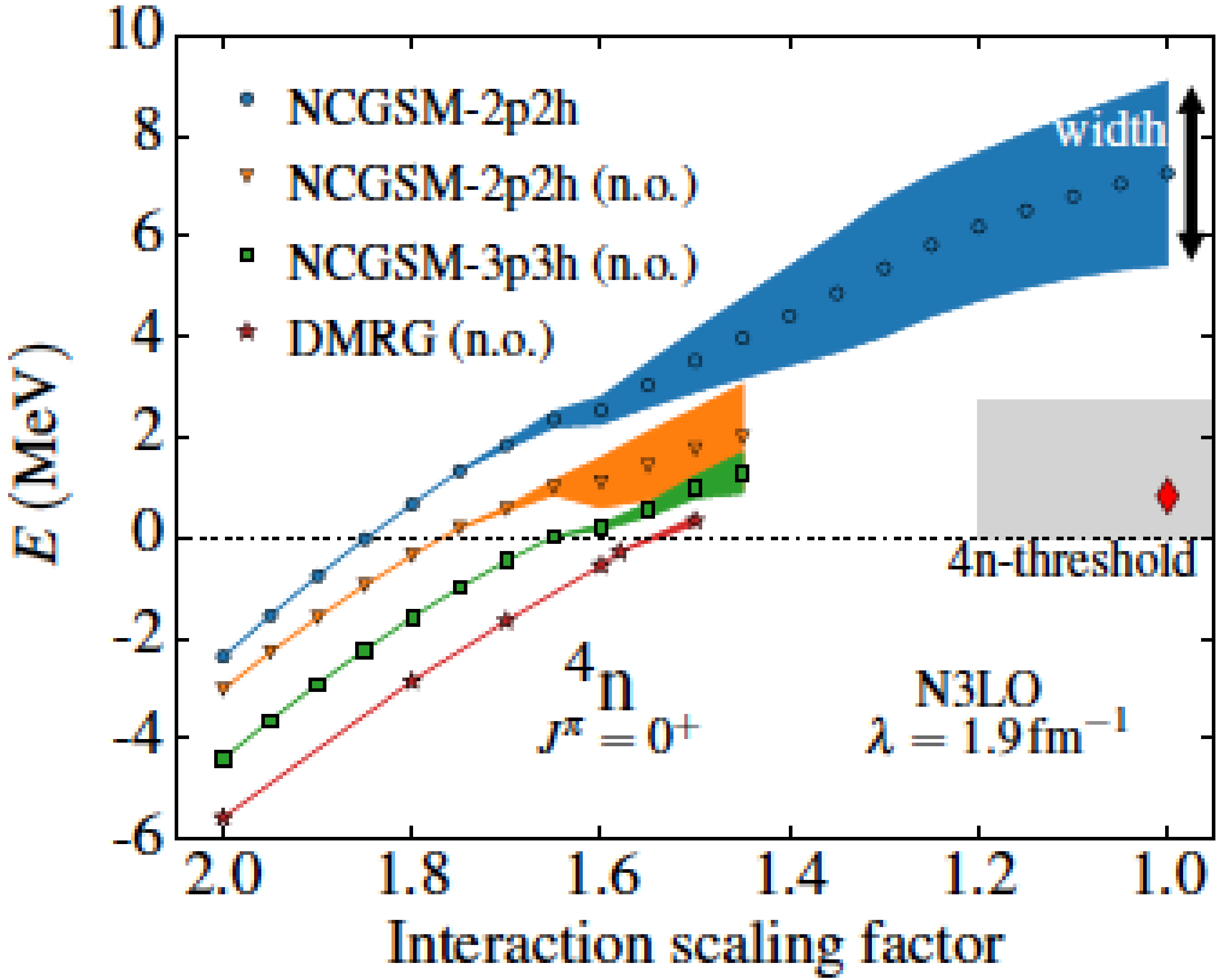
Tetraneutron

Energy (width) of J=0⁺ pole of the 4n system

	$\lambda = 1.7\,\mathrm{fm}^{-1}$	$\lambda = 1.9\,\mathrm{fm}^{-1}$	$\lambda = 2.1\,\mathrm{fm}^{-1}$
N3LO	7.27 (3.69)	7.28 (3.67)	7.28 (3.69)
$\mathrm{N2LO_{opt}}$	7.32 (3.74)	7.33 (3.78)	7.34 (3.95)
$\mathrm{N2LO_{sat}}$ *	7.24 (3.48)	7.22 (3.58)	7.27 (3.55)
JISP16		7.00 (3.72)	

- NCGSM results for 4n-system depend weakly on details of the chiral EFT interaction
- No dependence on the renormalization cutoff of the interaction weak dependence on the 3-, 4-body interactions

K. Fossez, et al, arXiv: 1612.01483v1[nucl-th]



Continuum is non-perturbative

IV. Summary and Outlook

IV. Summary and Outlook

1. The Berggren basis is appropriate for calculations of weakly bound/unbound nuclei.

2. Berggren basis has been applied successfully in an ab-initio GSM framework --> No Core Gamow Shell Model for weakly bound/unbound nuclei.

3. Diagonalization with DMRG makes calculations feasible for heavier nuclei using Gamow states.

4. Future applications to heavier nuclei and to nuclei near the driplines.

NCGSM for reaction observables

→ NCGSM is a structure method but overlap functions can be assessed.

→ Asymptotic normalization coefficients (ANCs) are of particular interest because they are observables… (Mukhamedzanov/Kadyrov, Furnstahl/Schwenk, Jennings)

→ Astrophysical interest

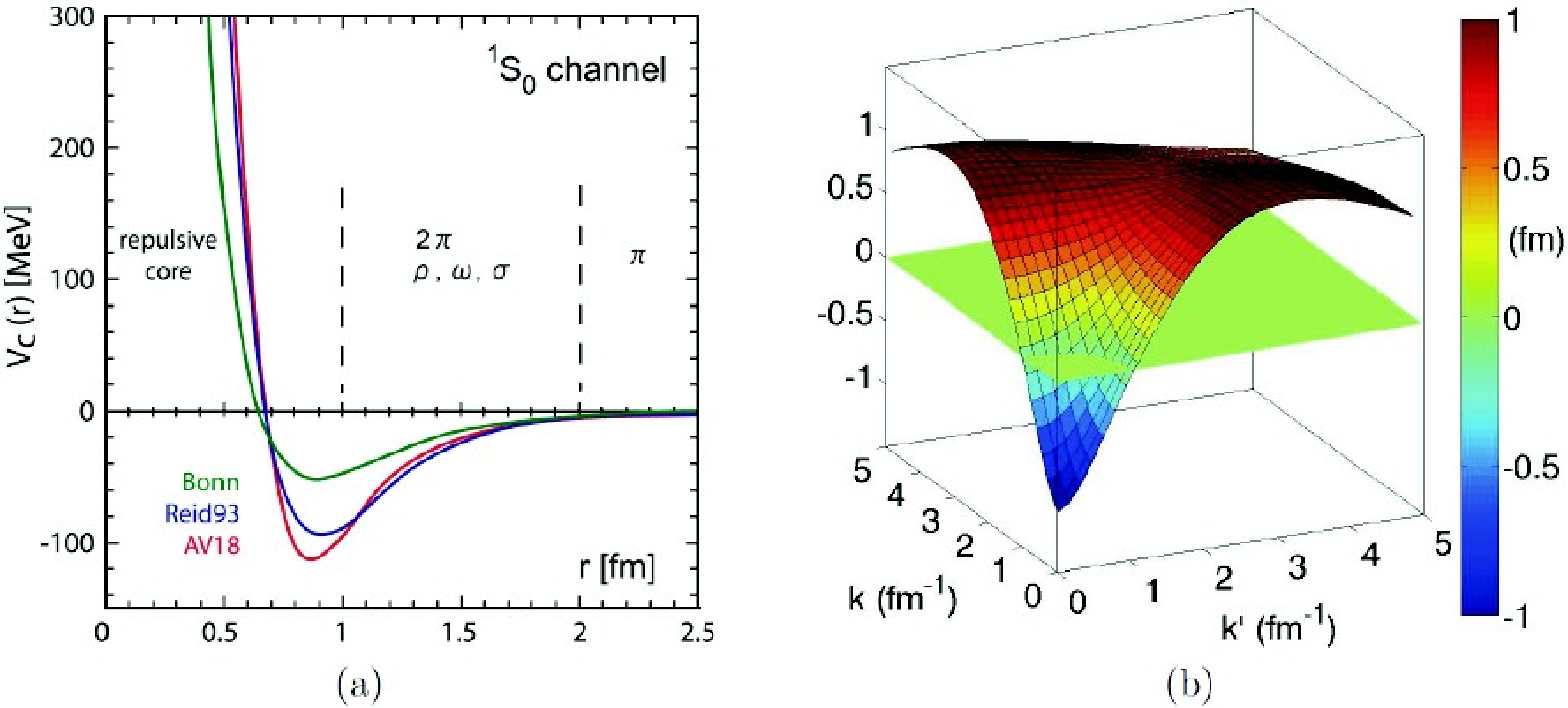
(see I. Thompson and F. Nunes “Nuclear Reactions for Astrophysics:…” book)

→ ANCs computing difficulties: (see also K.Nollett and B. Wiringa PRC 83, 041001,2011)

1) Correct asymptotic behavior is mandatory
2) Sensitivity on S1n …

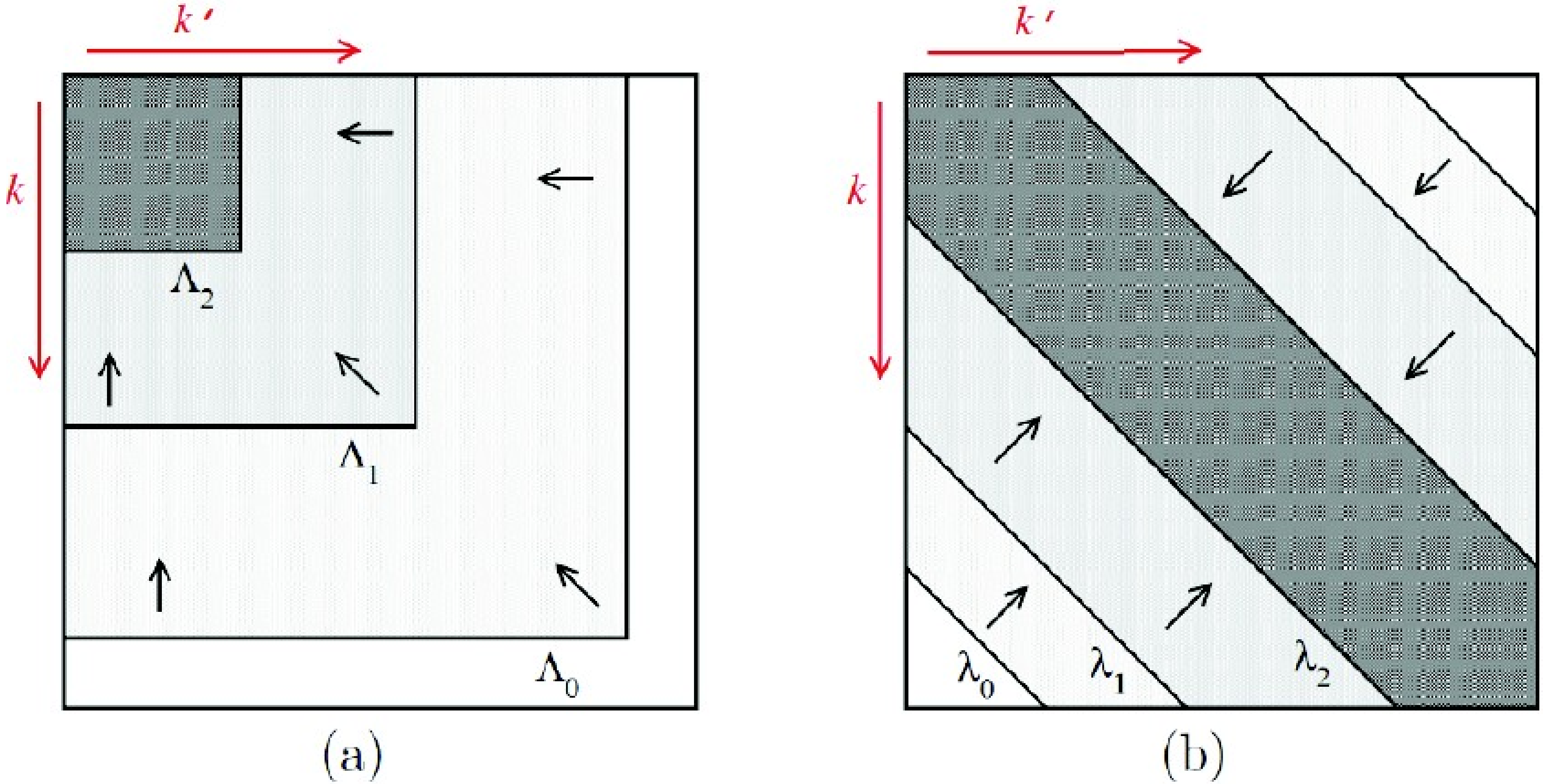
See also Okolowicz et al Phys. Rev. C85, 064320 (2012)., for properties of ANCs

Realistic two-body potentials in coordinate and momentum space



Repulsive core makes calculations difficult

Illustration on how the high momentum nodes are integrated out in the Vlowk (a) and in the SRG (b) RG methods



→ Need to decouple high/low momentum modes

✓ Achieved by V_{low-k} or Similarity RG approaches (e.g. SRG)

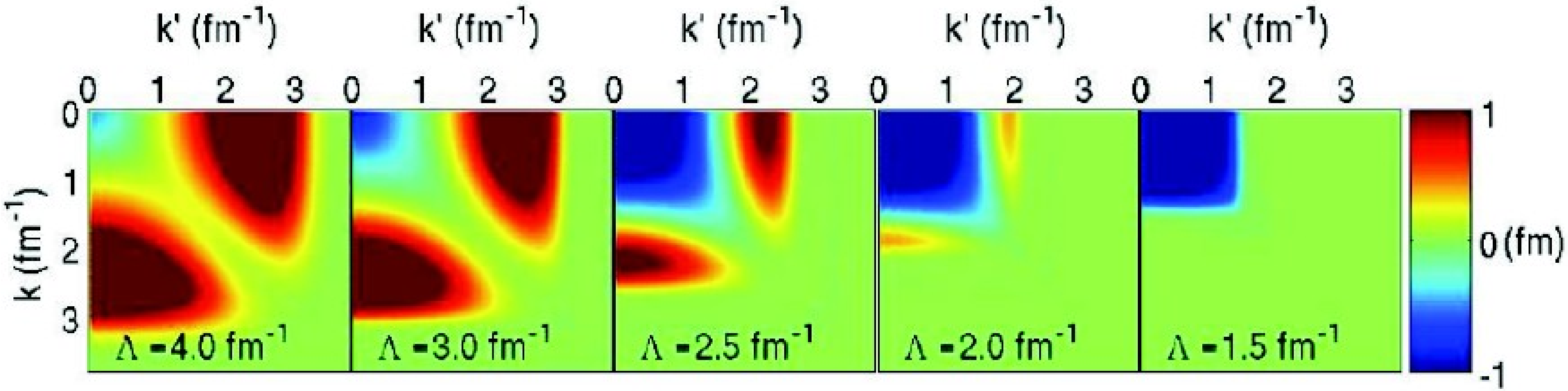
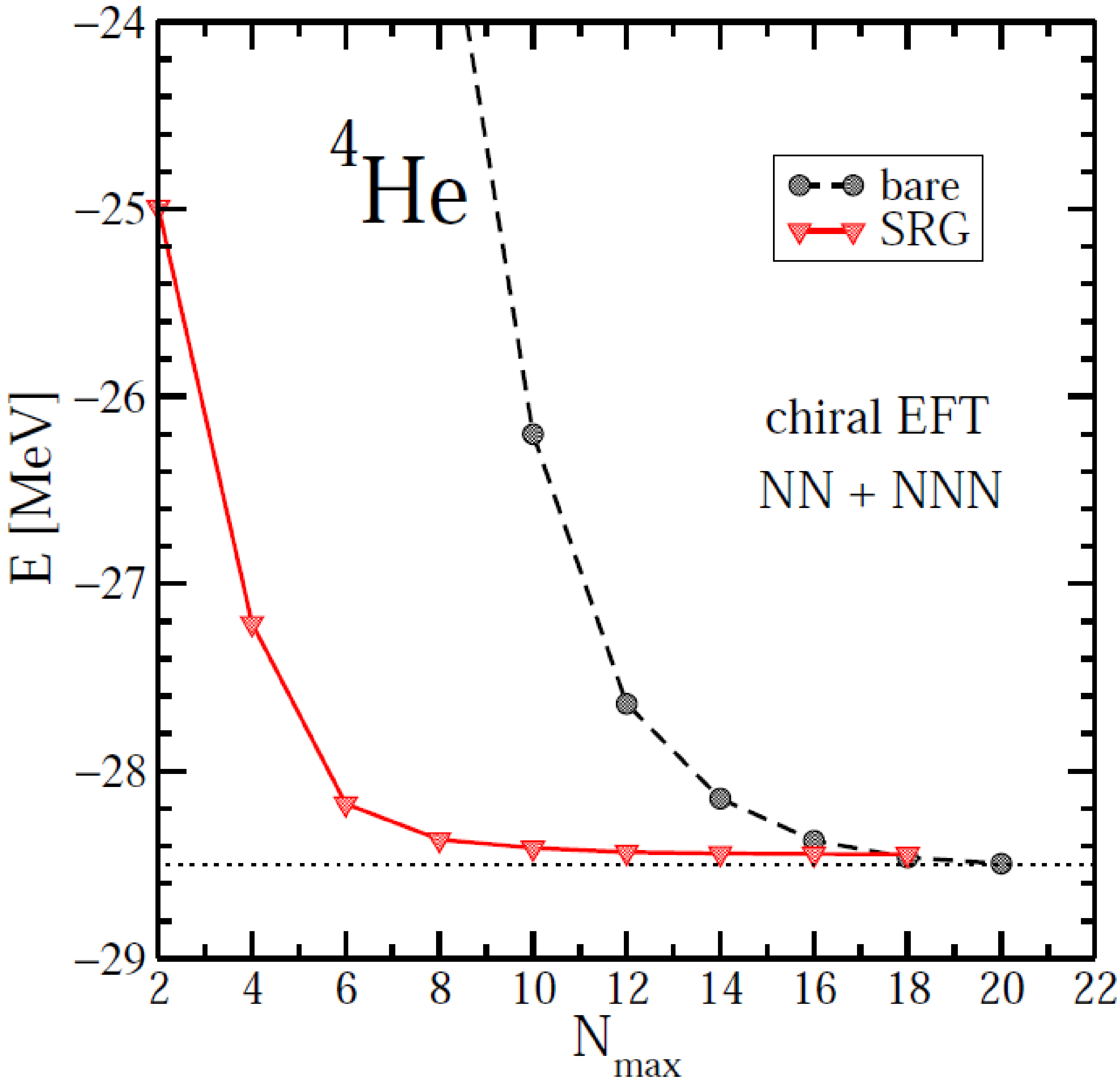


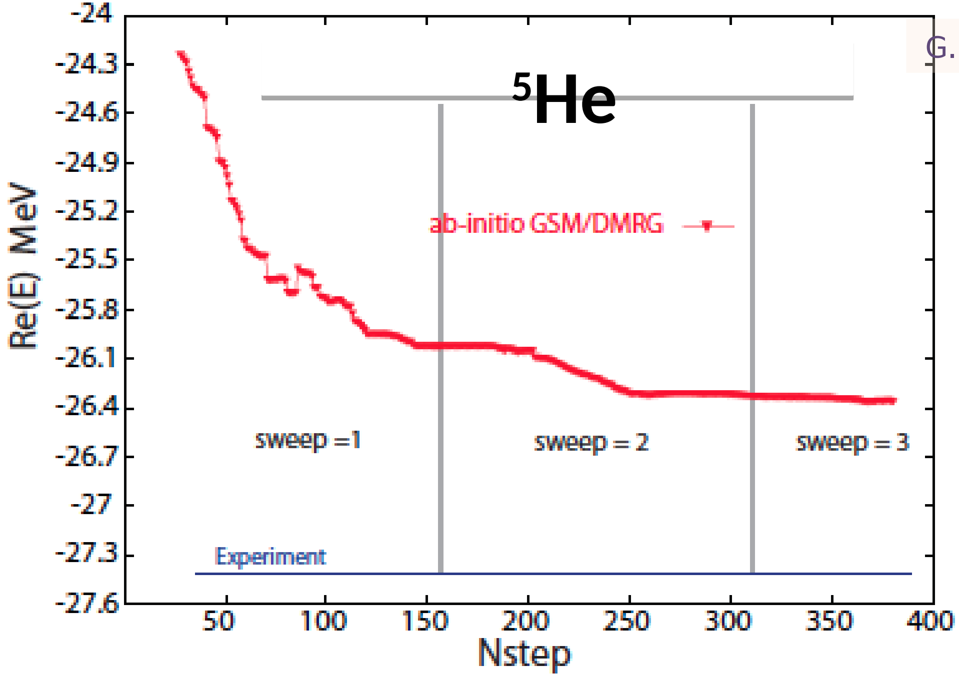
Fig. from S. Bogner et al Prog.Part.Nucl.Phys.65:94-147,2010

→ Observable physics is preserved (e.g. NN phase shifts) AND calculations become easier (work with the relevant degrees of freedom)

→ One has to deal with "induced" many-body forces...



^{4}He
bare
SRG
chiral EFT
NN + NNN
E [MeV]
−24
−25
−26
−27
−28
−29
2
4
6
8
10
12
14
16
18
20
22
N_{max}



G. Papadimitriou et al., PRC 88, 044318 (2013)

Interaction: chiral N^{3}LO $V_{low\text{-}k}$ with $\Lambda = 1.9\ fm^{-1}$

$E_{NCGSM} = -26.31\text{MeV}$

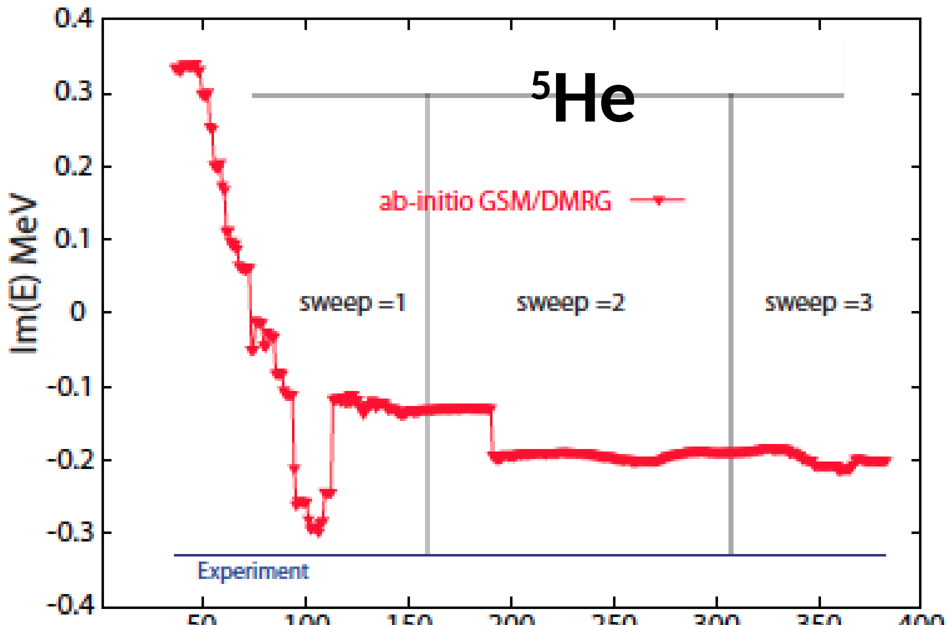
$\Gamma_{NCGSM} = 400\text{keV}$

$E_{Exp} = -27.4\text{MeV}$

$\Gamma_{Exp} = 648\text{keV}$

$E_{CCSD} = -24.8\text{MeV}$

$\Gamma_{CCSD} = 320\text{keV}$



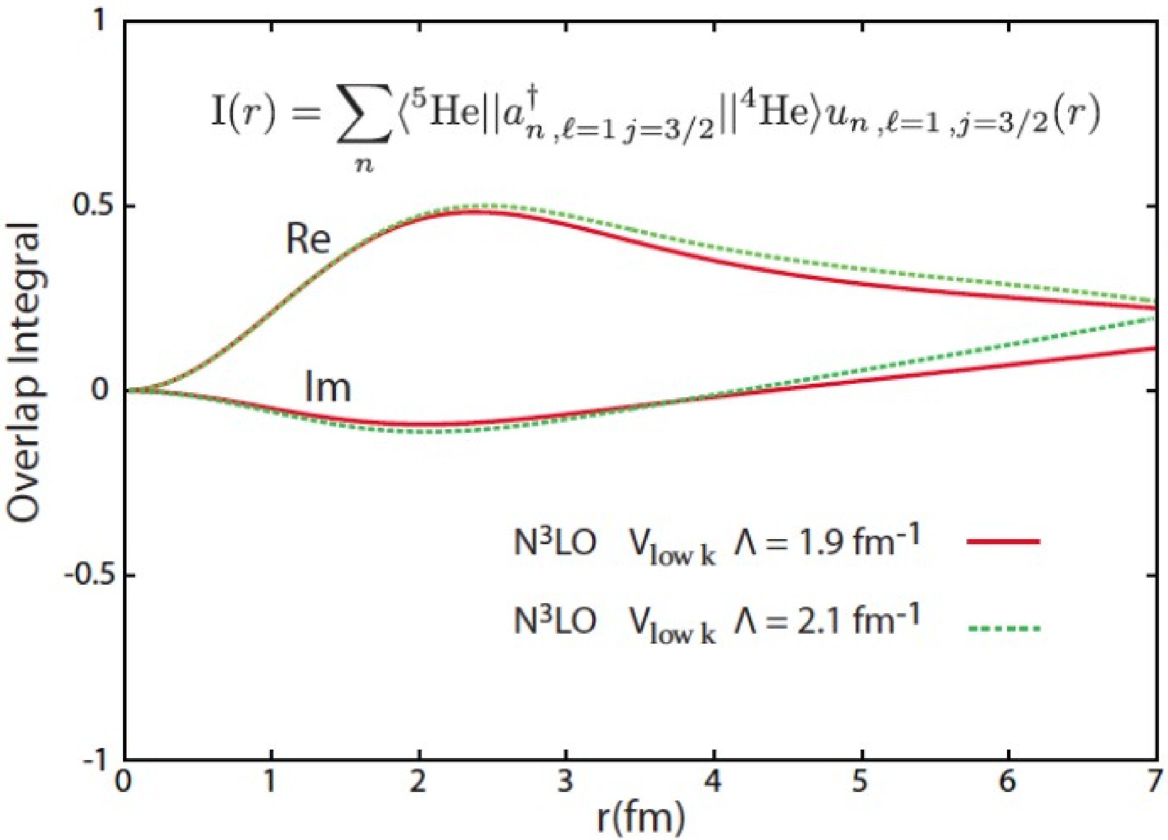
$S_{n;NCGSM} = -1.17\text{MeV}$

$S_{n;Exp} = -0.89\text{MeV}$

$S_{n;CCSD} = -2.51\text{MeV}$

Method	Energy (MeV)	Γ (MeV)
NCGSM$_{\text{DMRG}}$	1.17	0.400
"extended" R-matrix [78]	0.798	0.648
R-matrix [78]	0.963	0.985
NUBASE evaluation [85] [a]	0.890	0.651
^{3}He + t [86]	0.79	0.525

Results: Ab-initio overlaps in the NC-GSM



Overlap tail sensitive to S_{1n}

ANC ($\Lambda = 2.1$ fm^{-1}) = 0.255

S_{1n} ($\Lambda = 2.1$ fm^{-1}) = -1.8 MeV

$\Gamma_{\mathrm{diagonalization}}$ = 591 keV

Γ_{ANC} = 570 keV

⇓

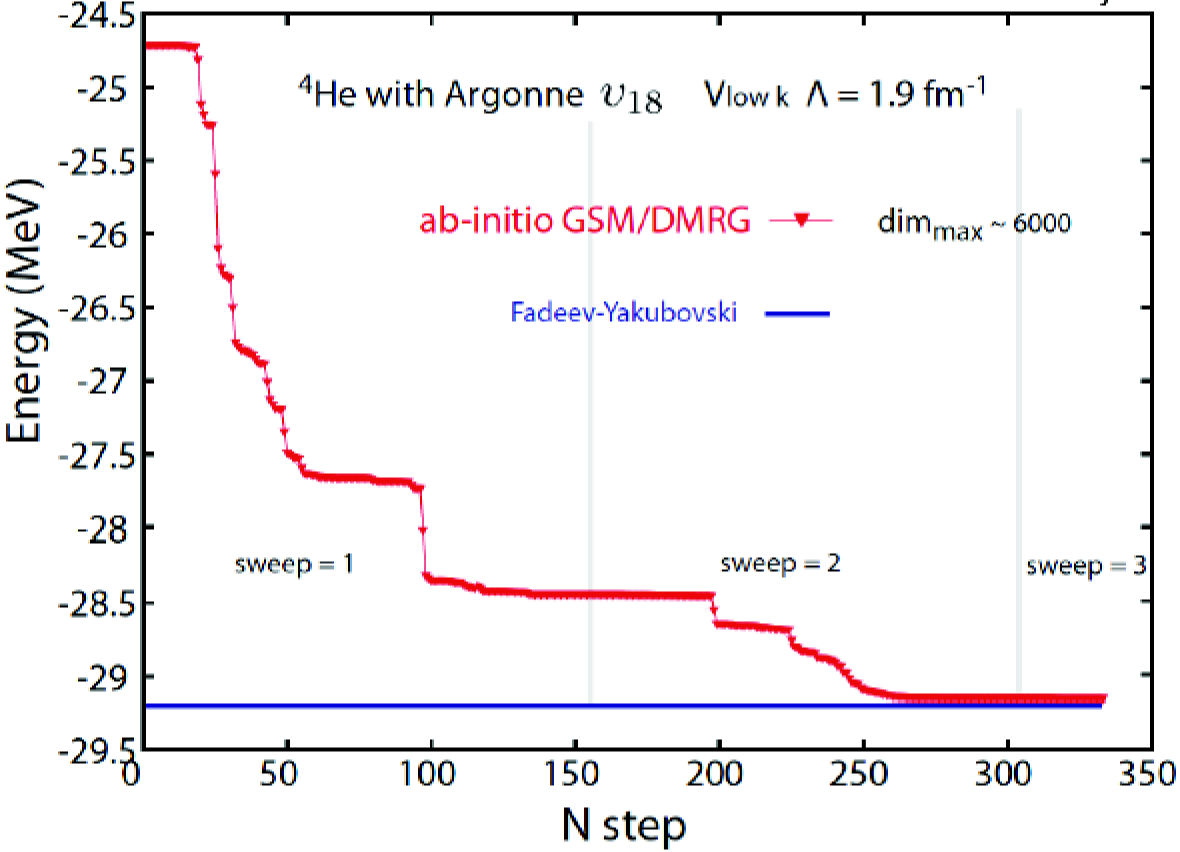
The width exhibits the correct behavior

S.F($\Lambda = 1.9$ fm^{-1}) = 0.62
S.F($\Lambda = 2.1$ fm^{-1}) = 0.66

^{5}He wavefunction fragmented in both cases.
depart from s.p. picture

Results: ^{4}He against Fadeev-Yakubovsky

G.Papadimitriou, J.Rotureau, B. Barrett, N. Michel, M.Ploszajczak arXiv:1301.7140
Submitted at Phys.Rev.C



- 2 neutrons
- 2 protons
- Pole space A:0s1/2 (p/n)
- Continuum space B:
  - p3/2,p1/2,s1/2 real energy continua
  - d5/2-d3/2, f5/2-f7/2, g7/2-g9/2 } H.O states
- 156 s.p. states total

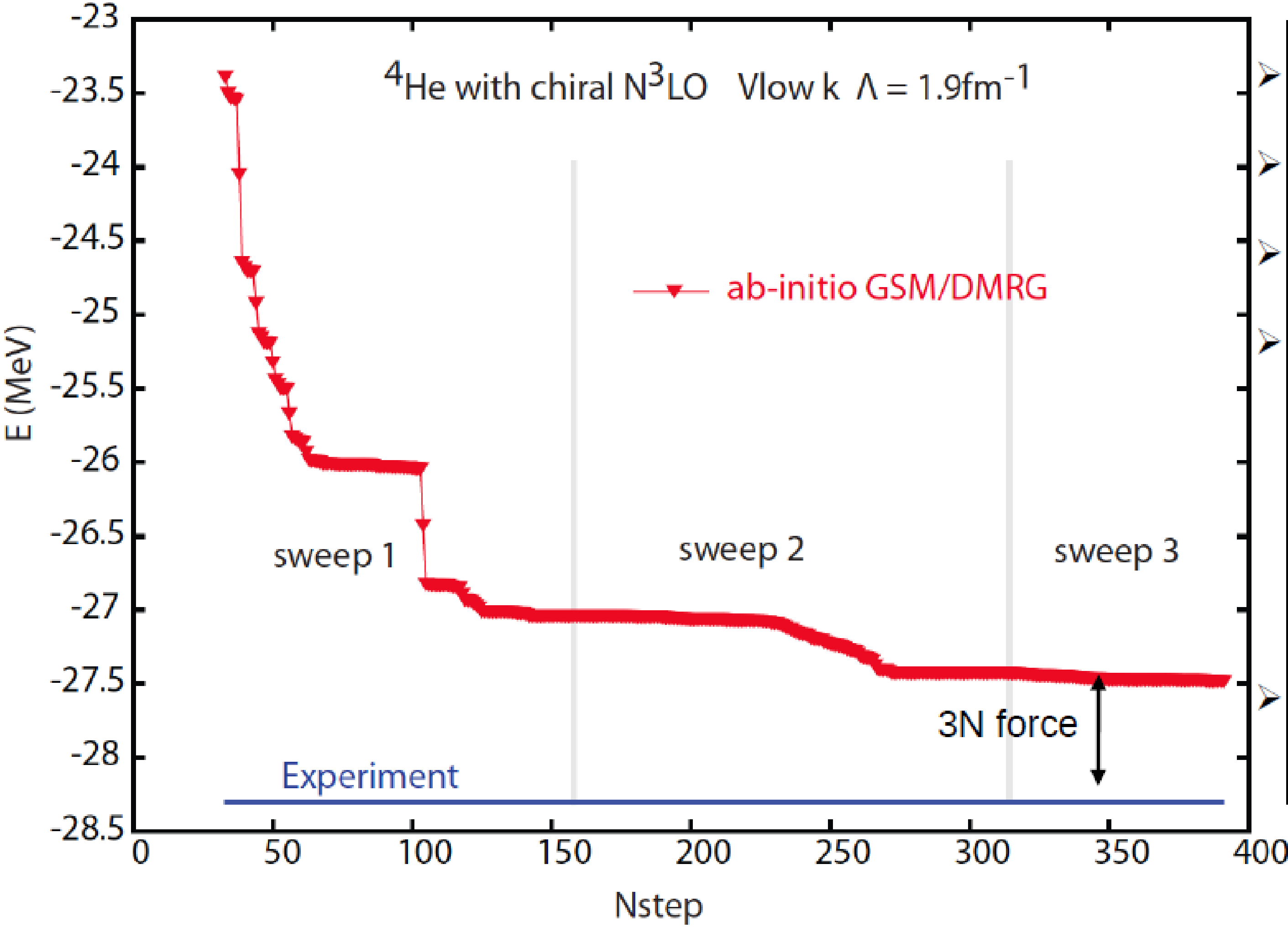
Dim for direct diagon: 119,864,088

$E_{ab\text{-}initio}$ = -29.15 MeV

E_{FY} = -29.19 MeV

Results: ^{4}He with chiral N^3LO

G.P., J.Rotureau, N. Michel, M.Ploszajczak, B. Barrett arXiv:1301.7140



- 2 neutrons
- 2 protons
- Pole space A:0s1/2 (p/n)
- Continuum space B: p3/2,p1/2,s1/2 real energy continua

  d5/2-d3/2
  f5/2-f7/2 H.O states
  g7/2-g9/2
- 156 s.p. states total

E_{N3LO} = -27.48 MeV

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

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

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

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

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

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

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

Effective Hamiltonian for NCSM

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

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

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

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

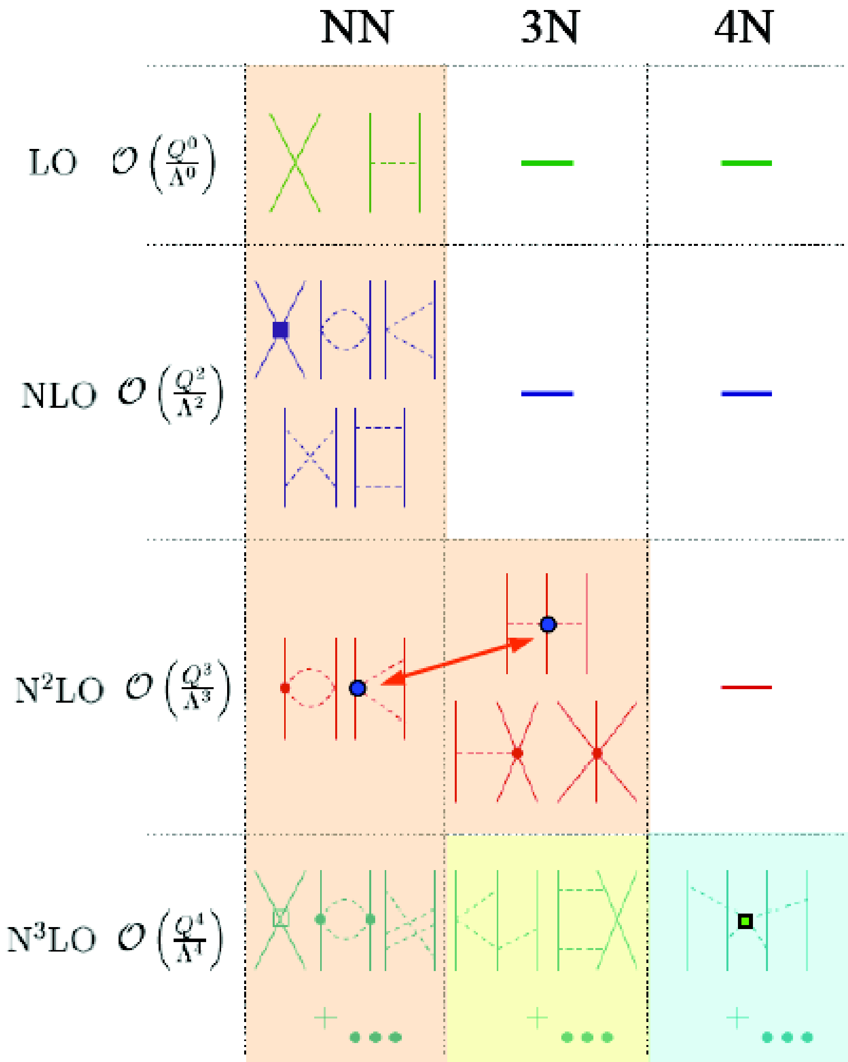
Two ways of convergence:

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

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

Chiral effective field theory (EFT) for nuclear forces

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

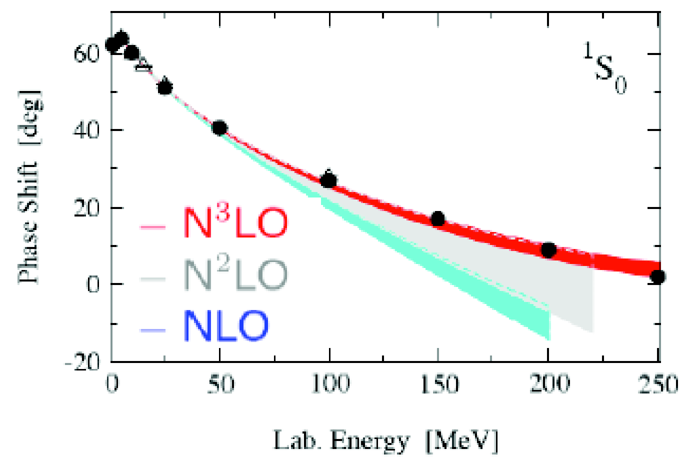


explains pheno hierarchy:
NN > 3N > 4N > …

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