From the No Core Shell Model to the No Core Gamow Shell Model using the Berggren basis

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INT-13-2b

August 8, 2013

Nuclei and Fundamental Symmetries: Theory Needs of Next-Decade Experiments

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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)

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

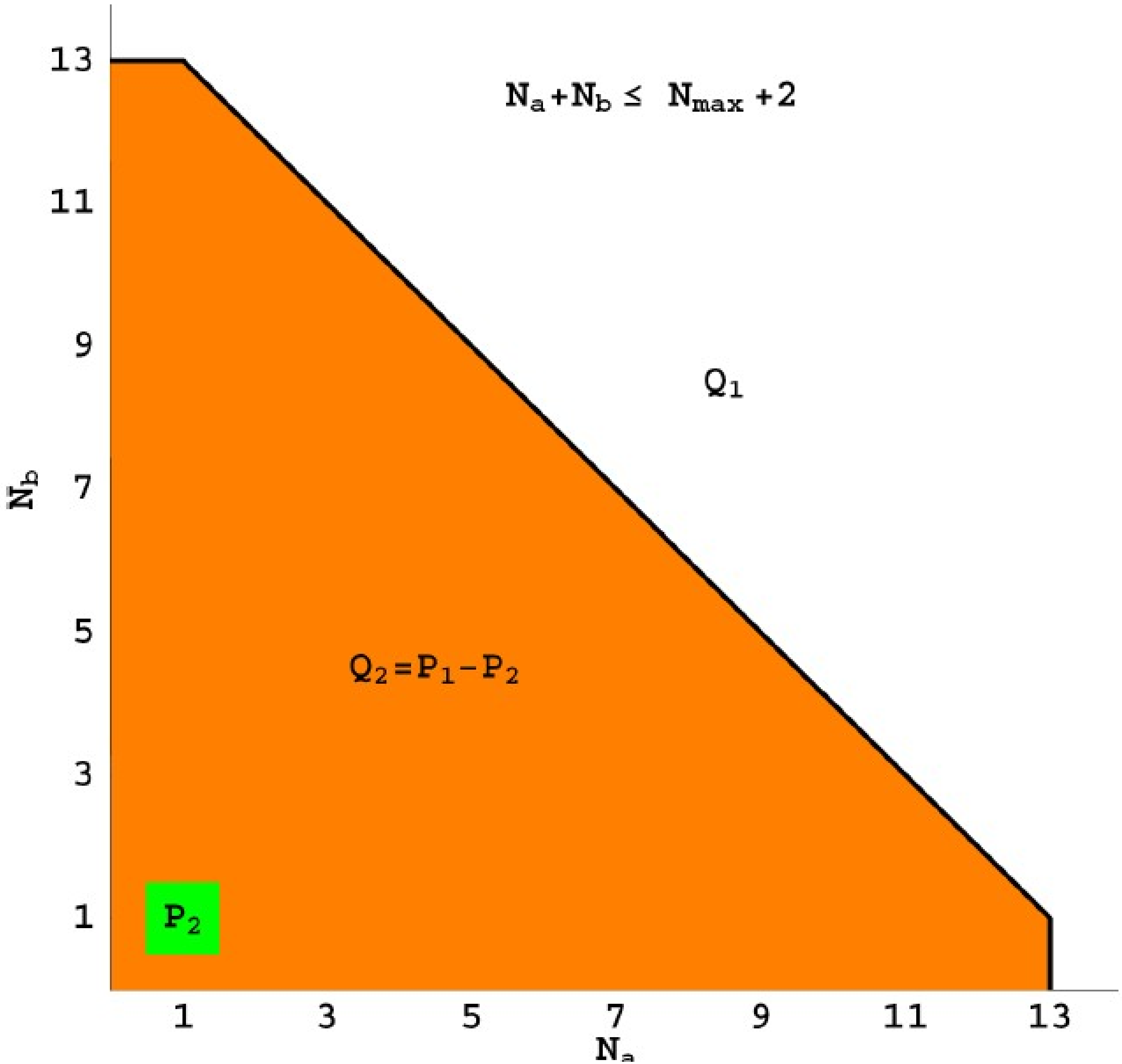
- Next, add CM harmonic-oscillator Hamiltonian

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

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}



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

From few-body to many-body

Ab initio
No Core Shell Model

Realistic NN & NNN forces

↓

Effective interactions in cluster approximation

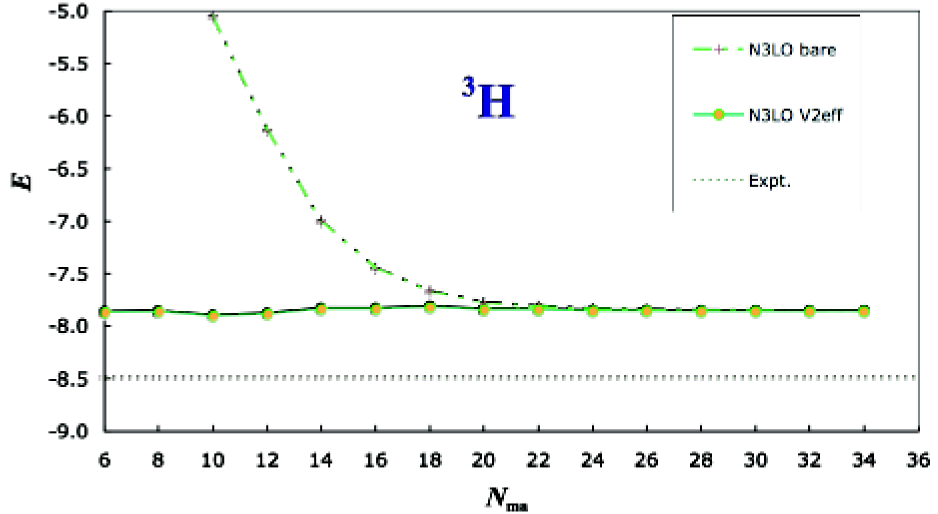
↓

Diagonalization of many- body Hamiltonian

↓

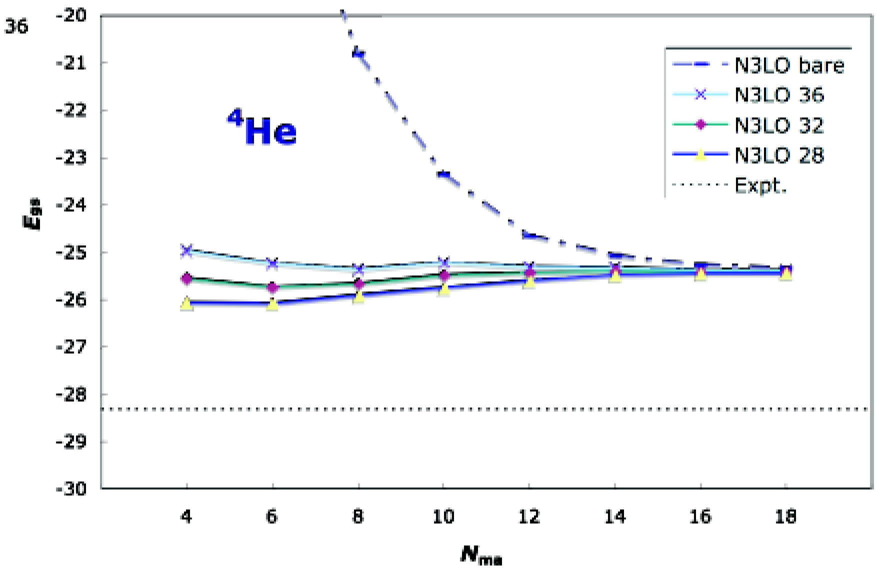
Many-body experimental data

- NCSM convergence test
  - Comparison to other methods



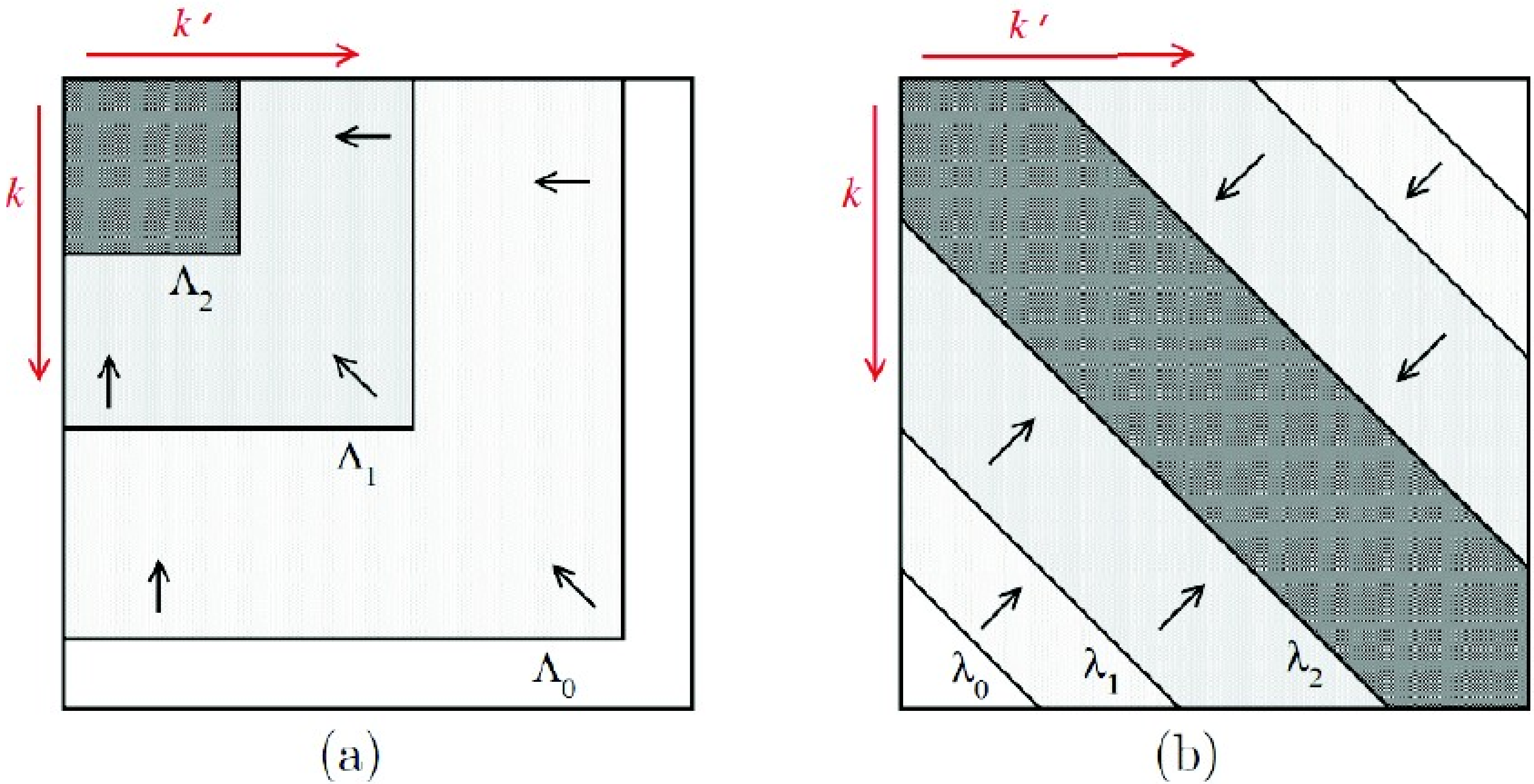
N^3LO NN	NCSM	FY	HH
^{3}H	7.852(5)	7.854	7.854
^{4}He	25.39(1)	25.37	25.38

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



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

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 $V_{low\text{-}k}$ or Similarity RG approaches (e.g. SRG)

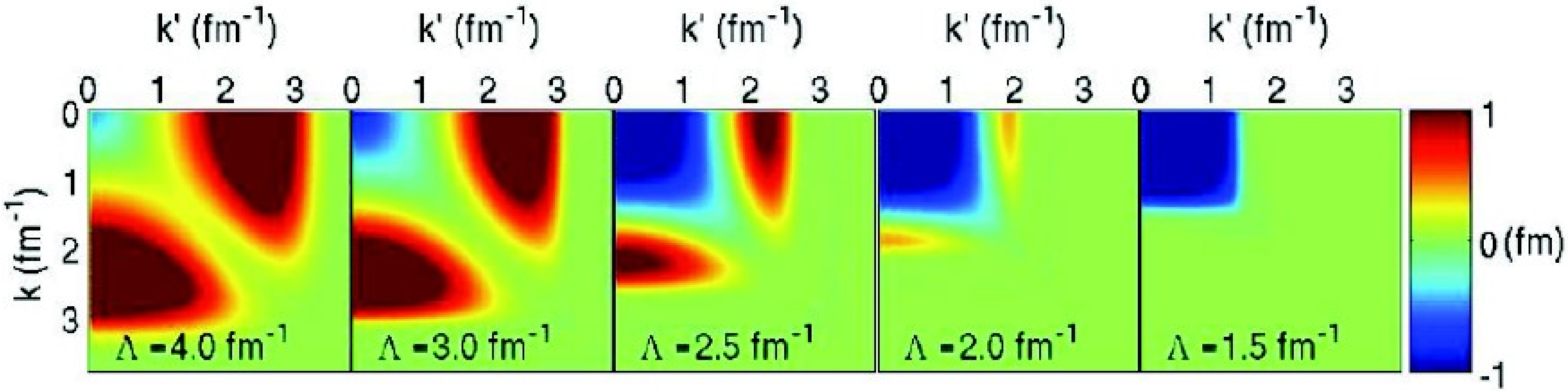
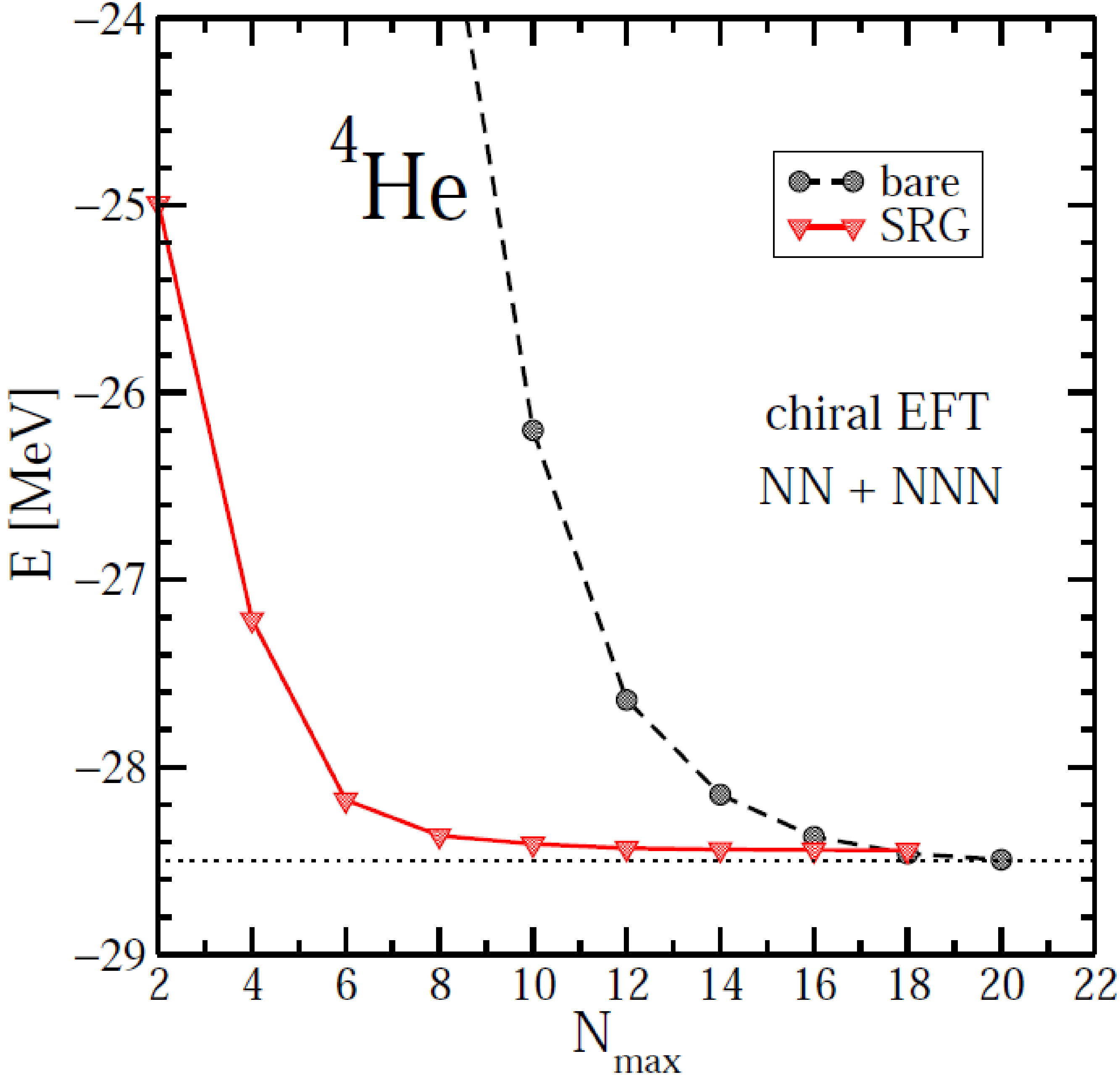


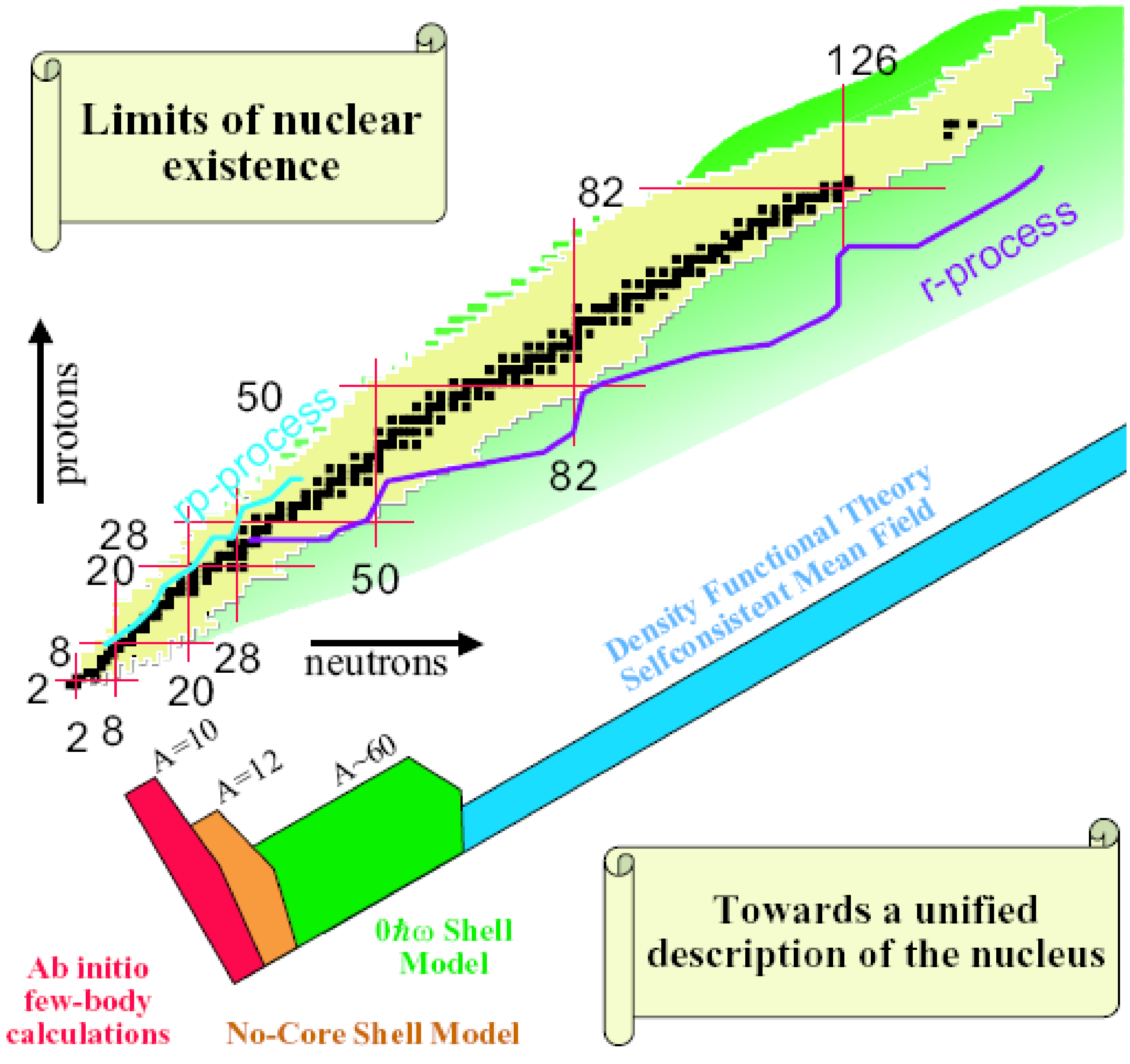
Fig. from S. Bogner et al Prog.Part.Nucl.Phys.65:94-147,2010

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

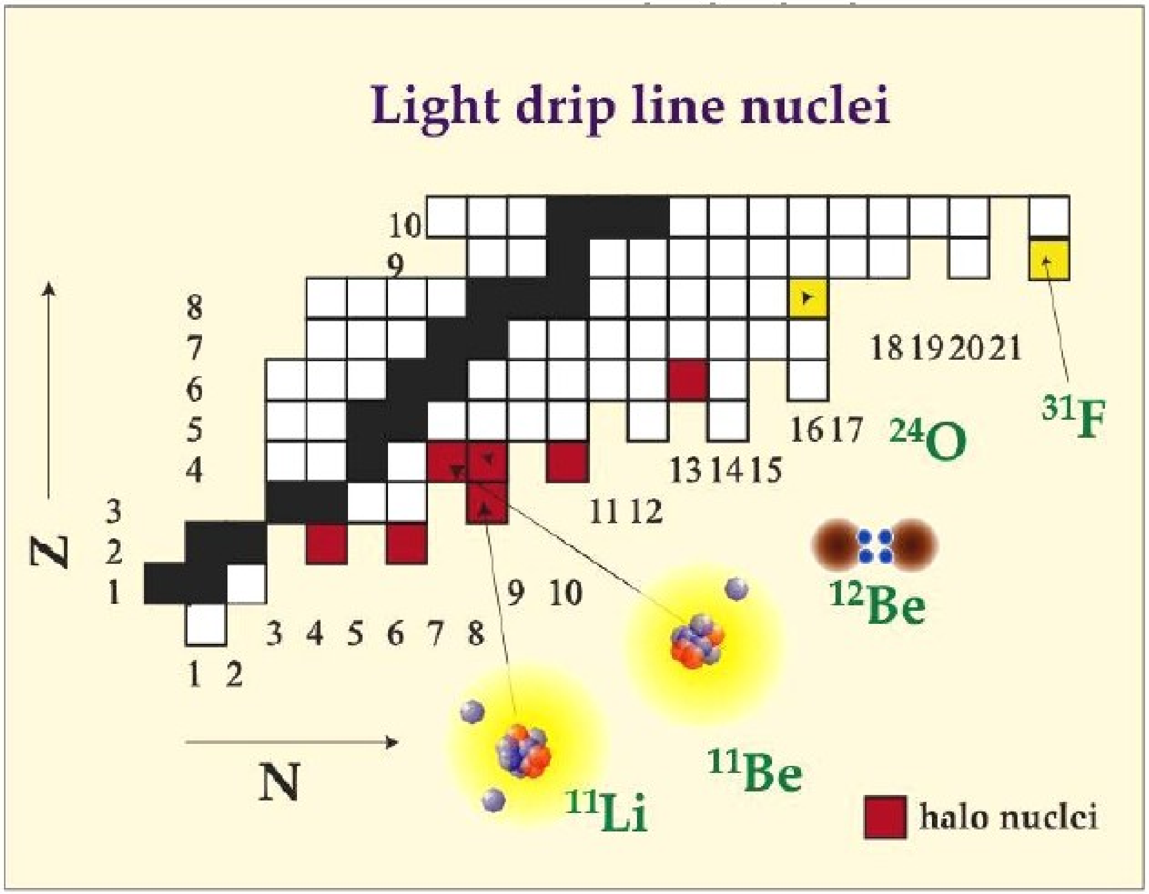
→ One has to deal with "induced" many-body forces…

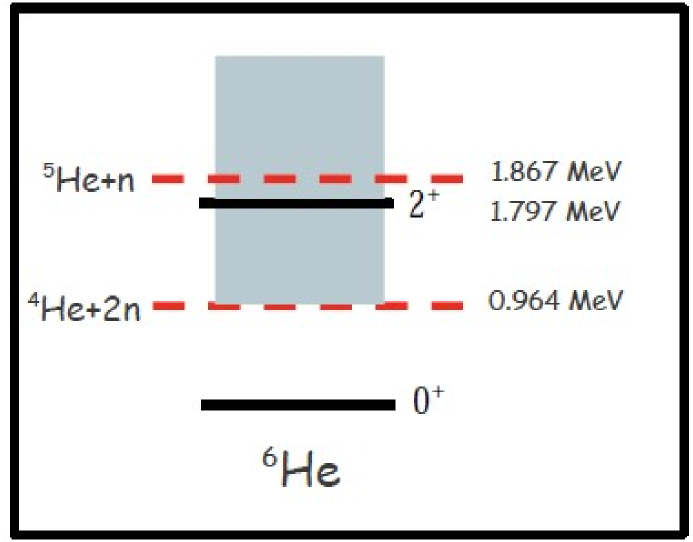


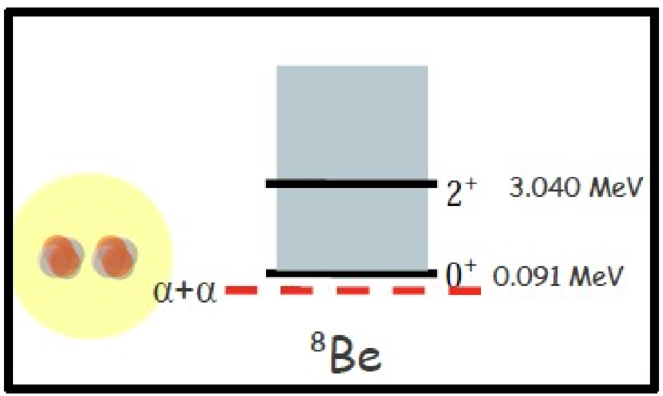
4He
bare
SRG
chiral EFT
NN + NNN
E [MeV]
N max
−24
−25
−26
−27
−28
−29
2
4
6
8
10
12
14
16
18
20
22

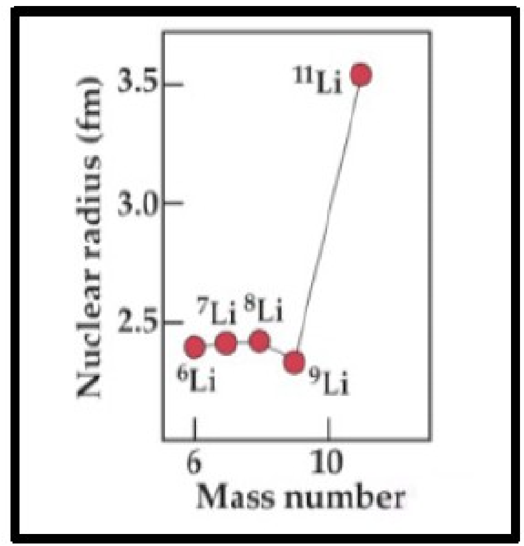


Limits of nuclear existence
protons
neutrons
126
82
82
50
50
28
20
8
2
28
20
2 8
rp-process
r-process
Density Functional Theory
Selfconsistent Mean Field
A=10
A=12
A~60
Ab initio
few-body
calculations
No-Core Shell Model
0ħω Shell
Model
Towards a unified
description of the nucleus

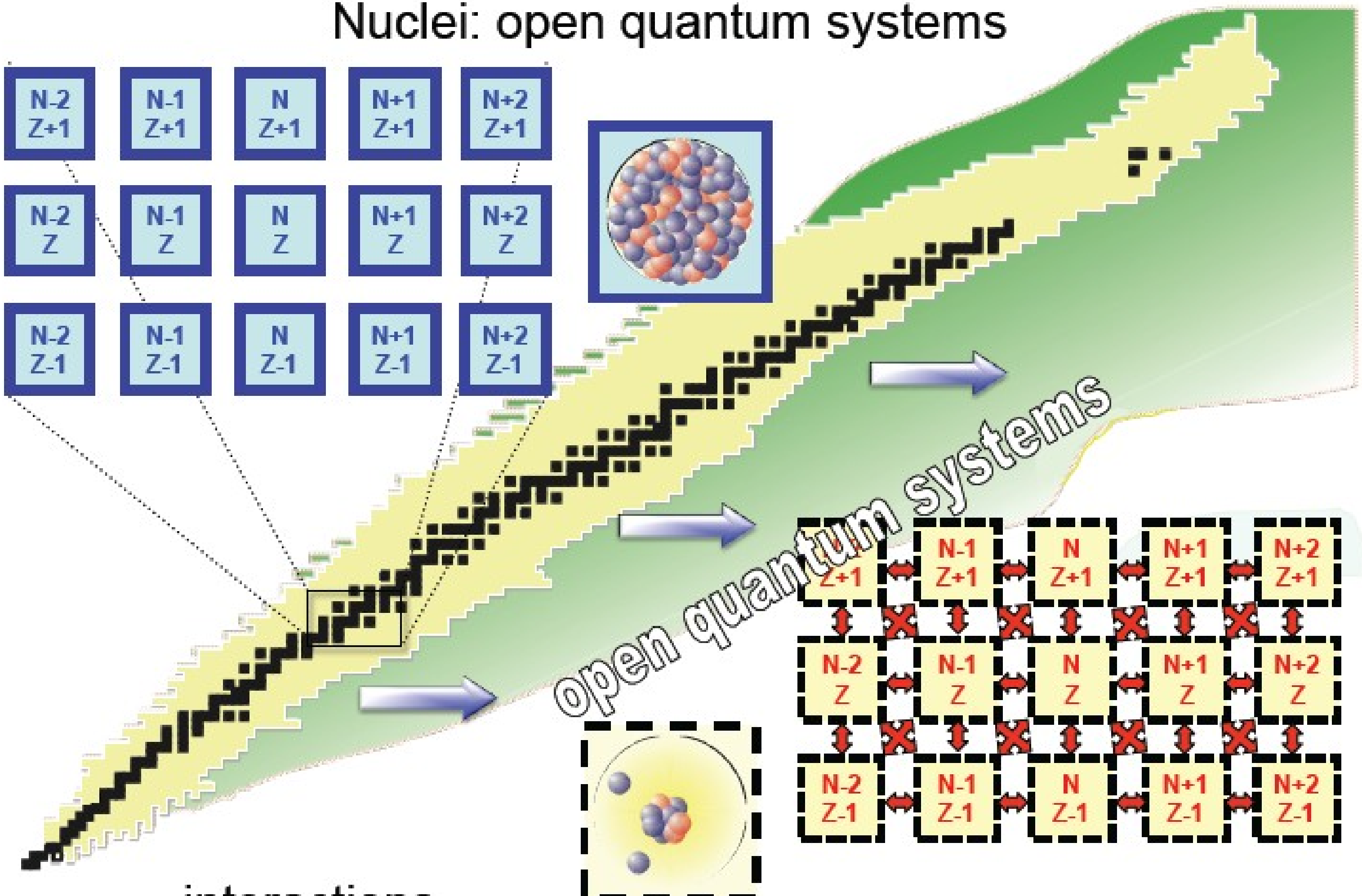

Light drip line nuclei
Z
N
1 2 3 4 5 6 7 8 9 10
1 2 3 4 5 6 7 8 9 10 11 12 13 14 15 16 17 18 19 20 21
^{11}Li
^{11}Be
^{12}Be
^{24}O
^{31}F
halo nuclei


$^{5}He+n$
1.867 MeV
2^+
1.797 MeV
$^{4}He+2n$
0.964 MeV
0^+
^{6}He

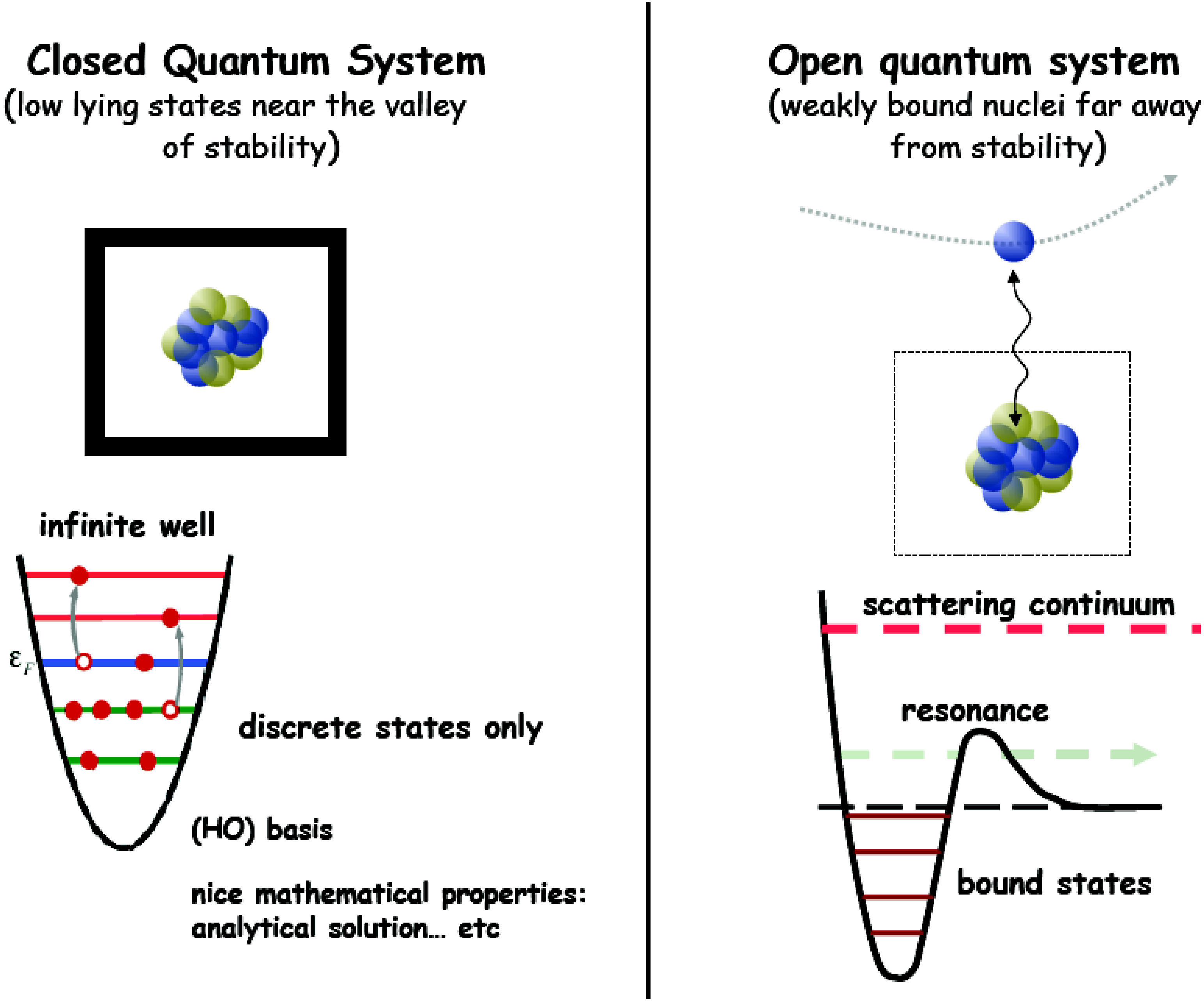

2^+
3.040 MeV
$\alpha+\alpha$
0^+
0.091 MeV
^{8}Be


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

Nuclei: open quantum systems



interactions
correlations
many-body techniques


Closed Quantum System
(low lying states near the valley of stability)
infinite well
ε_F
discrete states only
(HO) basis
nice mathematical properties: analytical solution... etc
Open quantum system
(weakly bound nuclei far away from stability)
scattering continuum
resonance
bound states

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)

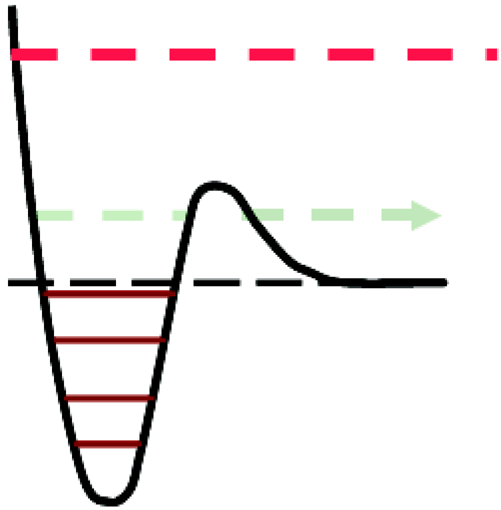
G. Hagen, T. Papenbrock, and M. Hjorth-Jensen, Phys. Rev. Lett. 104, 182501 (2013)

Green's Function Monte Carlo approach

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

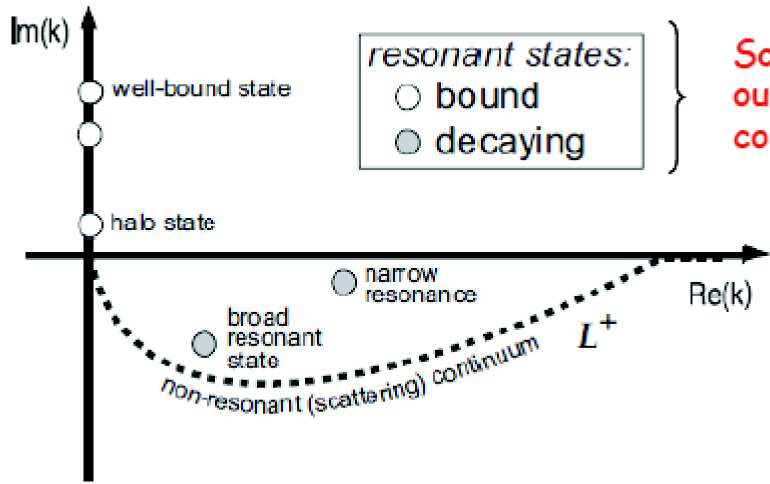
K. M. Nollett, Phys. Rev. C 86, 044330 (2012)

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



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

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



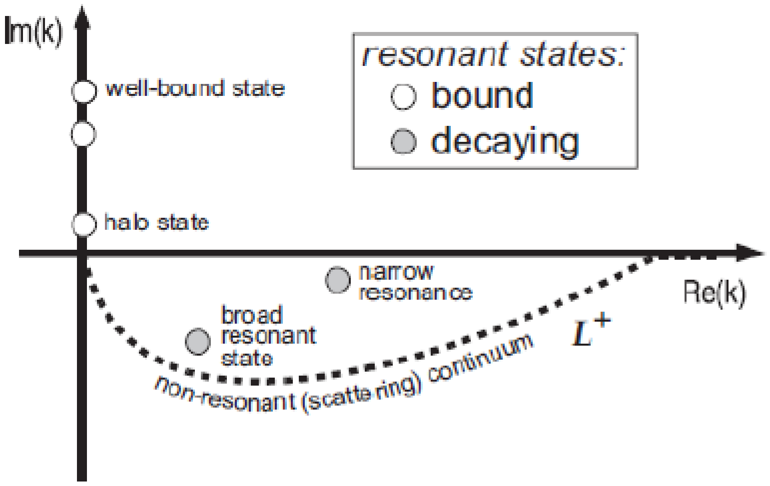
Solutions with outgoing boundary conditions

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

$$u_l(k,r)\sim C_+H_l^+(k,r)\,,r\rightarrow\infty\ \ \textit{bound states, resonances}$$

$$u_l(k,r)\sim C_+H_l^+(k,r)+C_-H_l^-(k,r)\,,r\rightarrow\infty\ \ \textit{scattering states}$$

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)

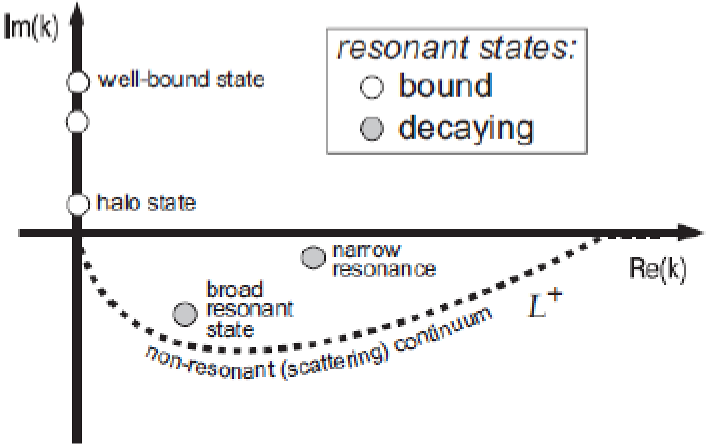
The shape of the contour is arbitrary, but it has to be below the resonance(s) position(s) (proof by T. Berggren)

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

The Density Matrix Renormalization Group (DMRG)

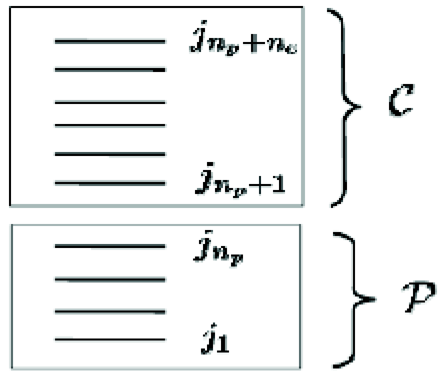
S.R White PRL 69 (1992) 2863
T.Papenbrock and D.Dean J.Phys.G 31 (2005) S1377
S.Pittel et al PRC 73 (2006) 014301
J.Rotureau et al PRC 79 (2009) 014304
J. Rotureau et al PRL 97 (2006) 110603

✓ **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:

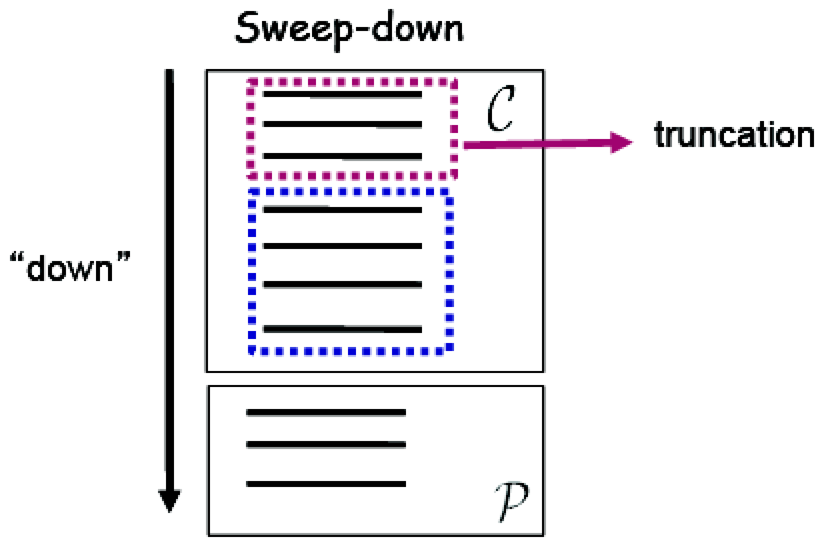
$$\rho^{J_c}_{c,c'} = \sum_p \Psi_{pc} \Psi_{pc'}$$

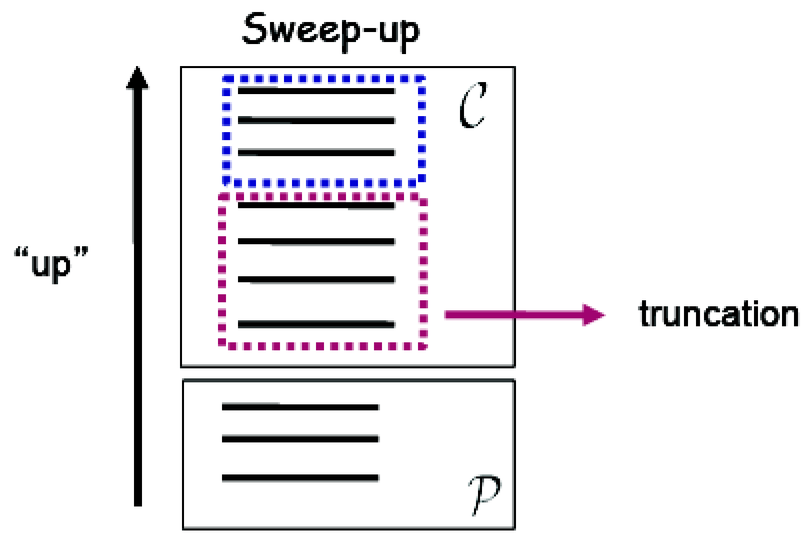
• truncation with the density matrix :

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

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

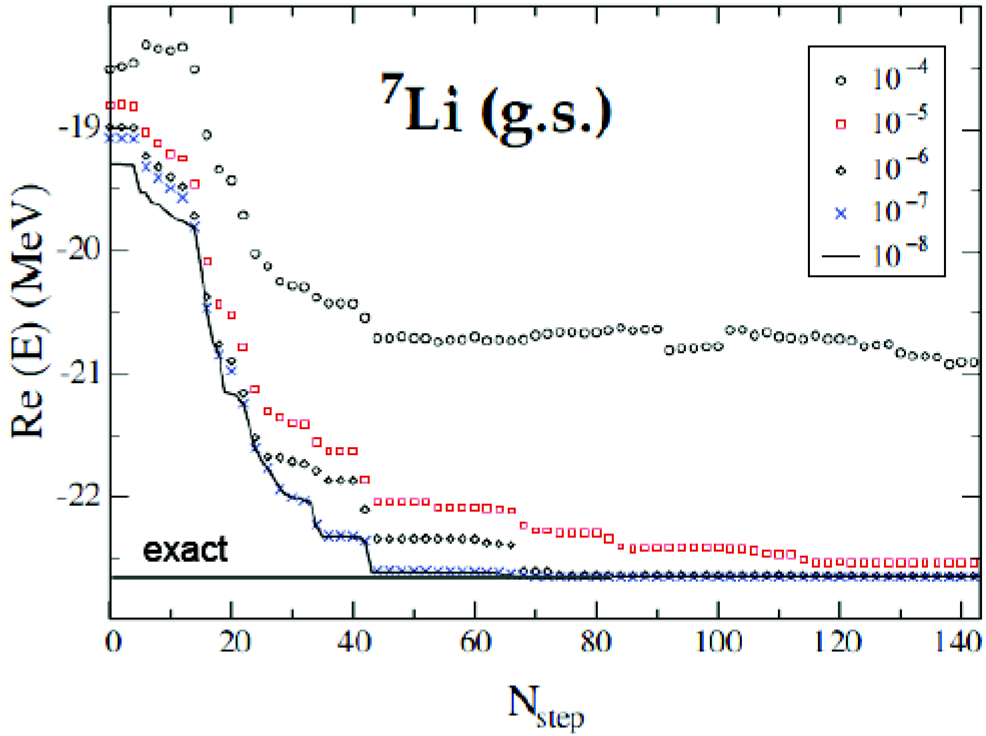
- The process is reversed...
- In each step (shell added) the Hamiltonian is diagonalized and N_{opt} states are kept.
- Iterative method to take into account all the degrees of freedom in an effective manner.
- In the end of the process the result is the same with the one obtained by "brute" force diagonalization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

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

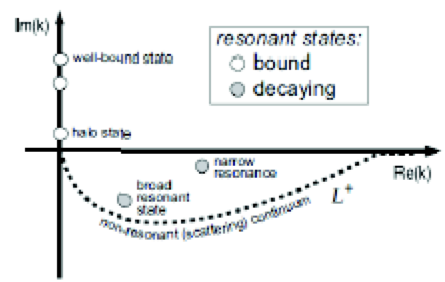
Small ε → more states of ρ are kept in each step

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

Gamow Shell Model in an ab-initio framework

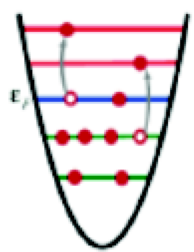
$$H = \frac{1}{A}\sum_{i<j}^{A} \frac{(\vec{p}_i - \vec{p}_j)^2}{2m} + V_{NN,ij} + \ldots \quad (1)$$

- 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. Λ_{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

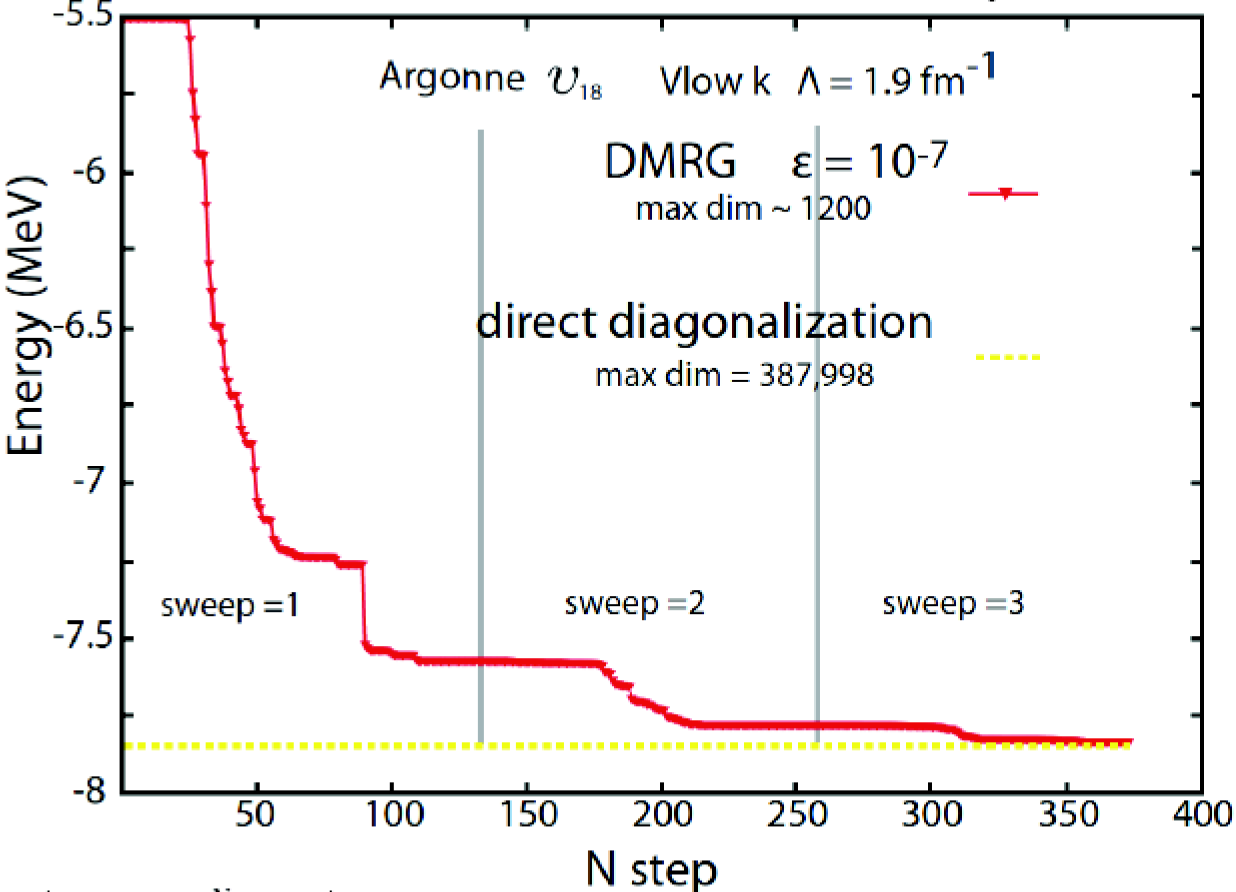


- Diagonalization of (1) → Applications to ^3H, ^4He, ^5He

III. NCGSM: Applications to Light Nuclei

Results: Triton

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



- 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

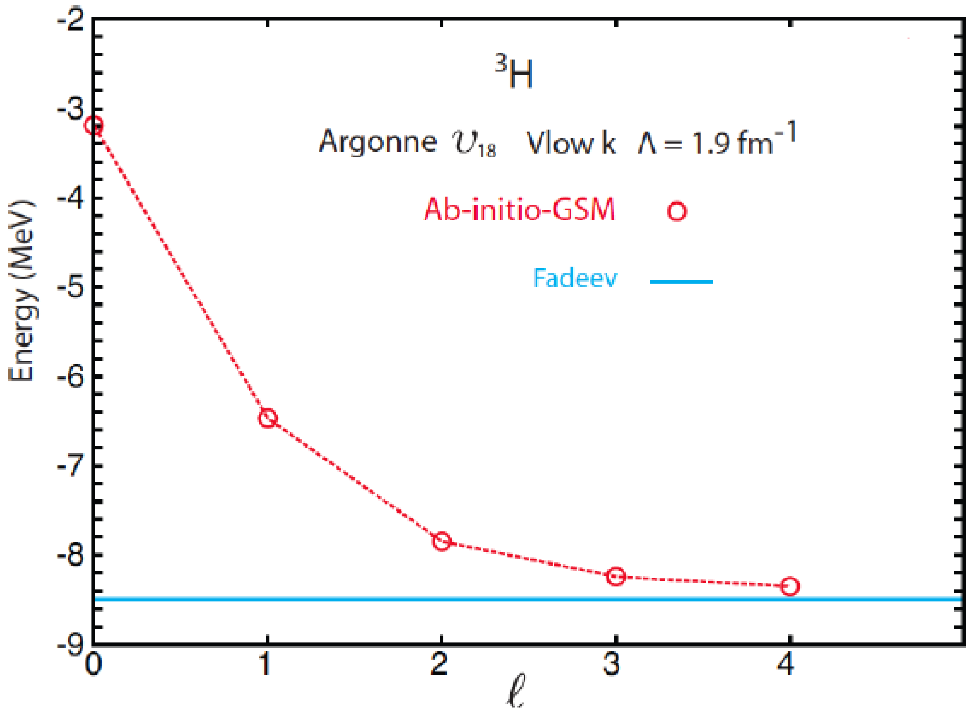
$$\left| 1 - \mathcal{R}e\left(\sum_{i=1}^{N_\rho} w_i\right)\right| < e$$

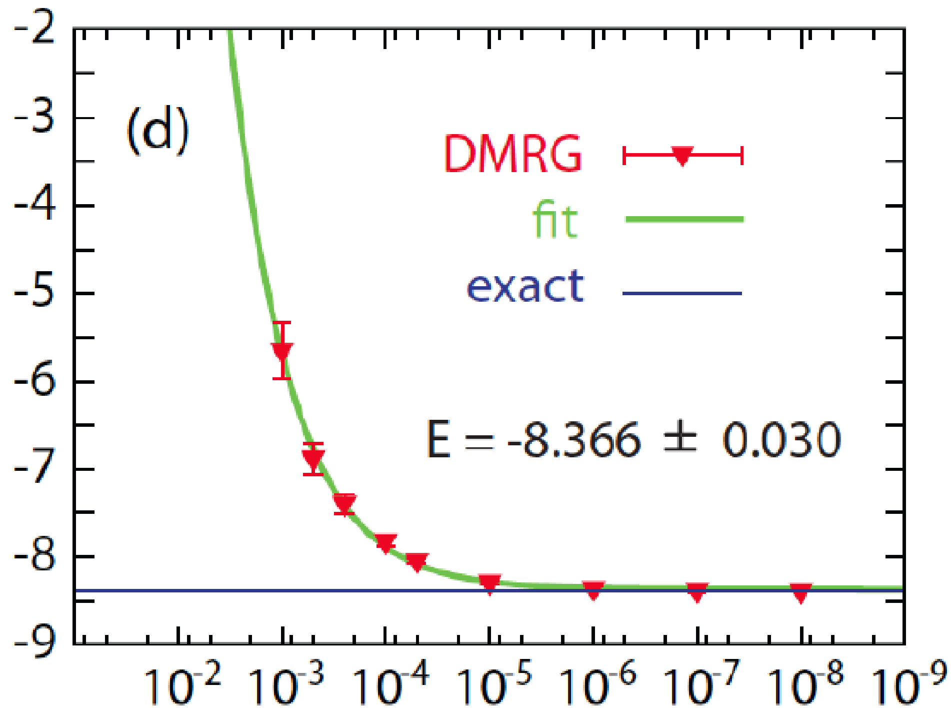
$$\sum_\alpha w_\alpha = 1$$

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





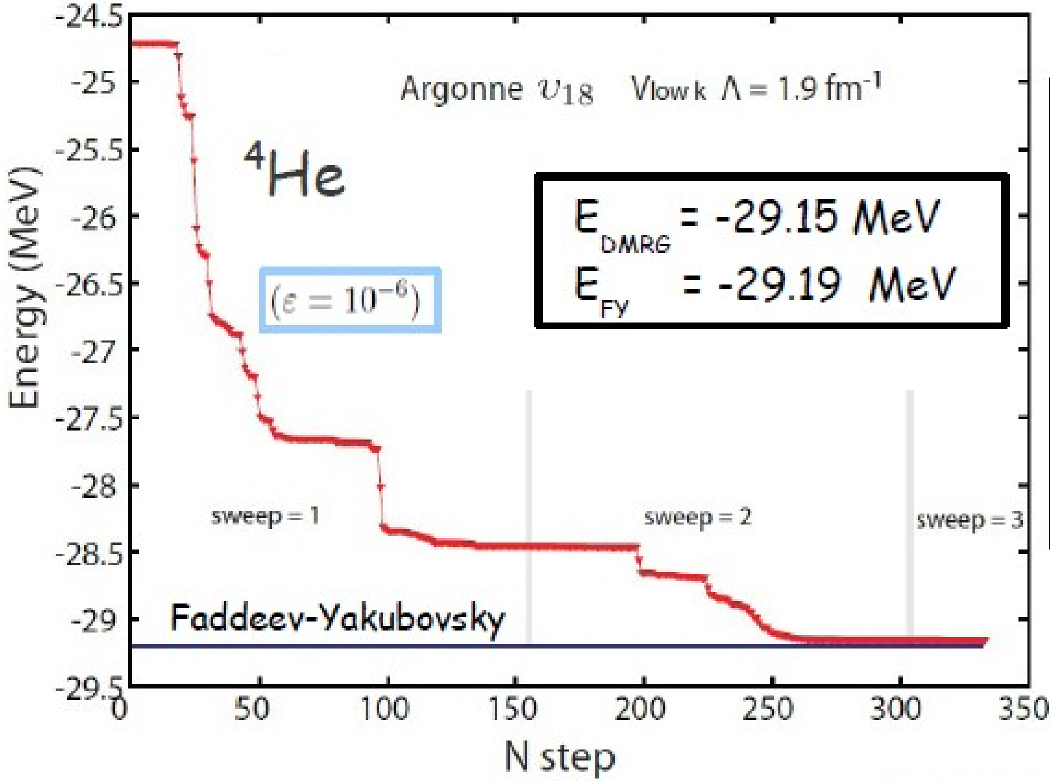
E_{Fadeev} = -8.47 MeV

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

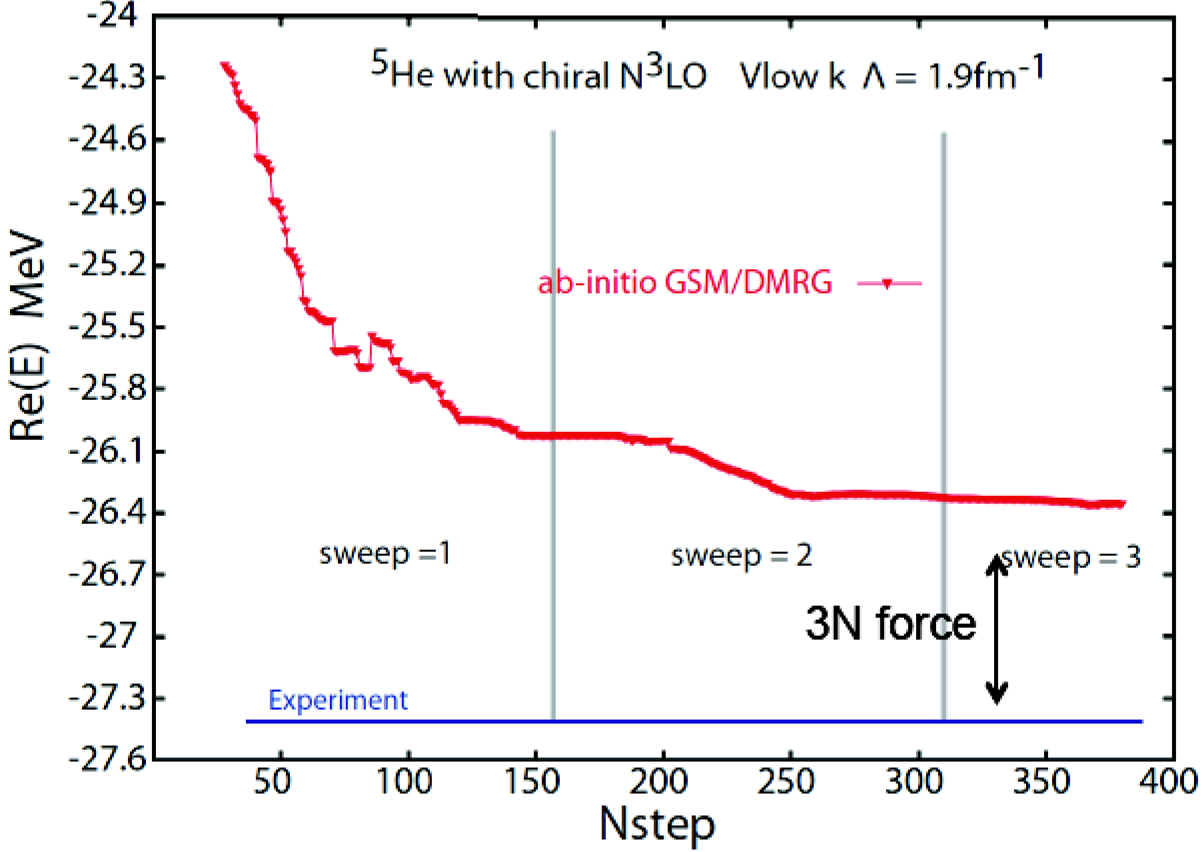
J-scheme dimension

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

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

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

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



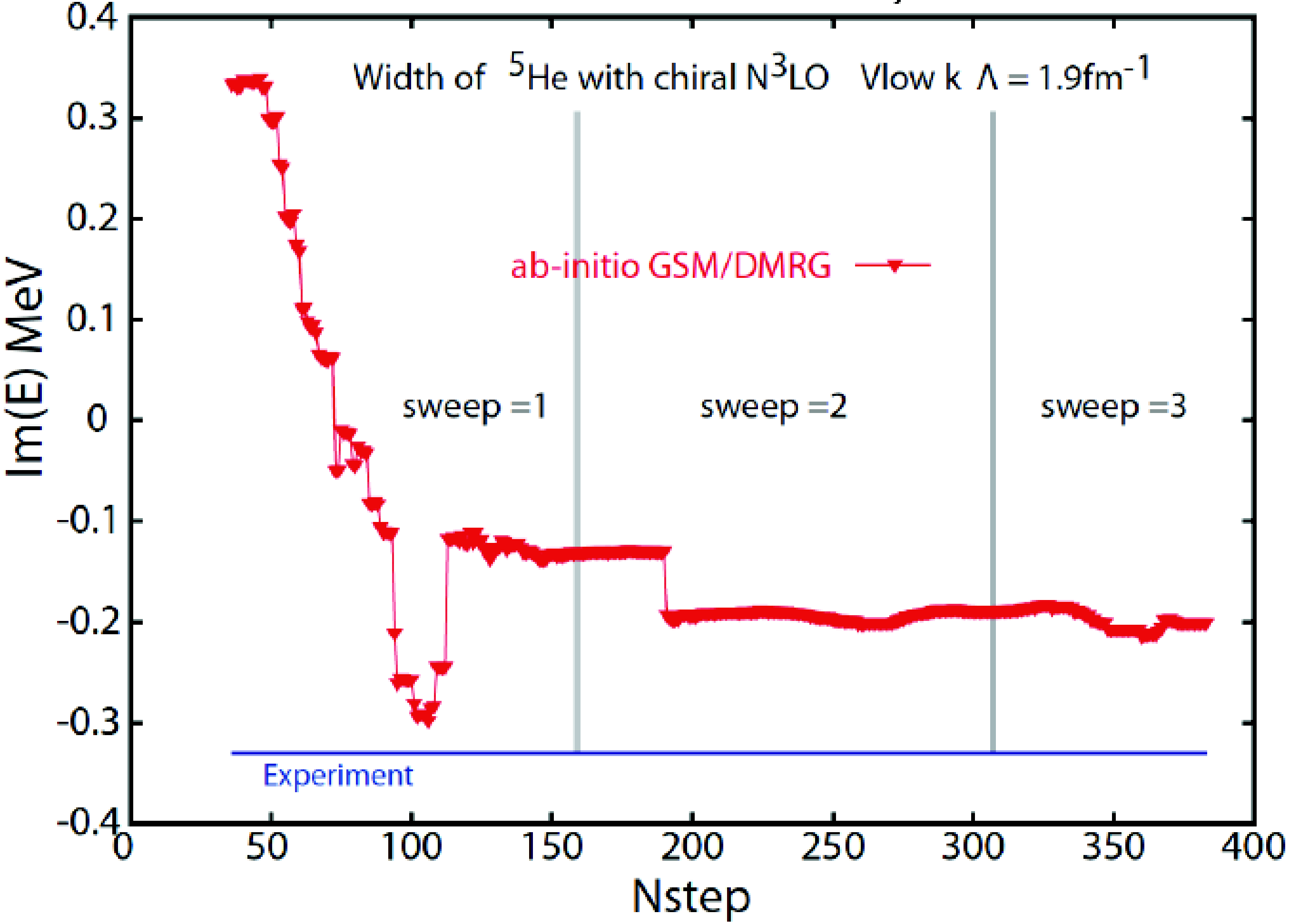
- 3 neutrons
- 2 protons
- Pole space A:0s1/2 (p/n) + 0p3/2 n resonant state
- Continuum space B:
  - p3/2 complex continuum
  - p1/2-s1/2 real continua
  - d5/2-d3/2, f5/2-f7/2, g7/2-g9/2 } H.O states
- 157 s.p. states total

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

DMRG dim ~ 10^5

Results: ^{5}He 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 ^{5}He reproduced within an ab-initio framework

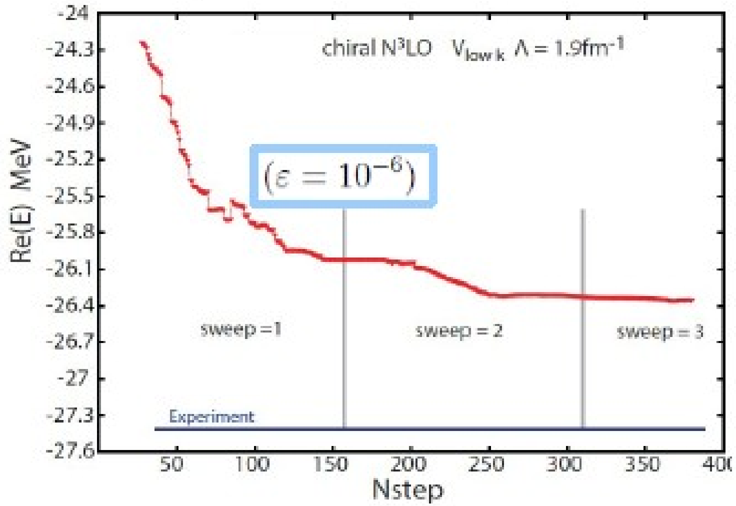
Satisfactory agreement of the **width** with experiment

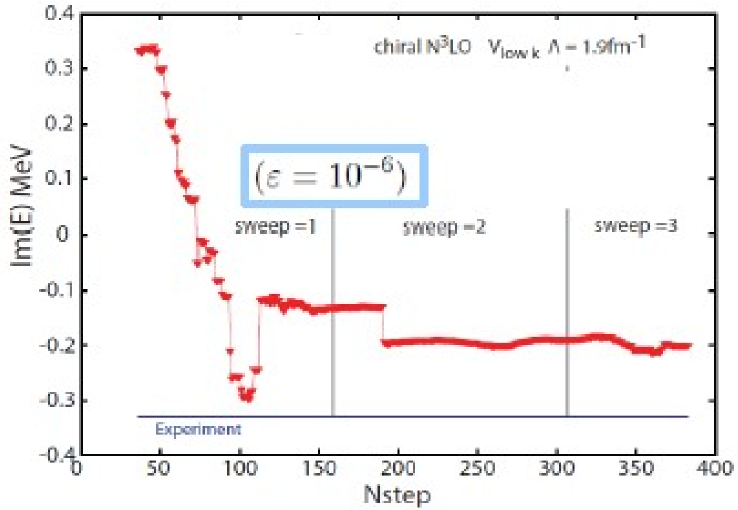
^5He

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)

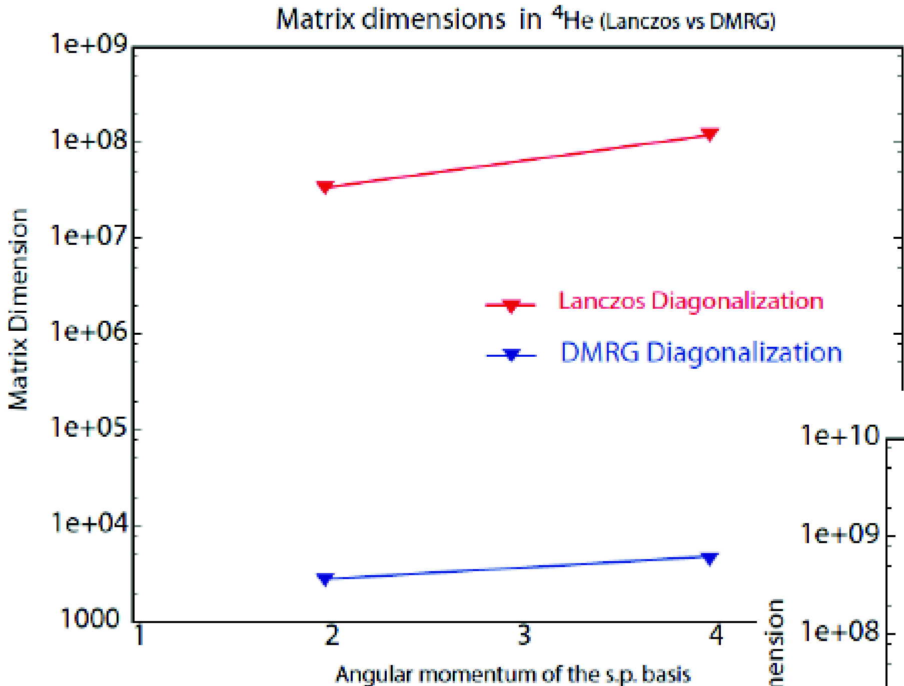
G. Hagen *et al*, PLB 656 (2007) 169.

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

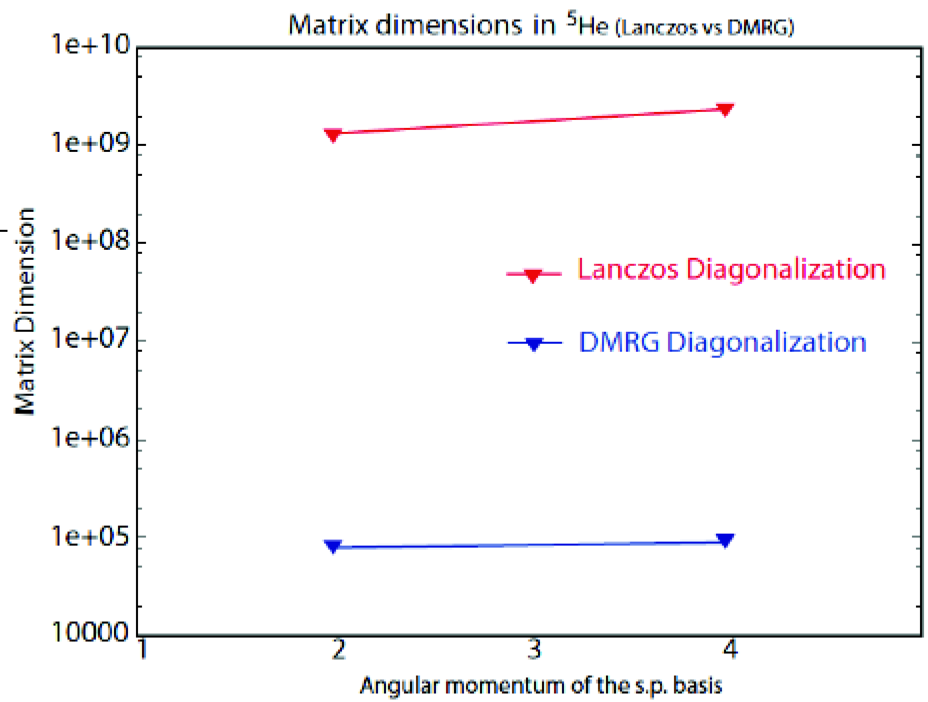
*D. R. Tilley, et al., Nucl. Phys. A 708, 3 (2002)

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



IV. Summary and Outlook

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

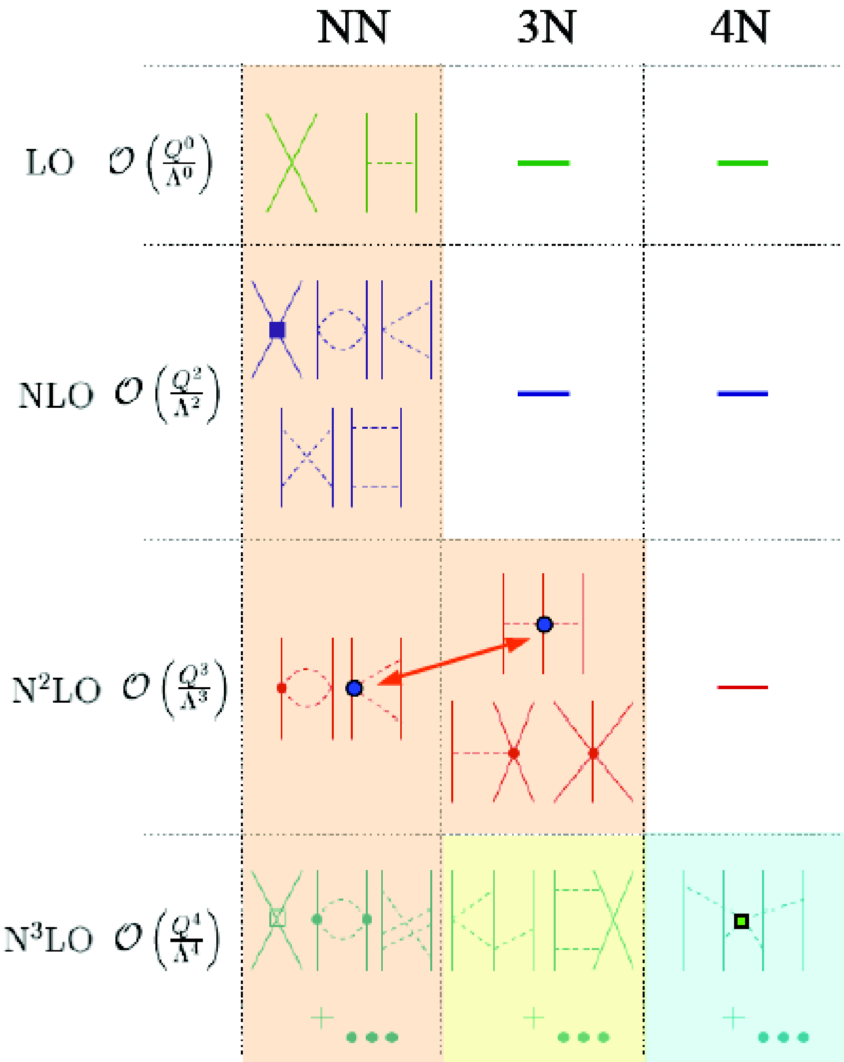
2. Berggren basis has been applied successfully in an ab-initio GSM framework --> No Core Gamow Shell Model for weakly bound/unbound nuclei.

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.

Chiral effective field theory (EFT) for nuclear forces

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

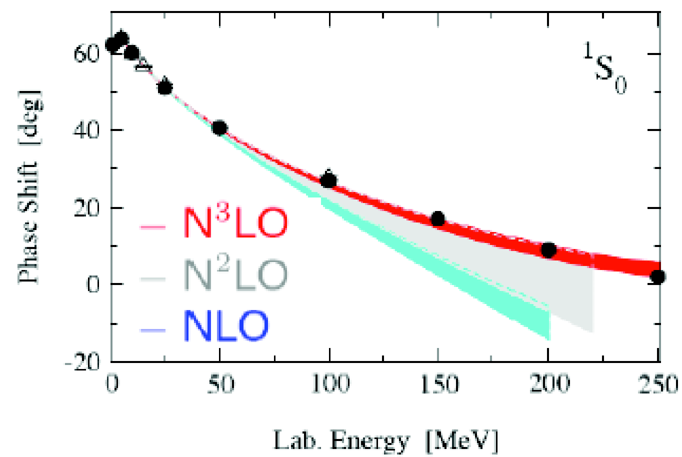


explains pheno hierarchy:
NN > 3N > 4N > …

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

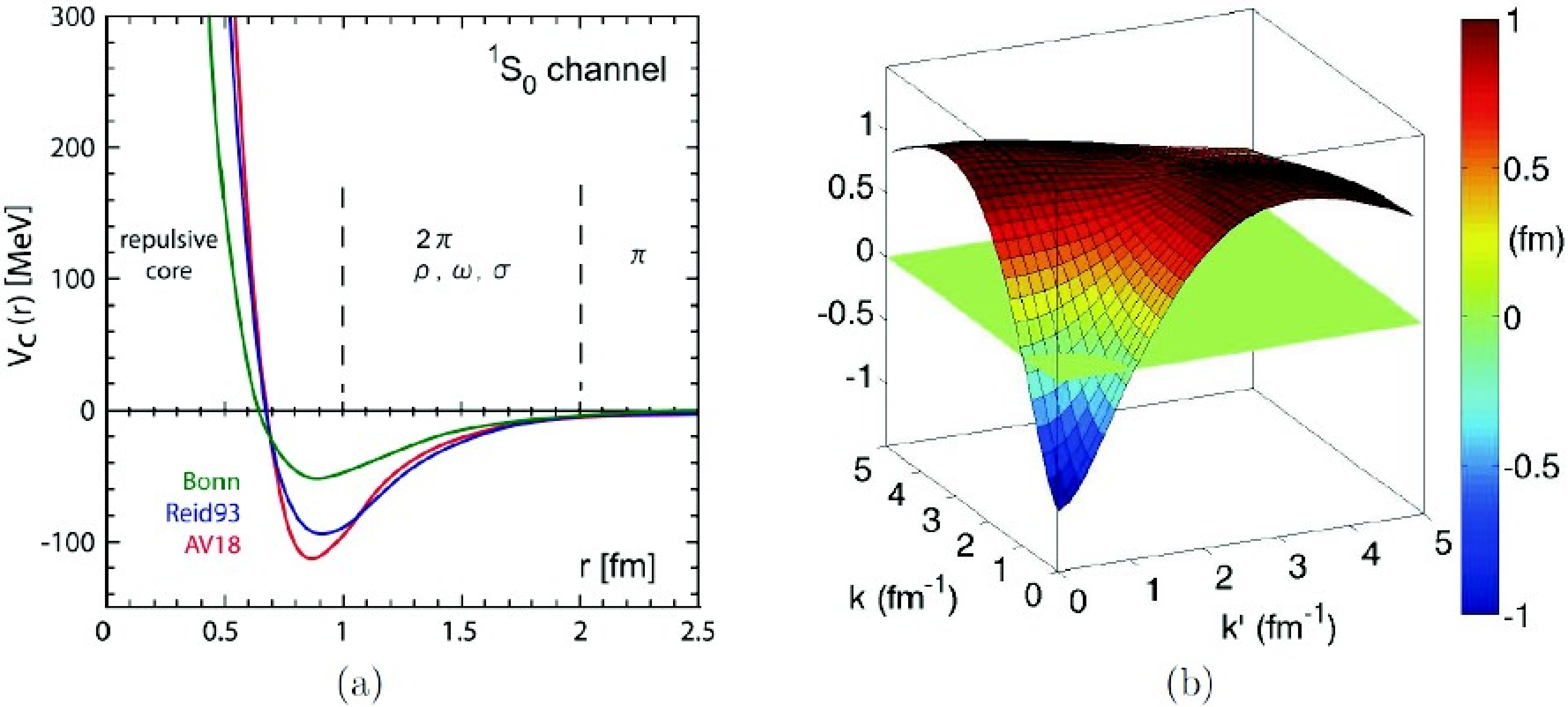
3N,4N: 2 new couplings to N^3LO!

theoretical error estimates



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

Realistic two-body potentials in coordinate and momentum space



Repulsive core makes calculations difficult

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

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

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

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

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

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

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;

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

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

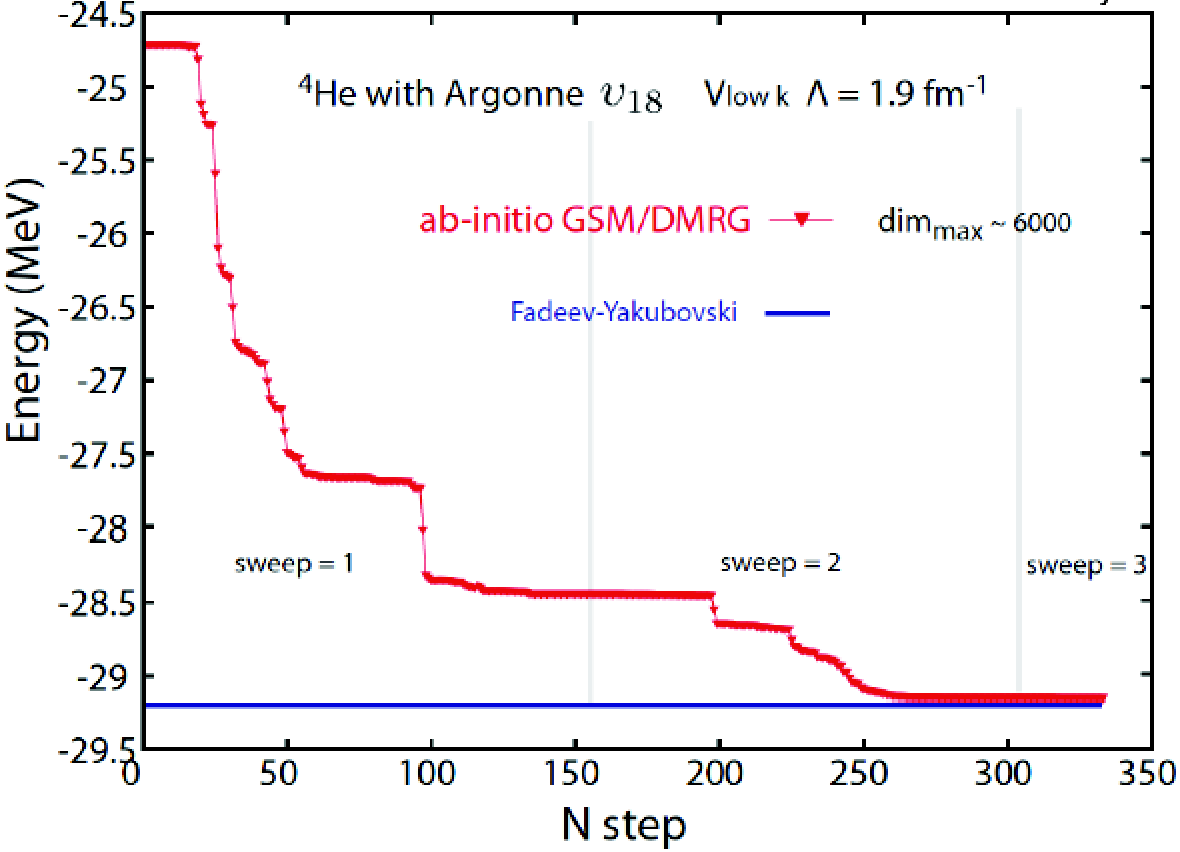
Two ways of convergence:

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: $H^{\mathrm{eff}}_{A,a} \rightarrow H_A$

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

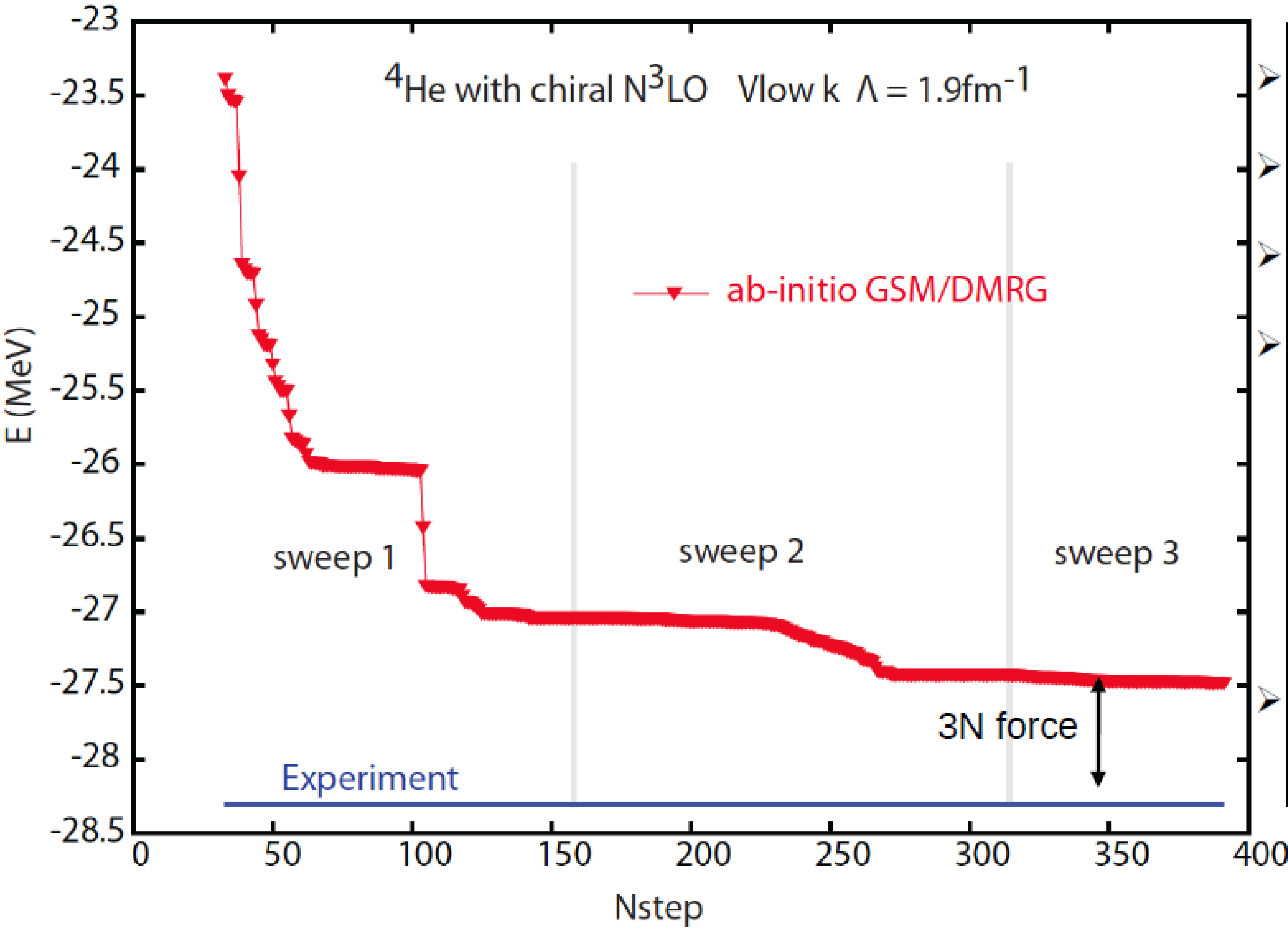
Dim for direct diagon: 119,864,088

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



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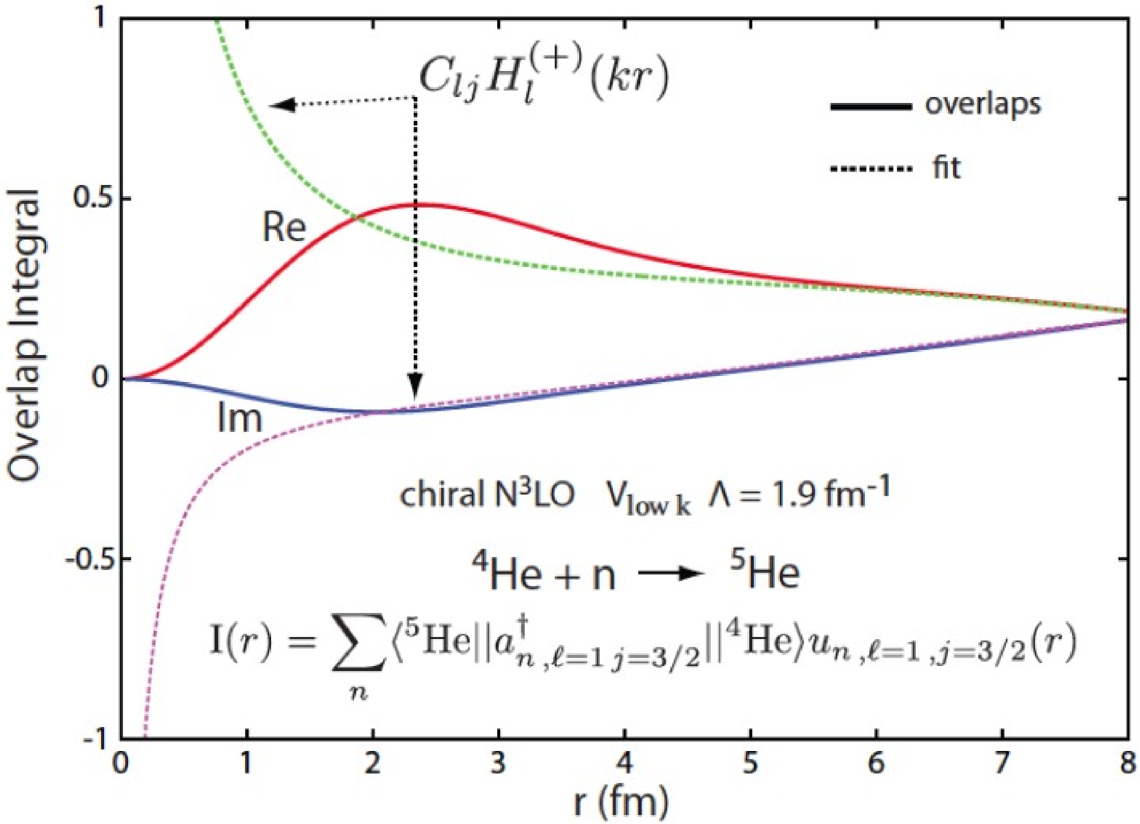
  d5/2-d3/2
  f5/2-f7/2 } H.O states
  g7/2-g9/2
- 156 s.p. states total

$E_{N3LO} = -27.48$ MeV

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

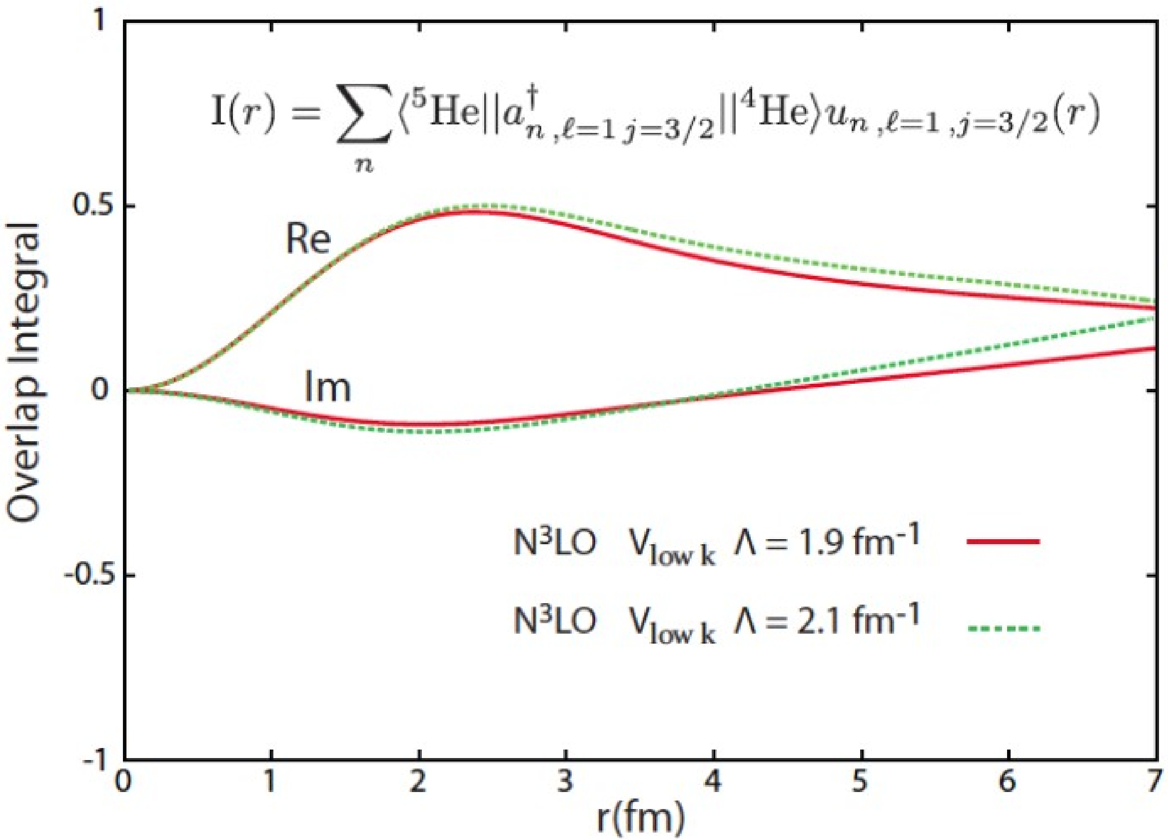
C = 0.197

and from (1)

Γ = 311 keV

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

Results: Ab-initio overlaps in the NC-GSM



Overlap tail sensitive to S_{1n}

ANC (Λ = 2.1 fm^{-1}) = 0.255

S_{1n} (Λ = 2.1 fm^{-1}) = -1.8 MeV

$\Gamma_{diagonalization}$ = 591 keV

Γ_{ANC} = 570 keV

The width exhibits the correct behavior

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

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