Microscopic description of exotic nuclei in the Berggren basis

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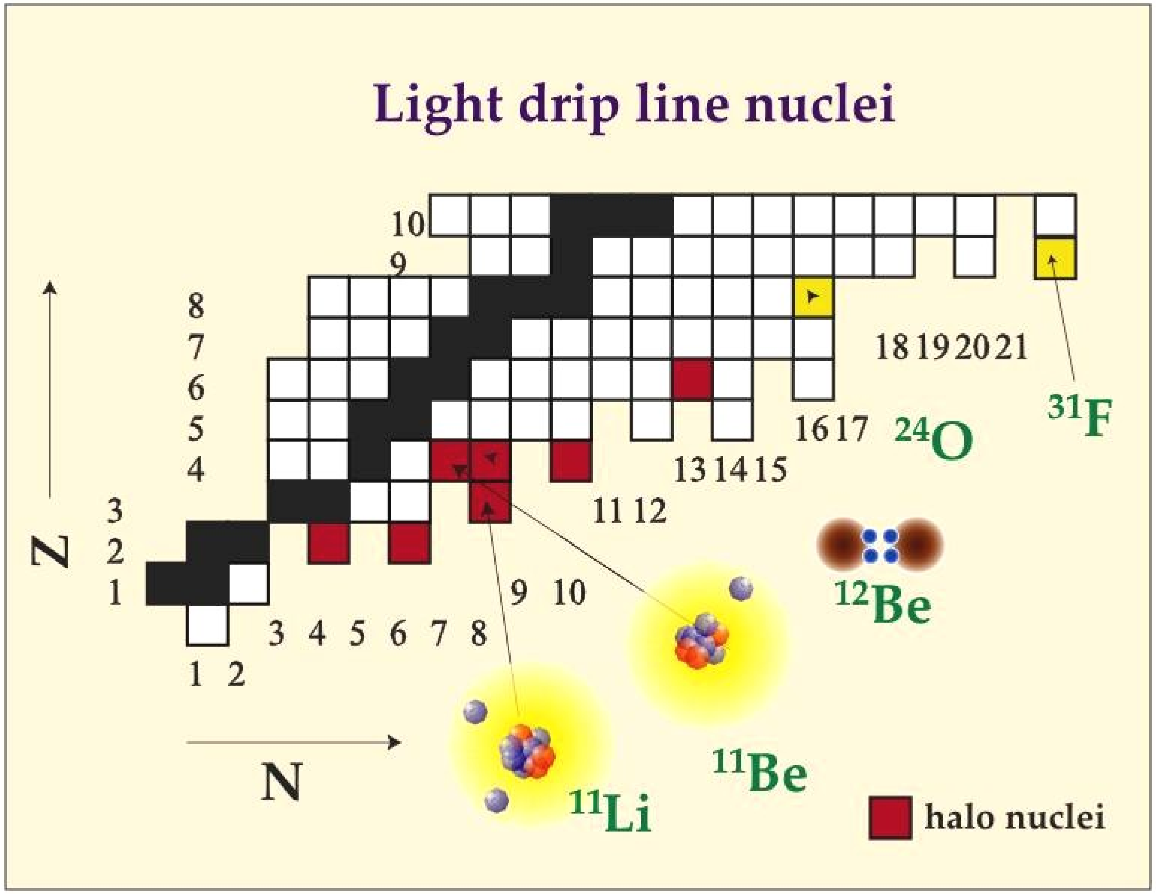
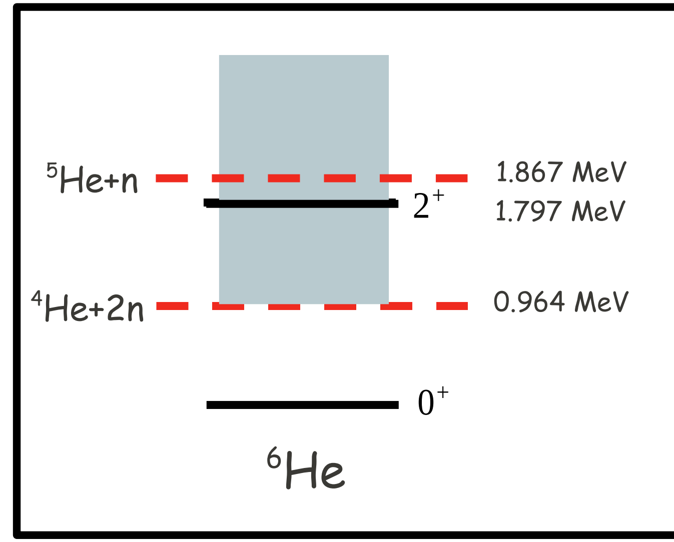
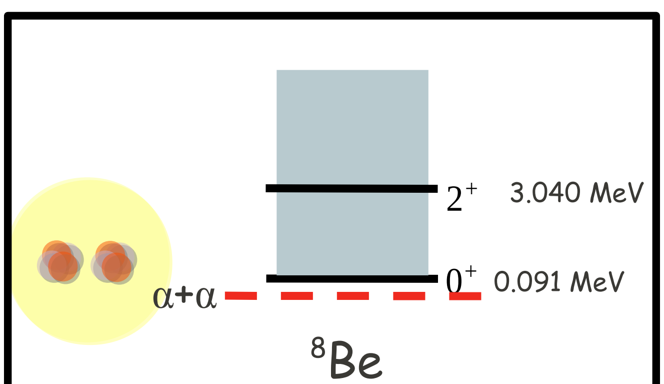
European Research Council
erc

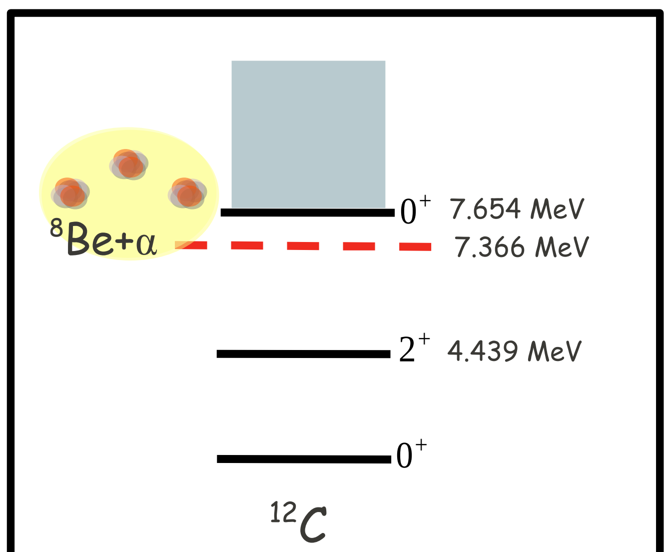
CHALMERS

Light nuclei from first principles, INT, October 3, 2012



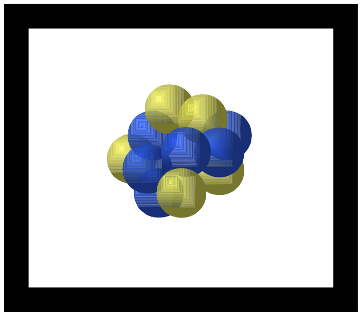




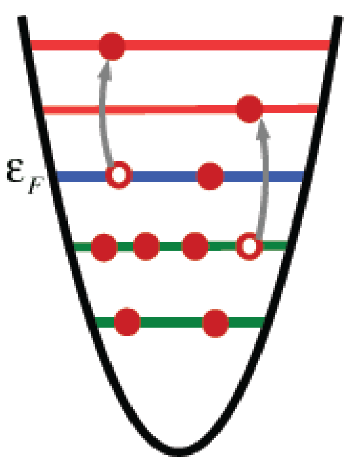


Importance of continuum in the structure of nuclei far from stability

Closed quantum systems



infinite well

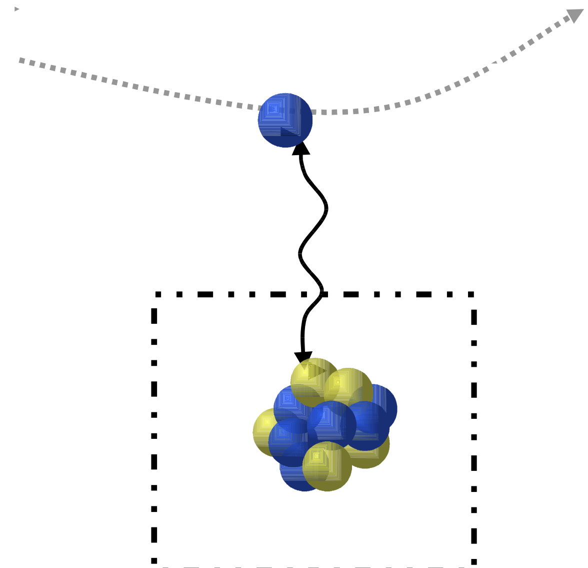


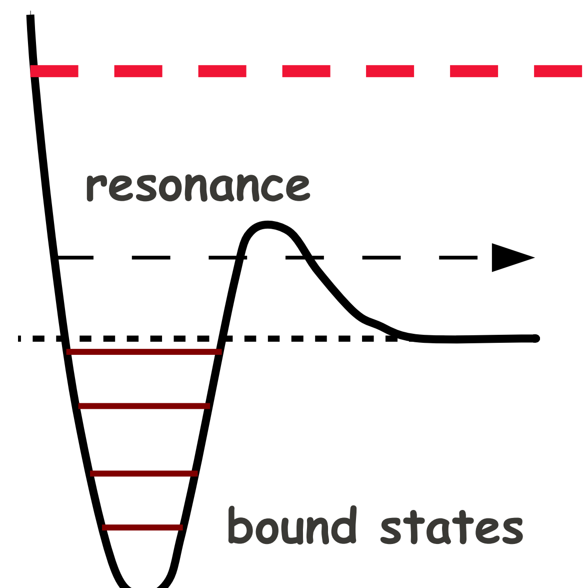
discrete states only,
HO basis usually

exact treatment of the
c.m, analytical solution...

Open quantum systems

(nuclei far from stability)

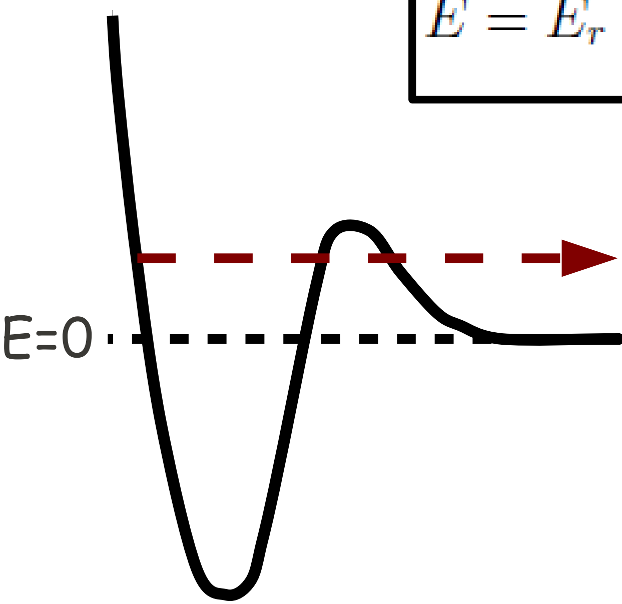


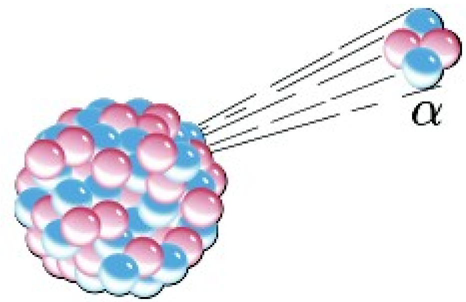


Gamow States

G. Gamow, Z. Phys. 51 (1928) 204

$$\tilde{E} = E_r - i\frac{\Gamma}{2}$$

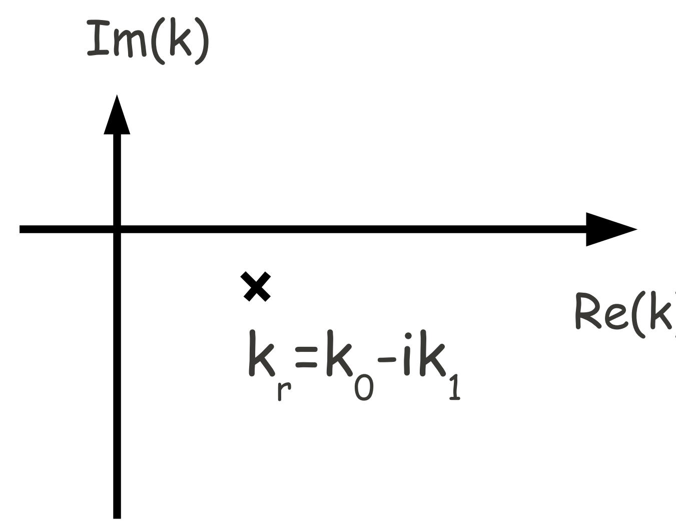




$$\Psi(t,r) = e^{\frac{-i\tilde{E}t}{\hbar}}\psi(r)$$

$$|\Psi(t,r)| \sim e^{-\frac{\Gamma t}{2\hbar}} e^{k_1 r}, r \to \infty$$

$$\left(-\frac{d^2}{dr^2} + \frac{2\mu}{\hbar^2}V(r) + \frac{l(l+1)}{r^2} - k^2\right)\psi(r) = 0$$

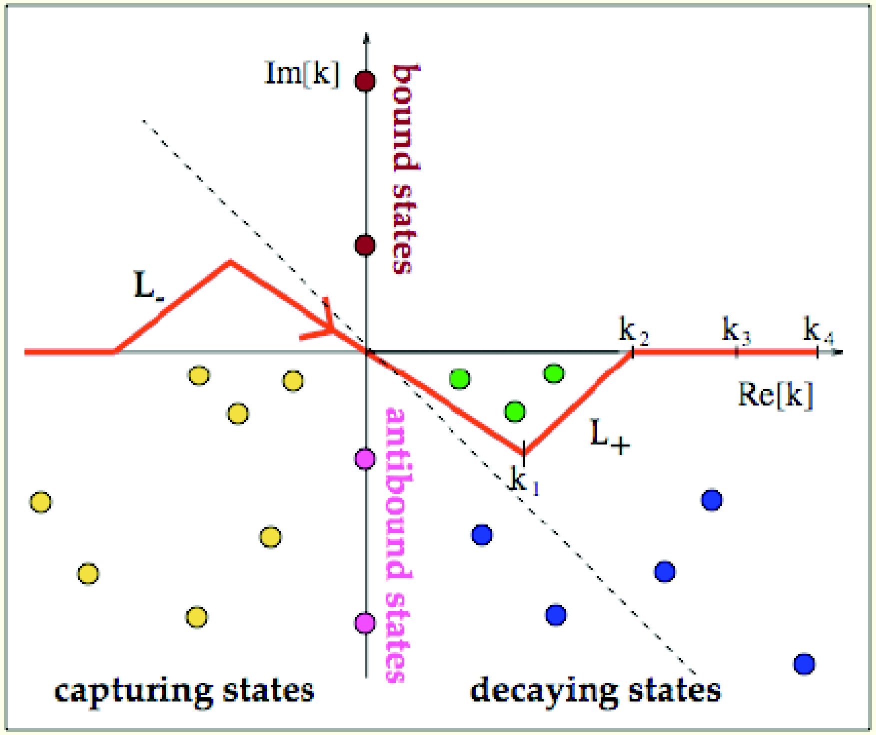


Boundary condition

$$\psi(r) \sim \mathcal{O}_l(kr) \sim e^{ikr}, r \to \infty$$

Gamow states and completeness relations

T. Berggren, Nucl. Phys. A109, 265 (1968); Nucl. Phys. A389, 261 (1982)
T. Lind, Phys. Rev. C47, 1903 (1993)



$$\sum_{n=b,r} |u_n\rangle\langle\tilde{u}_n| + \frac{1}{\pi}\int_{L_+} |u(k)\rangle\langle u(k^*)|\, dk = 1$$

particular case: Newton completeness relation

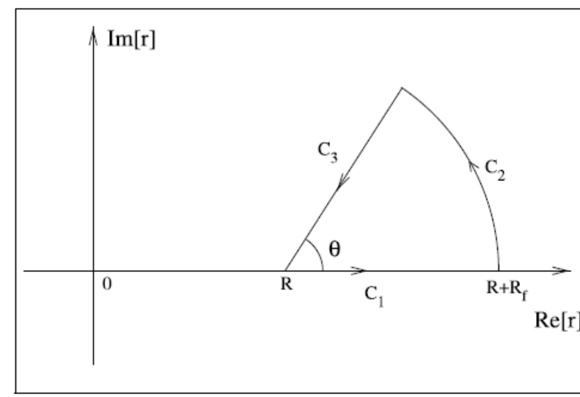
$$\sum_{n=b} |u_n\rangle\langle\tilde{u}_n| + \frac{1}{\pi}\int_{R} |u(k)\rangle\langle u(k^*)|\, dk = 1$$

Bound, resonant state

$$u(r) \to C_+ H^+_{l,\eta}(kr)$$

normalization of resonant states
with external complex scaling :

$$N_i = \sqrt{\int_0^R u_i^2(r)\,dr + \int_0^{+\infty} u_i^2(R + x\cdot e^{i\theta})\, e^{i\theta}\, dx}$$



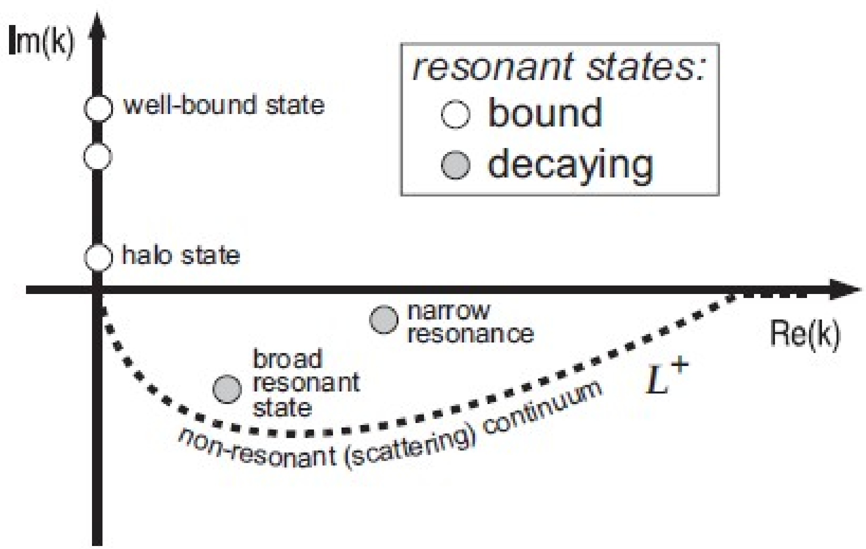
Complex scattering state

$$u(r) \to C_+ H^+_{l,\eta}(kr) + C_- H^-_{l,\eta}(kr)$$

$$C^+ C^- = \frac{1}{2\pi}. \quad \text{(normalisation)}$$

Gamow Shell Model

N. Michel *et al*, PRL 89 (2002) 042502; PRC67 (2003) 054311; PRC70 (2004) 064313
G. Hagen *et al*, PRC71 (2005) 044314
J.R *et al*, PRL 97 (2006) 110603
N. Michel *et al*, JPG (2009) 013101
G.Papadimitriou et al, PRC(R) 84 (2011) 051304



pole approximation: "0[th]" order approximation :

$$H^{p.a}|\Psi^{p.a.}\rangle = E^{p.a.}|\Psi^{p.a.}\rangle$$

Many-body resonance (bound) states have the largest overlap

$$|\langle\Psi^{p.a.}|\Psi\rangle|$$

i) discretization of continuum contour

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

ii) construction of many-body basis

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

iii) construction of Hamiltonian matrix

$$\langle SD_i|H|SD_j\rangle$$

(complex symmetric matrix)

iv) many-body spectrum:
bound,resonant and "spurious" continuum states

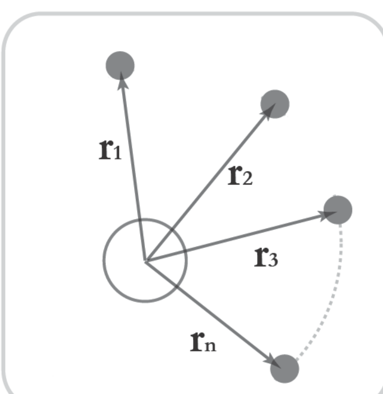
$$H = \sum_i \left[\frac{p_i^2}{2\mu} + U_i \right] + \sum_{i<j} \left[V_{ij} + \frac{1}{A_c} \vec{p}_i \vec{p}_j \right]$$

generic Hamiltonian for a GSM description of a nucleus as core+valence nucleon system

recoil term coming from the expression of *H* in the COSM coordinates. *No spurious states*

cluster Orbital Shell Model (COSM) coordinates

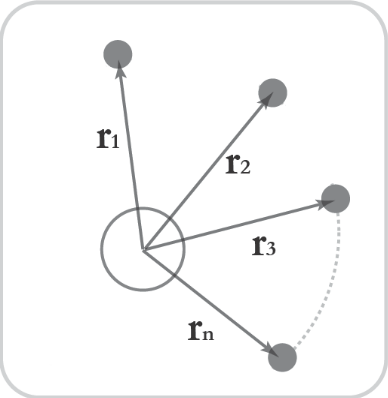
(Y. Suzuki et, Phys. Rev. C 38, 1 (1988))

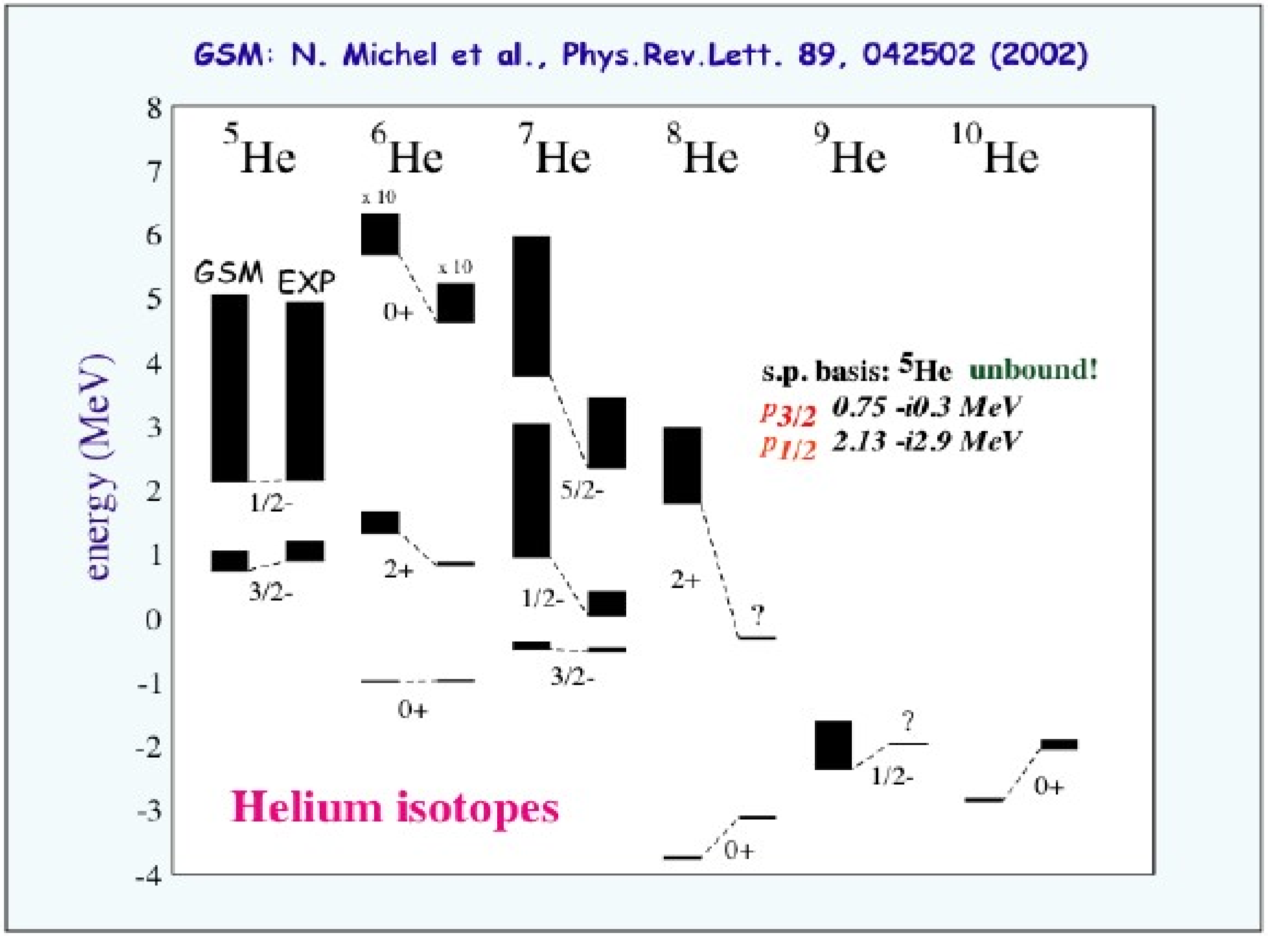


i) U_i core-nucleon potential

ii) V_{ij} phenomenological, realistic NN interaction

Helium chain (^{4}He core plus valence neutrons)



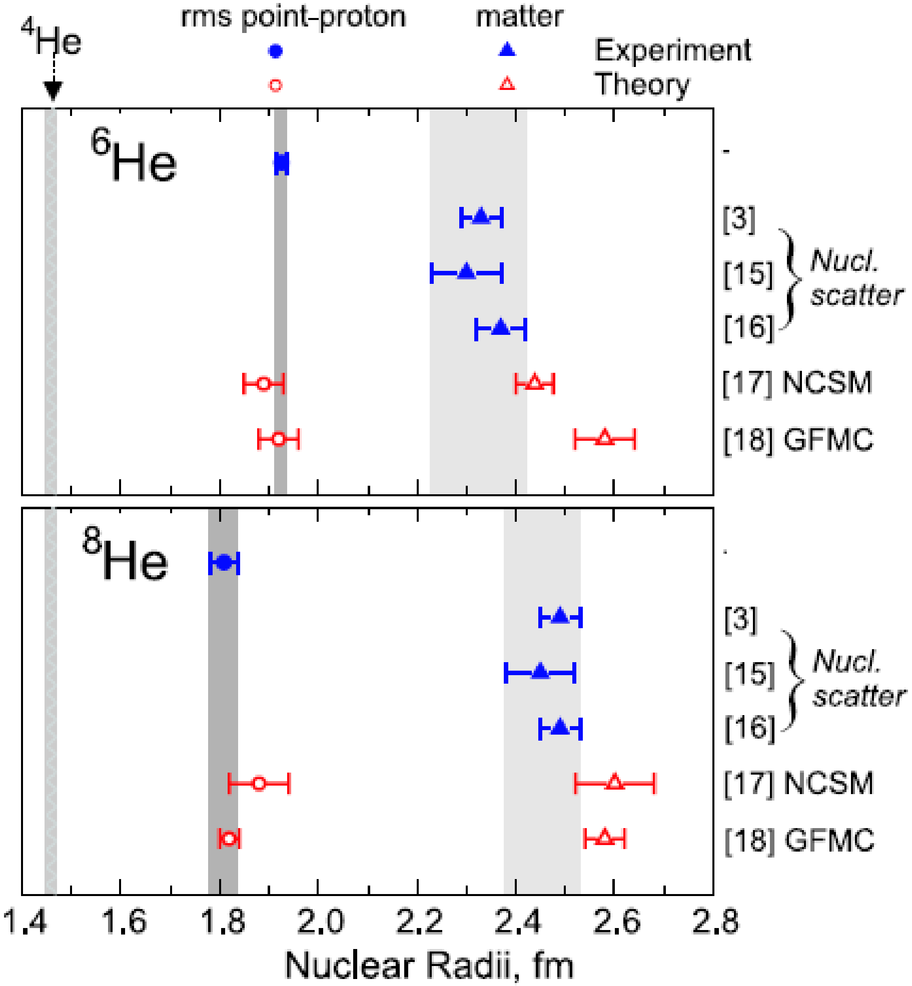


i) Woods-Saxon potential (^{4}He-n)

ii) two-body zero-range force (n-n)

pole approximation: $p_{3/2}$, $p_{1/2}$ resonance (^{5}He g.s and 1st excited state)

^6He, ^8He charge radii



(taken from P. Muller *et al* , PRL 99, 252501 (2007))

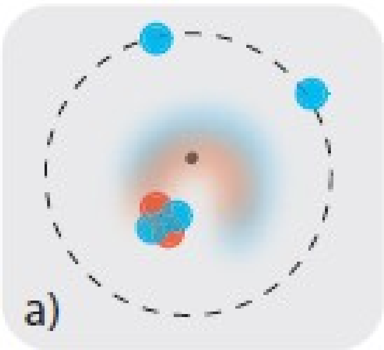
[16] E. Caurier *et al*, PRC 73, 021302 (R) (2006)
[17] S.C. Pieper, Riv. Nuovo Cim. 031, 709 (2008).

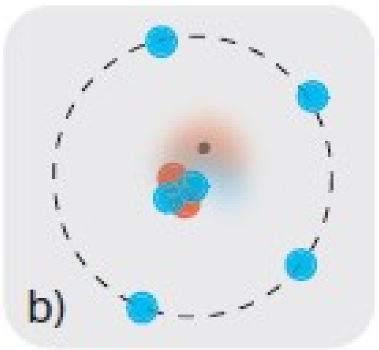
M. Brodeur et al.
PRL 108, 052504 (2012)

^6He =1.910±0.011 fm

^8He =1.835±0.019 fm

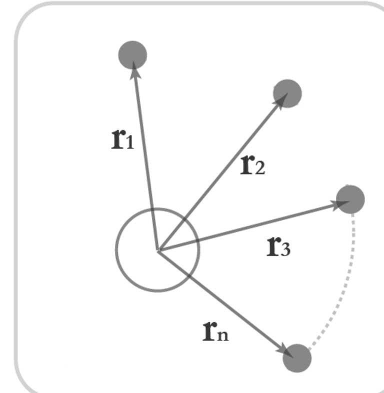
(point charge radius)





structural information on nuclear hamiltonian and nuclear many-body dynamics (the radial extent of the halo nucleus is reflected in the charge radius)

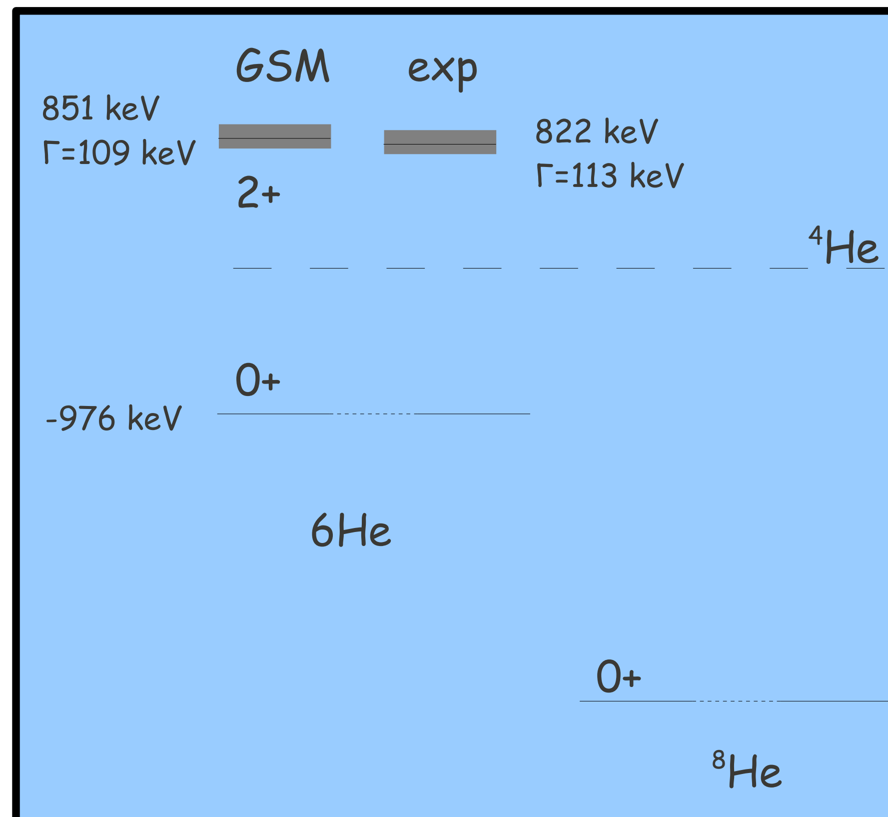
^{6}He,^{8}He Hamiltonian



- Woods-Saxon potential for ^{4}He-n (fitted to ^{5}He resonances)

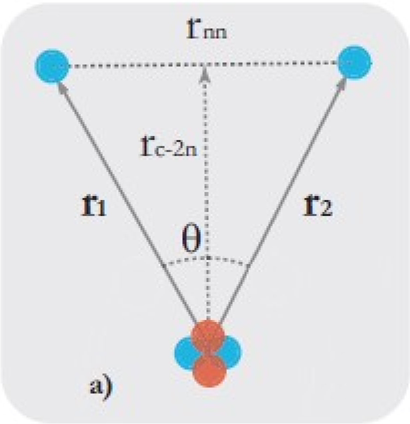
- "Minnesota like" interaction, 2 parameters (adjusted to ^{6}He,^{8}He g.s.)

- $p_{3/2}$ resonance + $p_{3/2}$ complex continuum
- $p_{1/2}$sd real continuum



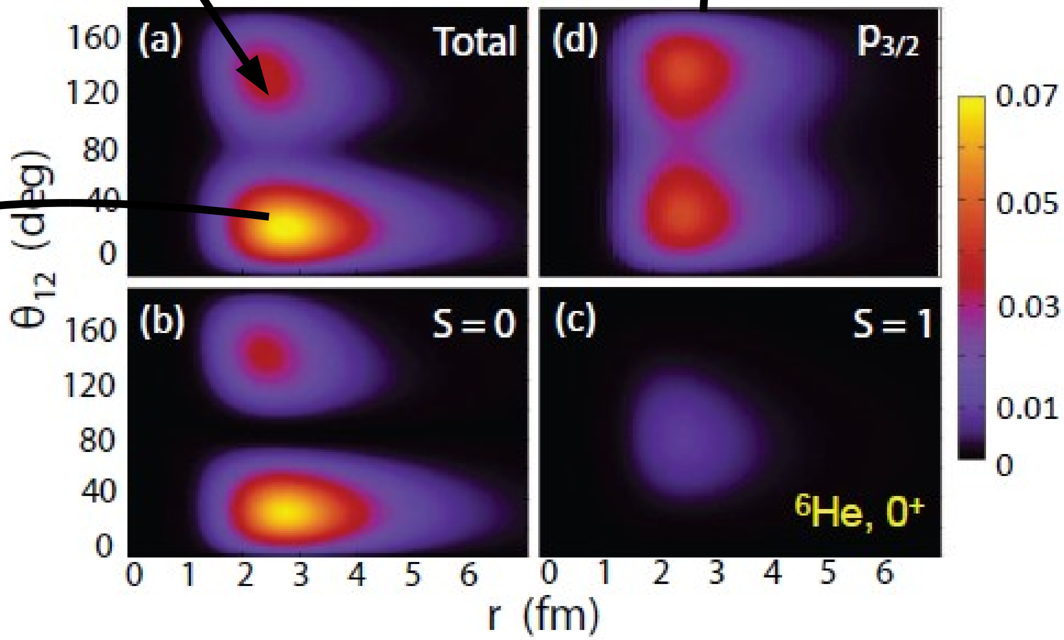
^{6}He g.s

two-neutron density $\rho_{nn}(r_1=r, r_2=r, \theta)$



cigar-like configuration

$p_{3/2}$ only, no $p_{1/2}$sd (continuum) shells



small components (~ 10 %) but dramatic effect !

"dineutron"-like configuration

S=0 ~ 87 %

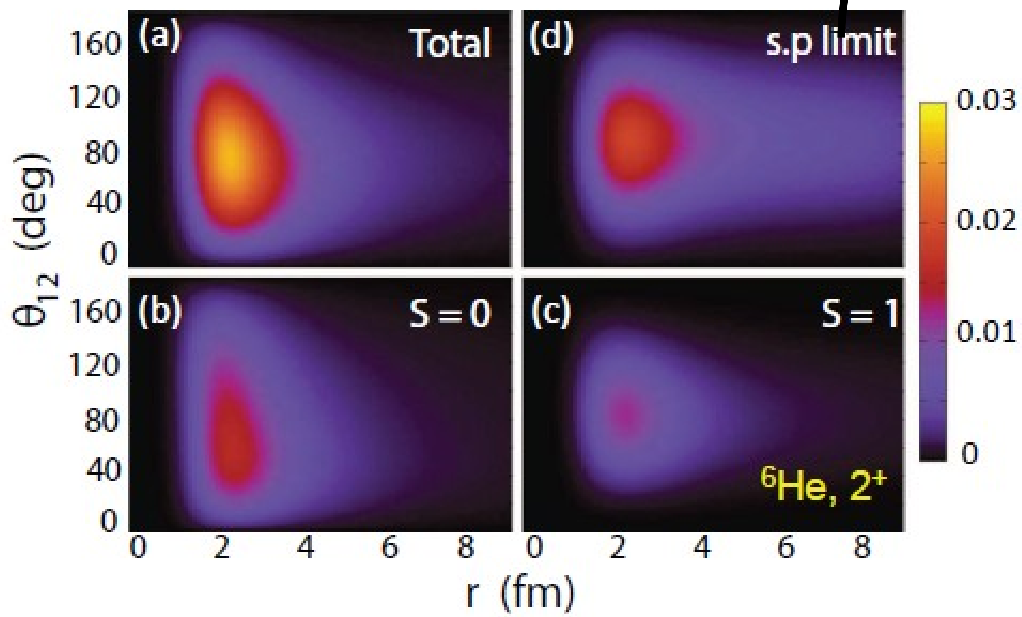
S=1 ~ 13 %

^{6}He *resonant* state $J^{\Pi}=2^{+}$

two-neutron density $\rho_{nn}(r_1=r, r_2=r, \theta)$

single particle "limit"

unbound state



S=0 ~ 66 %
S=1 ~ 33 %

G. Papadimitriou, A. T. Kruppa, N. Michel, W. Nazarewicz M. Płoszajczak and **J. R**, PRC 84 (2011)

Charge radii

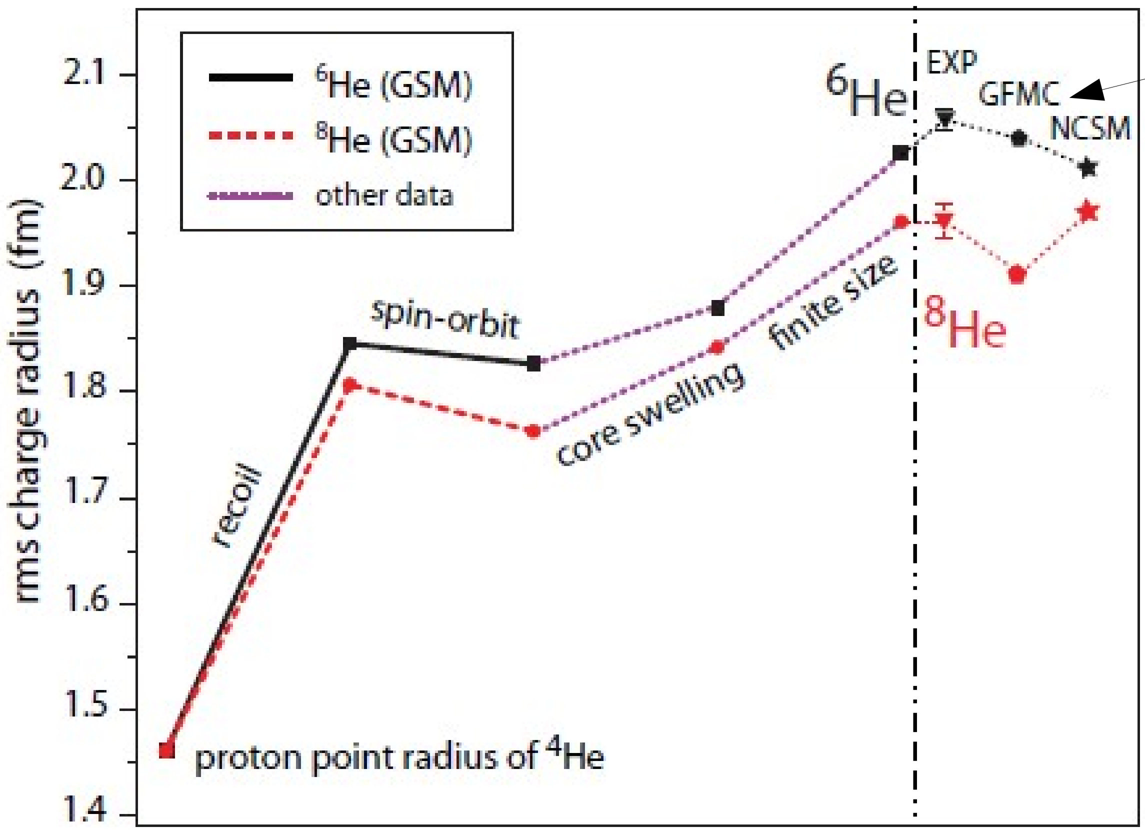
point proton radius — *finite size corrections*

$$\langle r^2_{ch}\rangle = \langle r^2_{pp}\rangle + \langle R^2_p\rangle + \frac{N}{Z}\langle R^2_n\rangle + \frac{3}{4M_p^2} + \langle r^2\rangle_{so}$$

$$\langle r^2_{pp}\rangle = \langle r^2_{pp}(^4He)\rangle + \langle recoil\rangle$$

- "swelling" of ^{4}He from GFMC
- recoil from GSM

nucleons charge radius + Darwin-Foldy term + Spin-Orbit contribution (obtained from GSM wf)



Experimental data and other theoretical approaches

	GSM	Exp
^{6}He	2.026 fm	2.059(7) fm
^{8}He	1.961 fm	1.959(16) fm

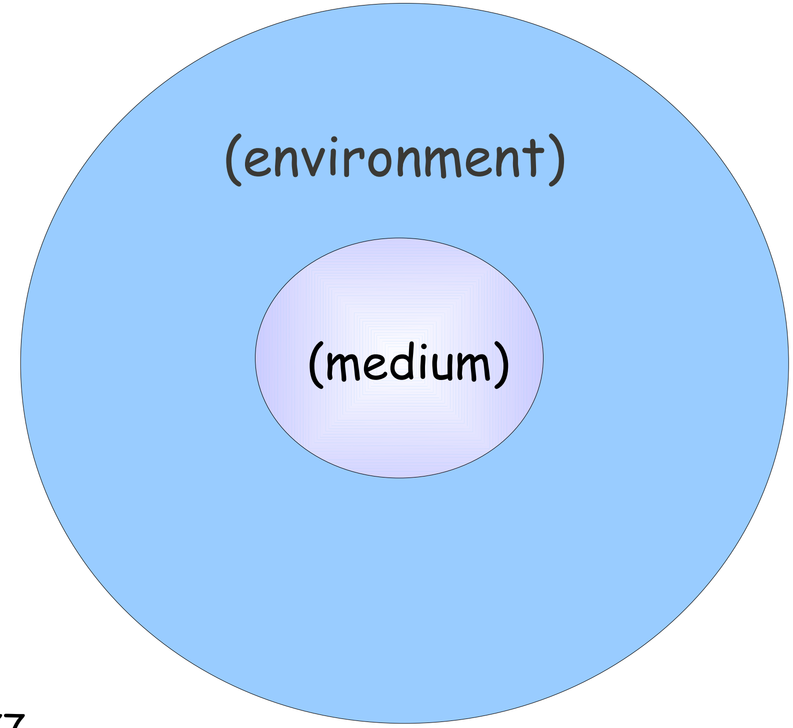
Density Matrix Renormalization Group (DMRG)

S. R. White, Phys. Rev. Lett. 69 (1992) 2863
S. R. White, Phys. Rev. B 48 (1993) 10345
S.R. White et al, Phys. Rev. B 48 (1993) 3844

lattice models, spin chain, quantum dots, atomic nuclei.......

Reduction of the number of degrees of freedom + renormalization

* Separation into a 'medium' and 'environment'
* Truncation of degrees of freedom in the environment

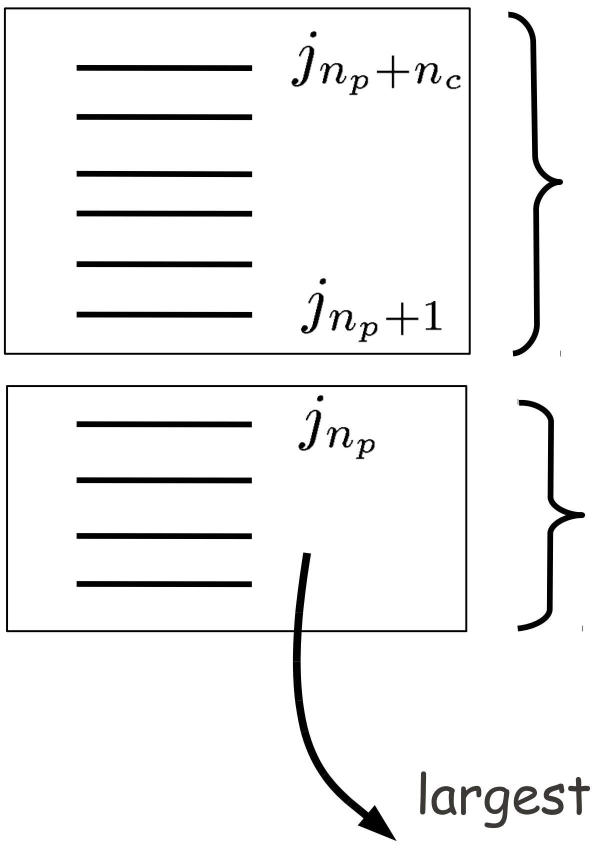


Application for nuclei

- T.Papenbrock et al J.Phys.G 31 (2005) S1377
- J. R et al, PRL 97 (2006) 110603
- S.Pittel et al PRC 73 (2006) 014301 (R)
- B. Thakur et al, Phys. Rev. C 78 (2008) 041303(R)
- J.R et al, PRC 79 (2009) 014304

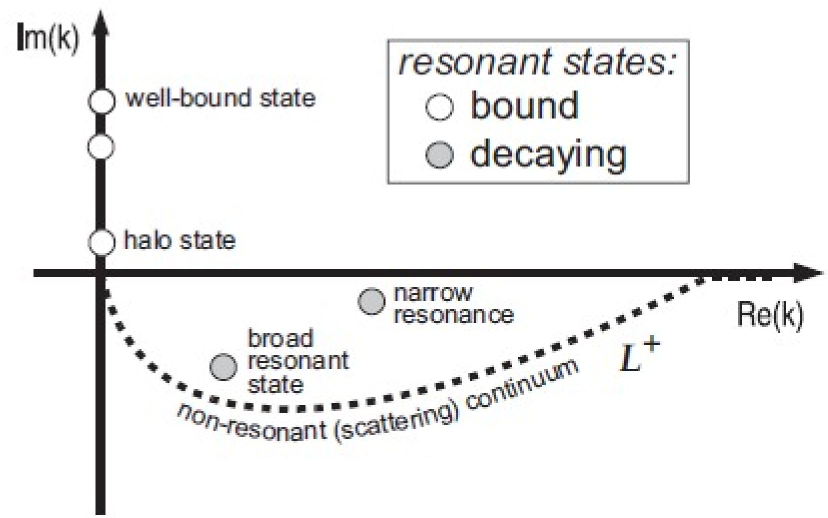
GSM+DMRG

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



C: non -resonant continuum

P:pole space

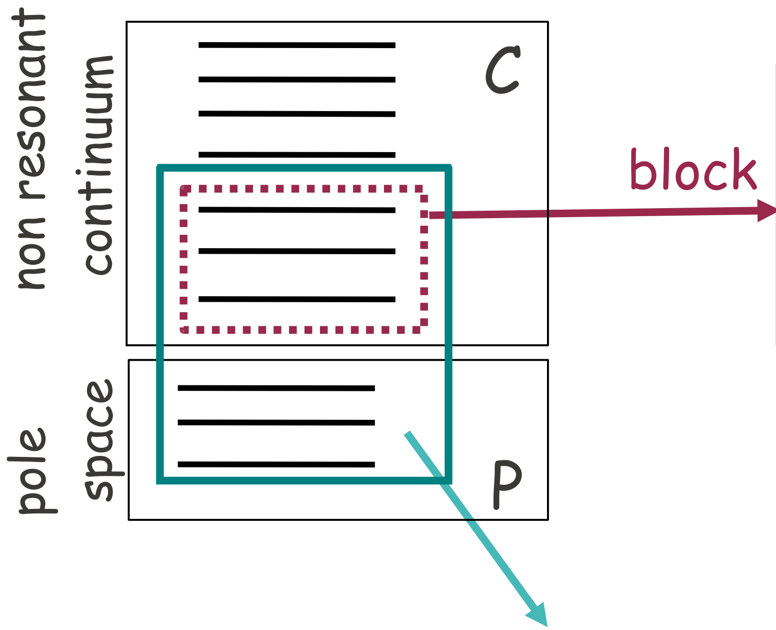


largest contribution to the GSM wave function

DMRG → truncation in environment C

Warm up phase

Construction of 2nd quantization operators and states in P and C



$|c\rangle$: states with 0,1,...n nucleons

operators : $a_i^\dagger, (a_j^\dagger a_k^\dagger)^K, [(a_i^\dagger a_j^\dagger)^{K_1} \tilde{a}_k]^{K_2} \ldots$

shells in C added one by one

one step=one shell

* diagonalization in the superblock →

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

(state with the largest overlap with the pole approx)

* singular value decomposition

*diagonalization of the density matrix :

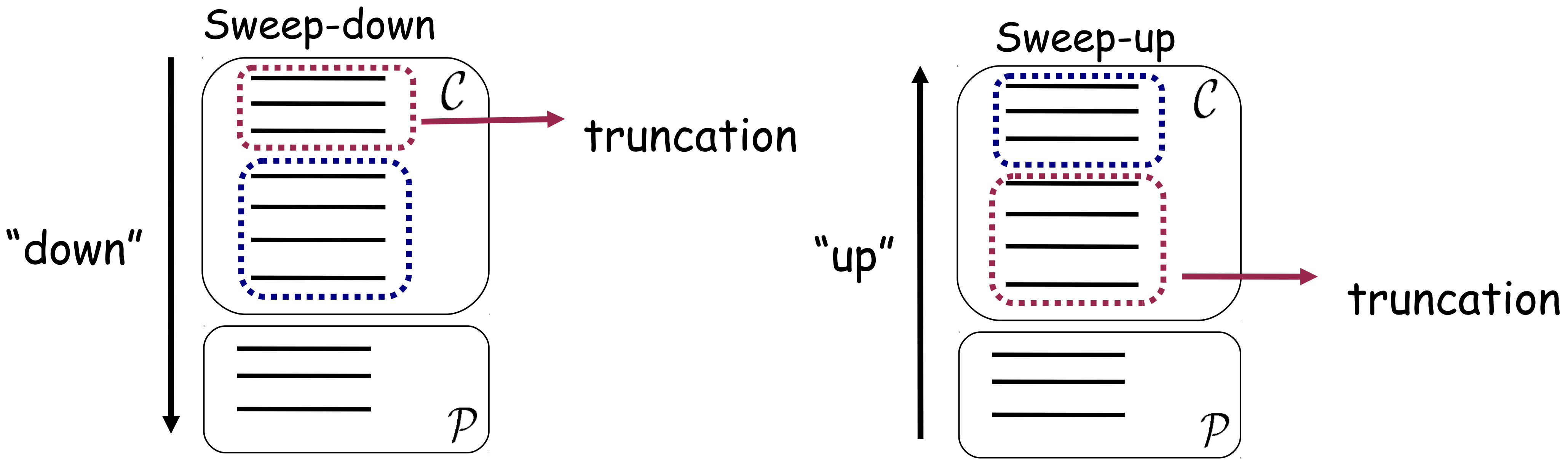
$$\rho^{J_c}_{c,c'} = \sum_p \Psi_{pc} \Psi_{pc'}$$

→ eigenstates with "largest" eigenvalues are kept.

Eigenvalues of the density are probabilities :

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

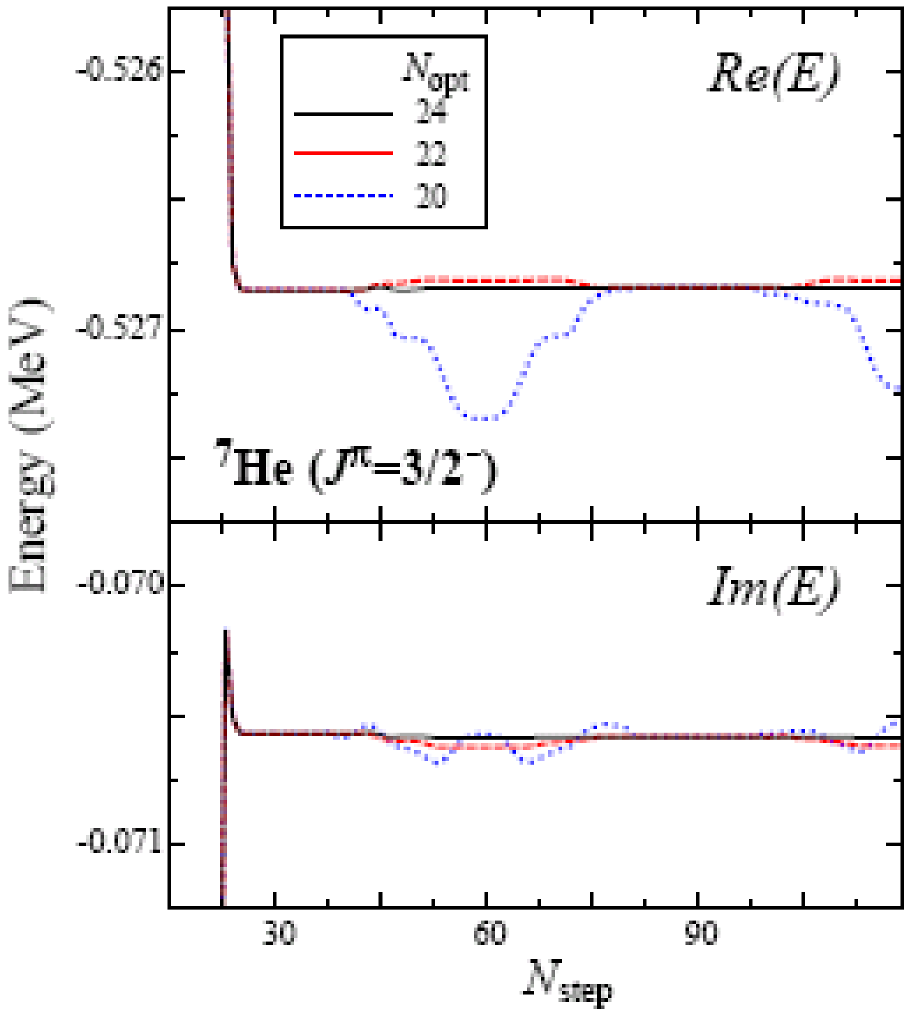
Sweeping phase



^7He g.s.

^4He core + 3 neutrons

Convergence of the energy as a function of DMRG iteration



- pole space : $0p_{3/2}$,$0p_{1/2}$
- continuum space : $p_{3/2}$,$p_{1/2}$ (30 shells each)

Woods-Saxon + Surface Gaussian two-body interaction :

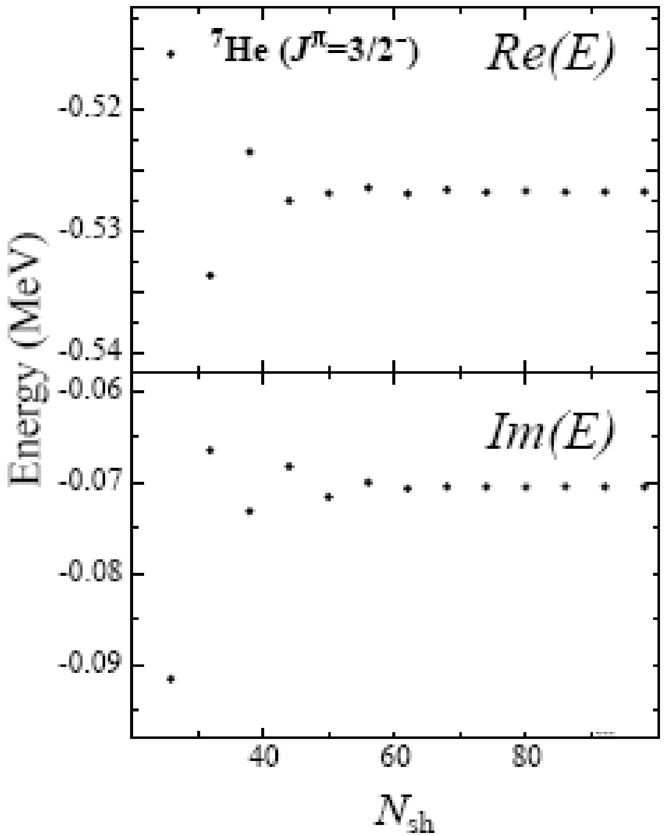
$$V_{i,j}^{J,T} = V_0(J,T)\exp\left[-\left(\frac{\mathbf{r_1}-\mathbf{r_2}}{\mu}\right)^2\right]\delta(|\mathbf{r_1}|+|\mathbf{r_2}|-2R_0)$$

Shell Model dimension=83948
largest matrix in DMRG=1143

(J.R *et al.*, PRL 97 (2006) 110603)

^{7}He g.s.

Convergence of the real (top) and imaginary part (bottom) of the g.s. energy as a function of the total number of shells



Shell Model dimension

6149 ⟷ 332171

DMRG dimension:

941 ⟷ 1001

Very good scaling

with number of shells !

DMRG truncation at N_{opt}=22

Ab-Initio calculations in the Berggren basis

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

i) NN potential:

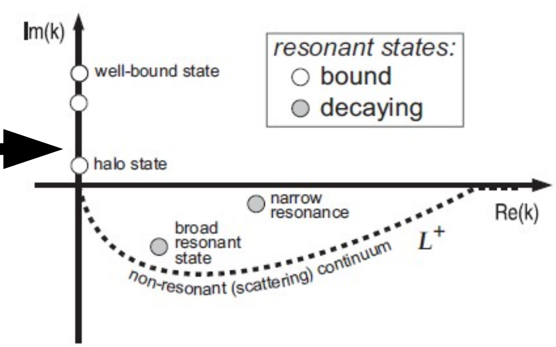
* AV18 (R.B. Wiringa et al PRC 51 (1995) 38)
* N^{3}LO (D.R.Entem et al PRC(R) 68 (2003) 041001)

} softened by v_{low-k} with Λ = 1.9 fm-1
(S. Bogner et al, Phys. Rep. 386 (2003) 1)

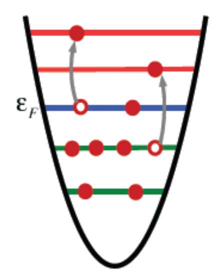
(For comparison with Faddeev, Faddeev-Yakubovsky and Coupled Cluster)

ii) single particle states:

a) s- and p-shells from Hartree-Fock potential ⟷

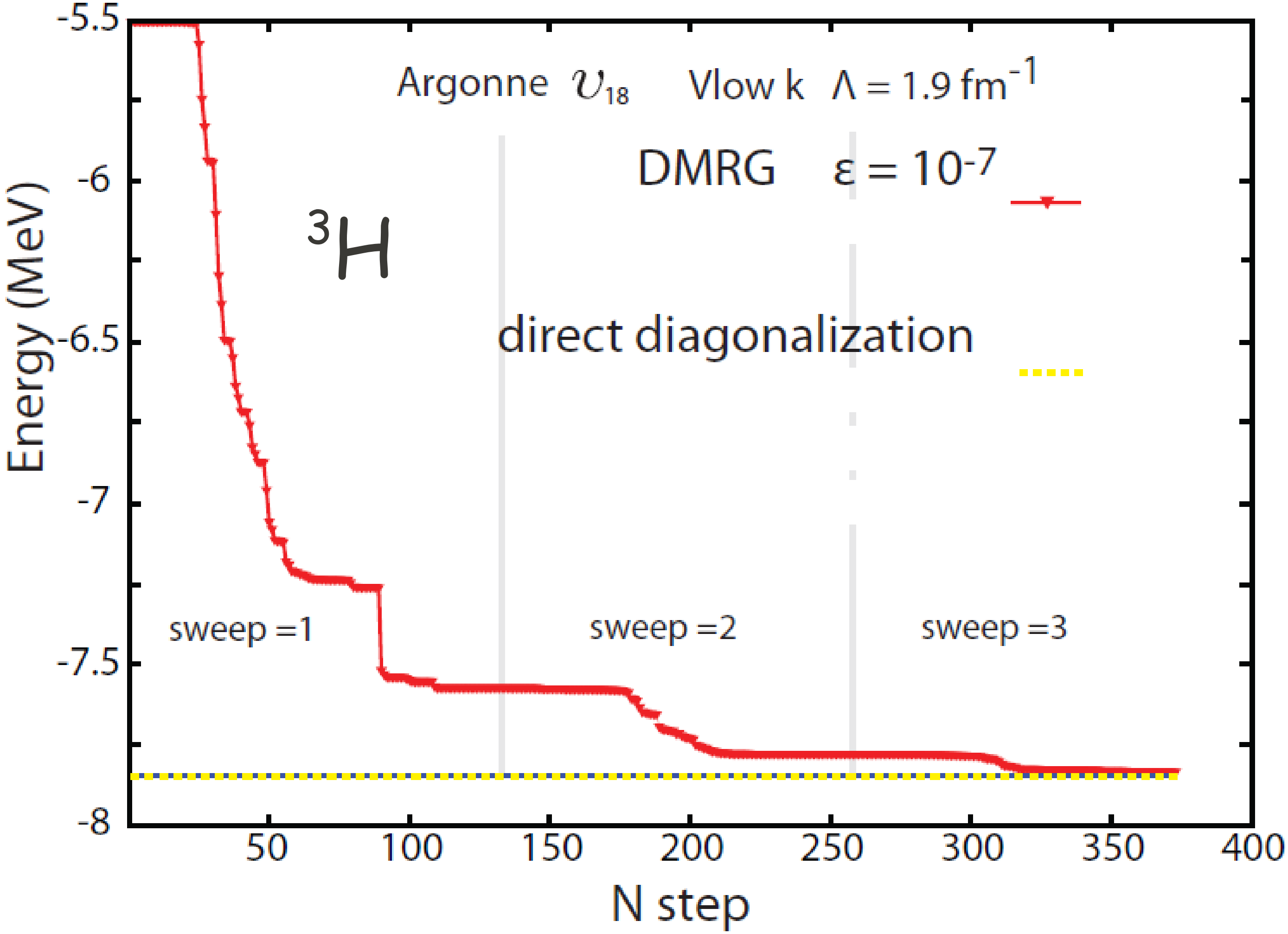


b) for l>1, shells of the Harmonic Oscillator



iii) Resolution with DMRG

Calculations of ^{3}H, ^{4}He and ^{5}He



Shells

$0s_{1/2}(p)$:E=-9.231 MeV
$0s_{1/2}(n)$:E=-11.765 MeV

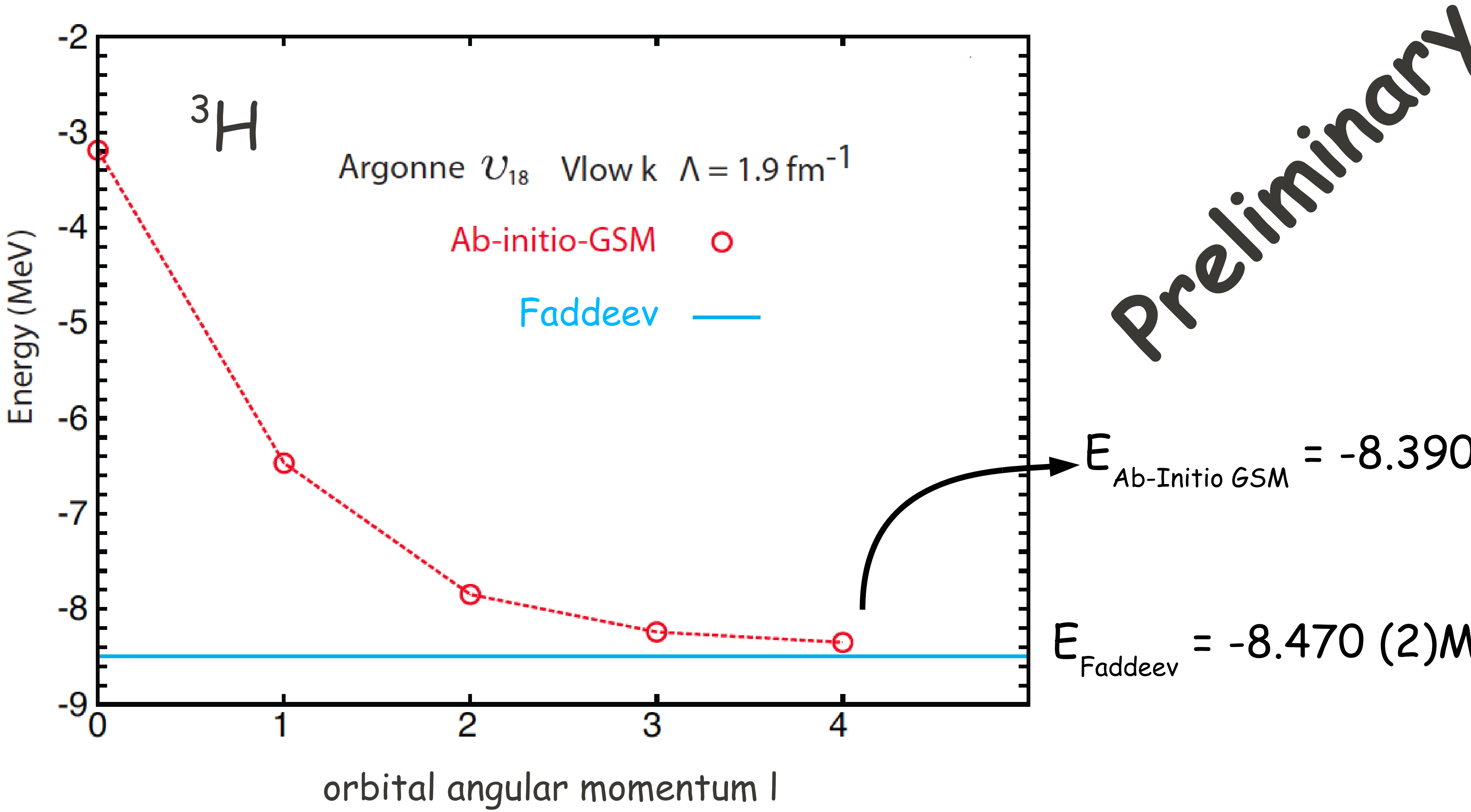
$s_{1/2},p_{3/2},p_{1/2},s_{1/2}$ real energy continua

$d_{5/2},d_{3/2}$ H.O states

130 s.p. in total

GSM full diagonalisation: dim= 123,835
DMRG : dim~ 1200

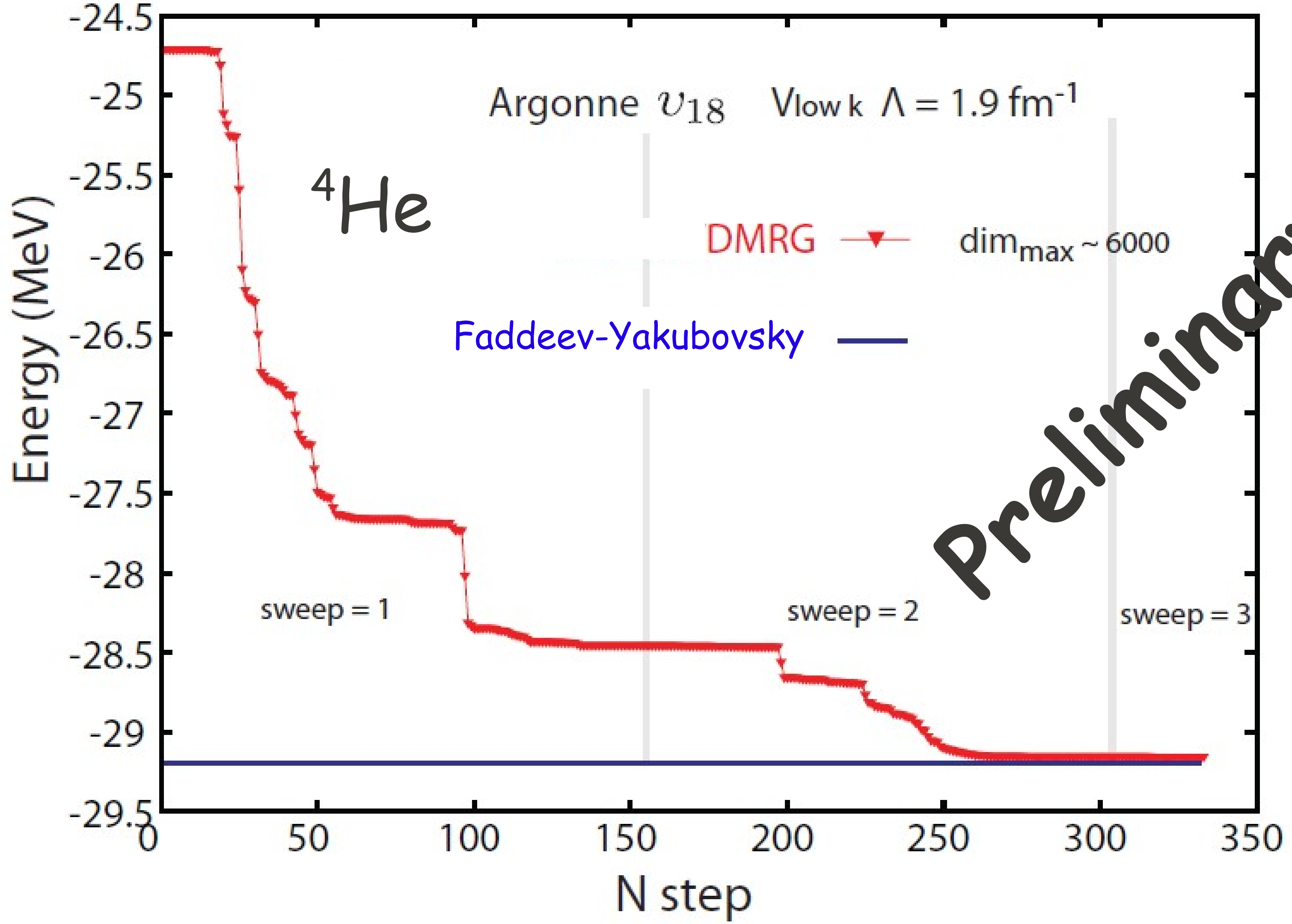
E_{exact}=-7.840 MeV
E_{DMRG}=-7.832 MeV



$E_{Ab\text{-}Initio\ GSM} = -8.390 MeV$

$E_{Faddeev} = -8.470\ (2) MeV$

Faddeev result from Nogga et al, PRC 70 (2004) 061002, 2004



Shells

$0s_{1/2}$(p) :E=-23.304 MeV

$0s_{1/2}$(n) :E=-24.334 MeV

$s_{1/2}, p_{3/2}, p_{1/2}, s_{1/2}$ real energy continua

d,f,g H.O states

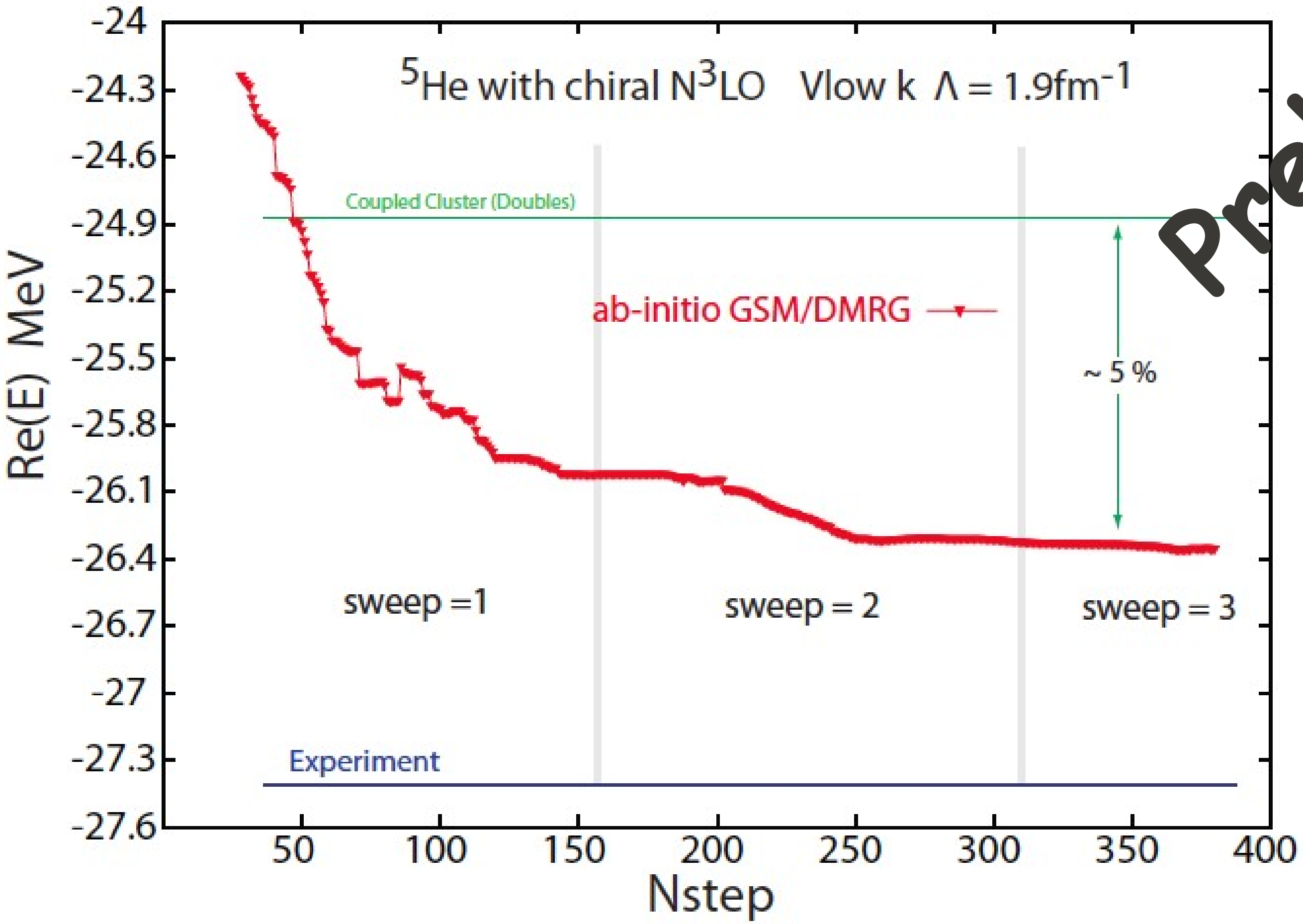
156 s.p. in total

GSM full dim=6,230,512

DMRG : dim~ 6000

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

$E_{Faddeev\text{-}Yakubovsky}$ = -29.19 (5) MeV



Preliminary

Shells

$0s_{1/2}$(p) :E=-23.291 MeV
$0s_{1/2}$(n) :E=-23.999 MeV

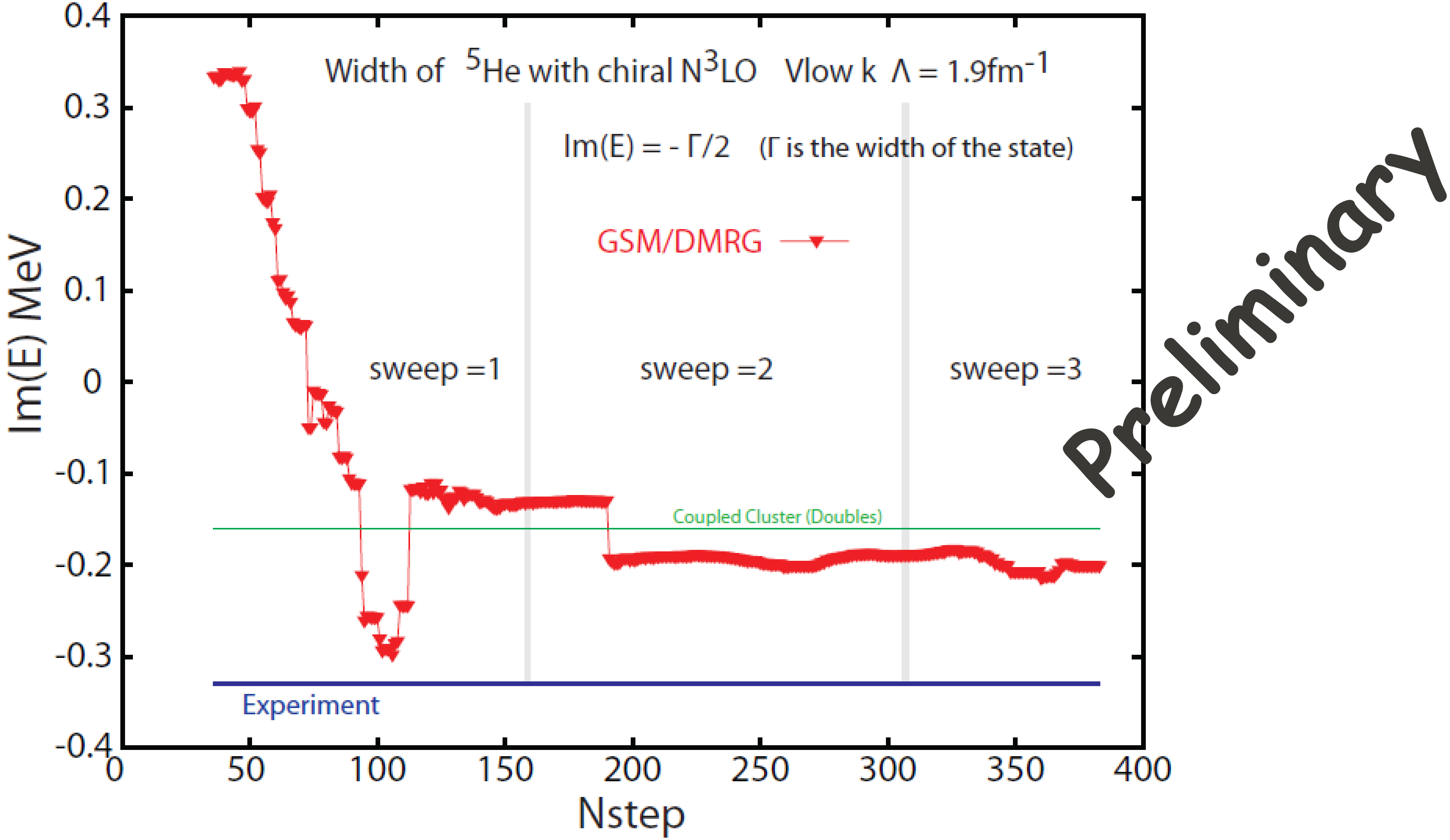
$0p_{3/2}$(n): E (1.194,-0.633)
$p_{3/2}$(n) complex contour (discretized)

$s_{1/2}$,$p_{3/2}$,$p_{1/2}$,$s_{1/2}$ real energy continua

d,f,g H.O states

157 s.p. in total

GSM full dim=1,379,196,439
DMRG : dim~ 1.10^5



Width of ^{5}He with chiral N^{3}LO Vlow k $\Lambda = 1.9 fm^{-1}$
Im(E) = - Γ/2 (Γ is the width of the state)
GSM/DMRG
sweep =1
sweep =2
sweep =3
Coupled Cluster (Doubles)
Experiment
Im(E) MeV
Nstep
0.4
0.3
0.2
0.1
0
-0.1
-0.2
-0.3
-0.4
0
50
100
150
200
250
300
350
400
Preliminary

Microscopic description of exotic nuclei in the Berggren basis

(Shell Model approach with coupling to the continuum)

i) Gamow Shell Model for helium isotopes, charge radius

ii) Ab-Initio approaches for (exotic) light nuclei with DMRG

Perspectives:

^{11}Li description as 7 nucleons above ^{4}He core, Oxygen isotopes with ^{22}O as a core, Ab-Initio description of Hydrogen chain.....

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