

Ab initio description of light nuclei in the Berggren basis

J. Rotureau



CHALMERS

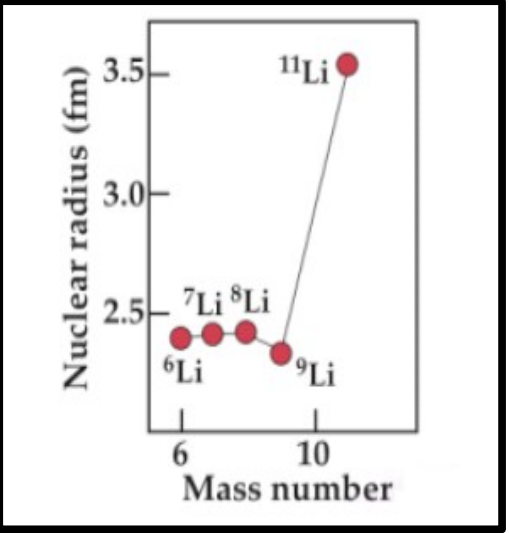
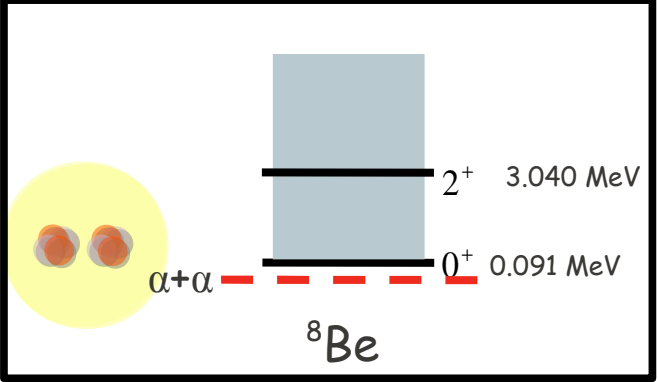
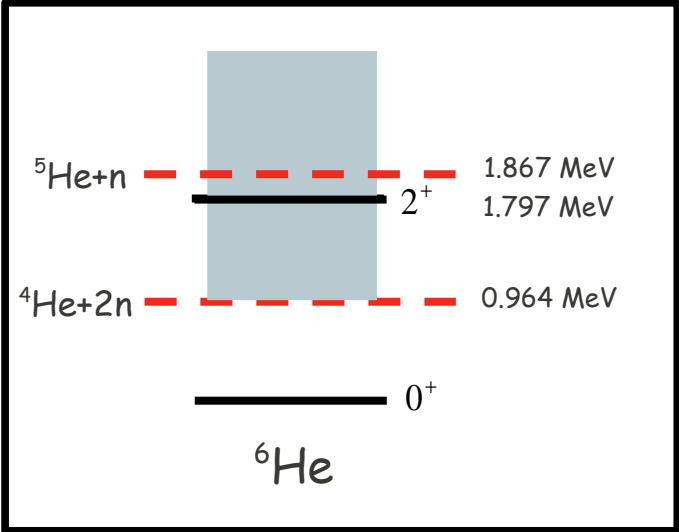
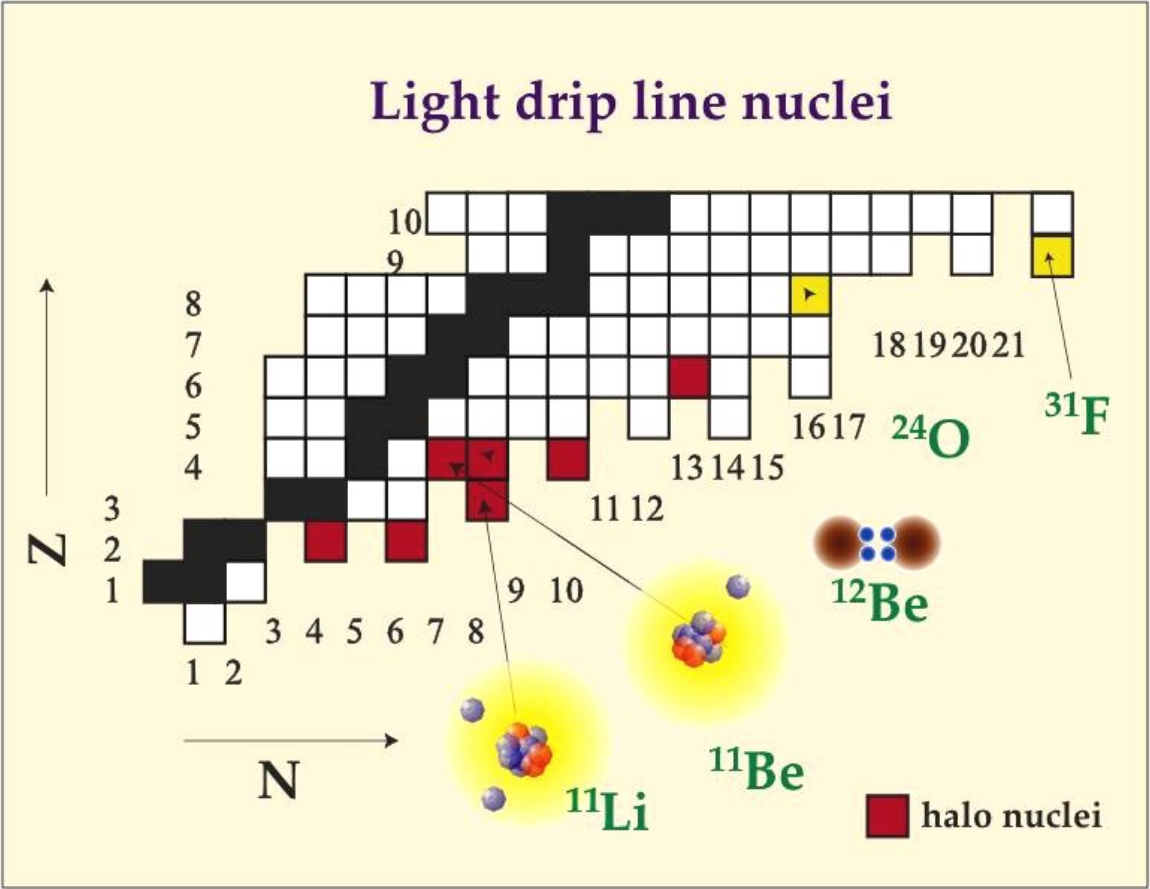
European Research Council



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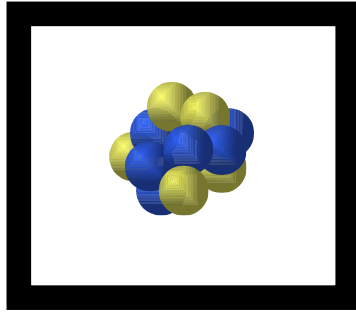
**International Conference on Nuclear Theory
in the Supercomputing Era, Ames, May 2013**

Impact of continuum for nuclei far from stability

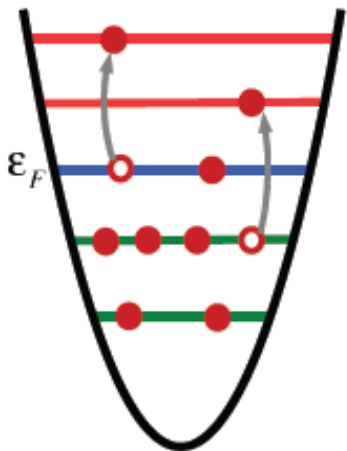


Closed quantum systems

(nuclei near the valley of stability)



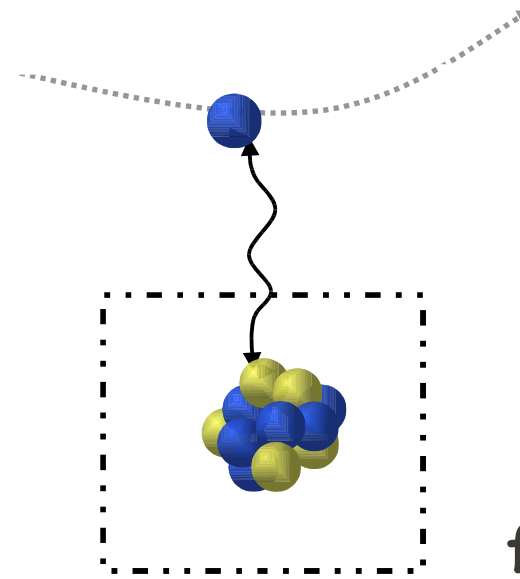
nucleons in bound shells



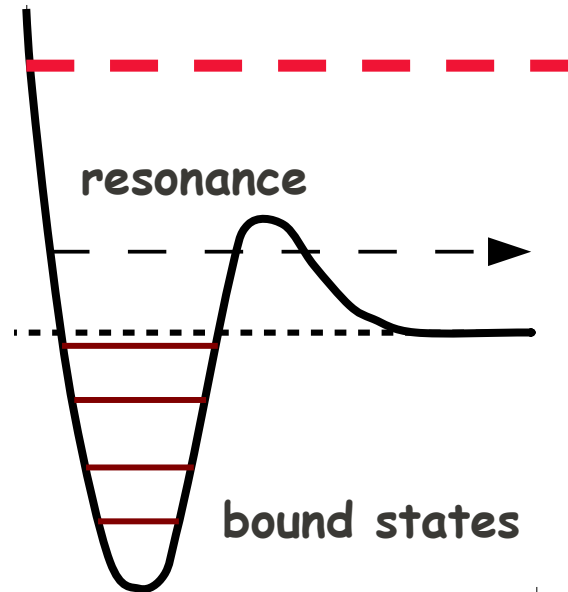
-> usually HO basis
-> exact treatment of the center of mass, analytical wavefunctions...

Open quantum systems

(nuclei far from stability)



finite-depth potential

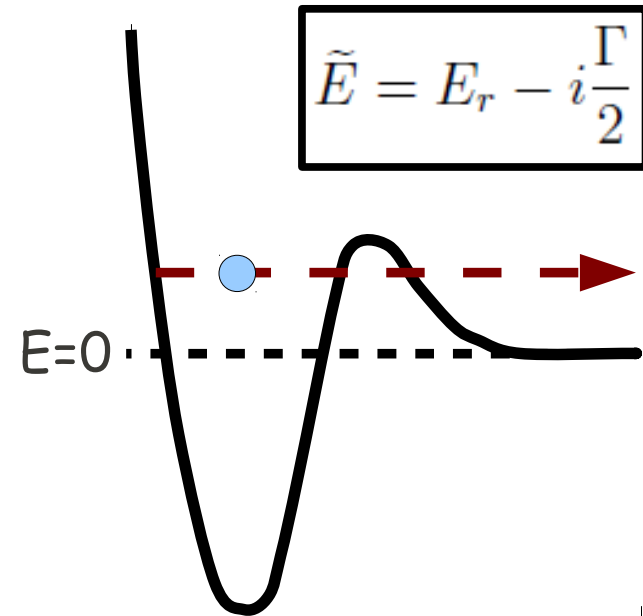


-> Woods-Saxon, Hartree-Fock potential.....
-> bound, resonant, continuum shells

see also talks by G.Hagen, P. Navratil, M Caprio, M. Hjorth-Jensen

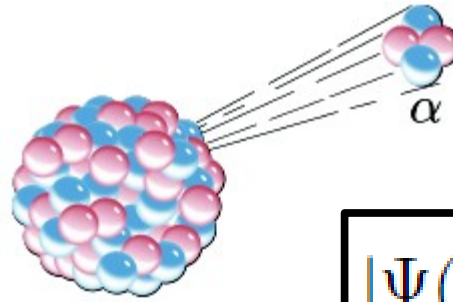
Gamow States

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



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

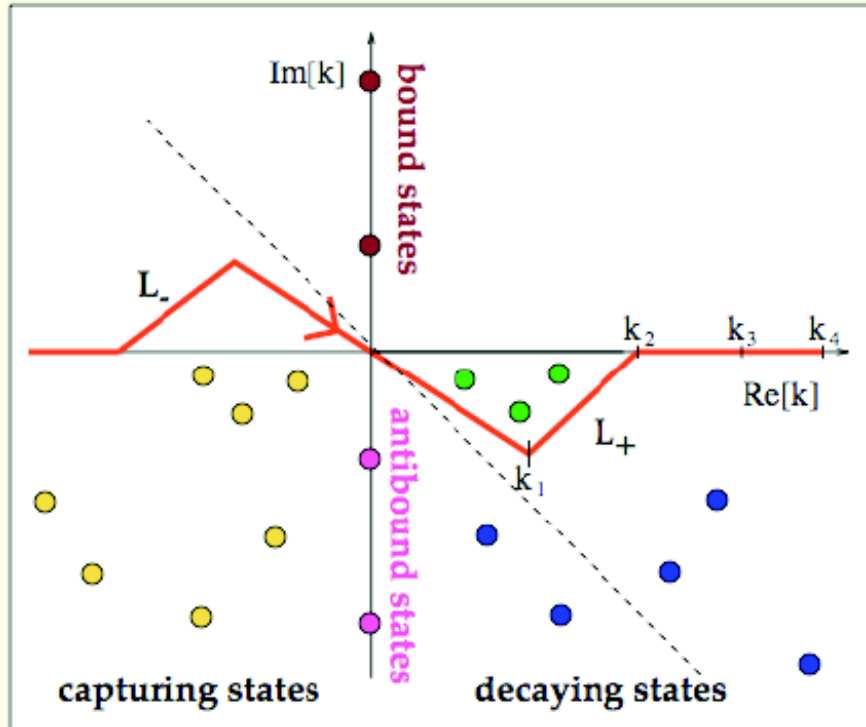
$$\Psi(t, r) = e^{\frac{-i\tilde{E}t}{\hbar}} \psi(r)$$



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

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

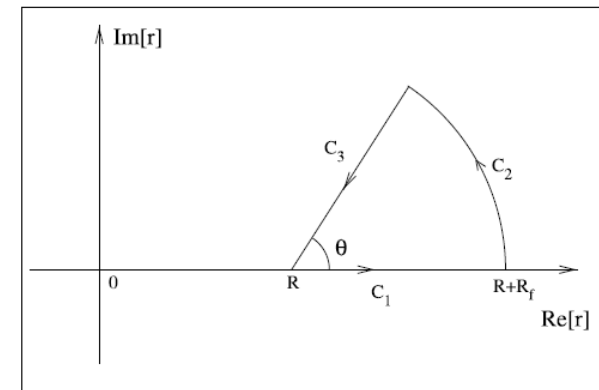
$$\sum_{n=b} |u_n \rangle \langle \tilde{u}_n| + \frac{1}{\pi} \int_R |u(k) \rangle \langle u(k^*)| dk = 1$$

Bound, resonant state

$$u(r) \rightarrow C_+ H_{l,\eta}^+(kr)$$

normalization of resonant states
with external complex scaling :

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

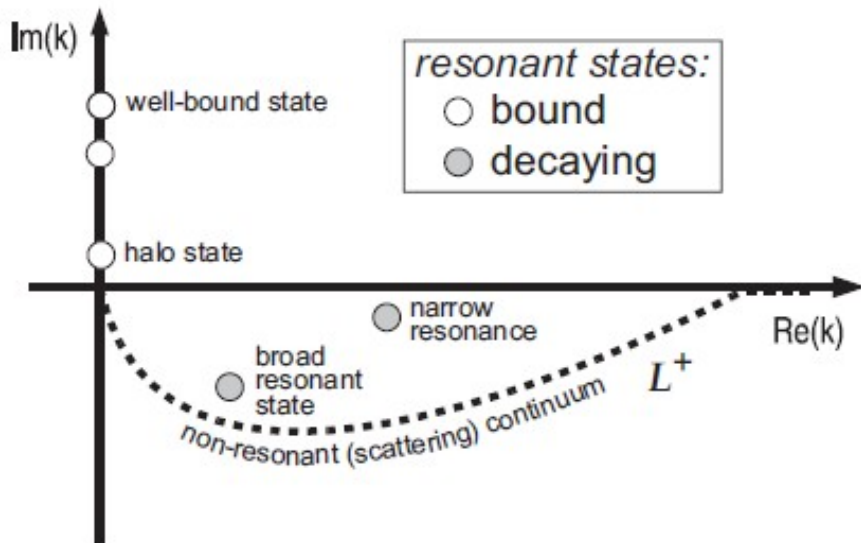


Complex scattering state

$$u(r) \rightarrow C_+ H_{l,\eta}^+(kr) + C_- H_{l,\eta}^-(kr)$$

Gamow Shell Model (GSM)

N. Michel *et al*, J.Phys. G36 (2009) 013101



"Shell Model in the Berggren basis"

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

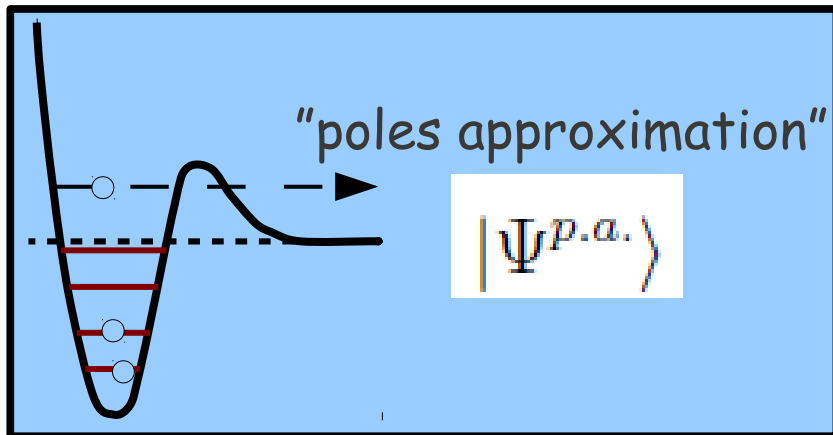
$$|SD_i\rangle = |u_{i1}\dots\dots u_{iA}\rangle$$

iii) construction of Hamiltonian matrix

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

(complex-symmetric matrix)

iv) \rightarrow many-body bound, resonant and continuum states

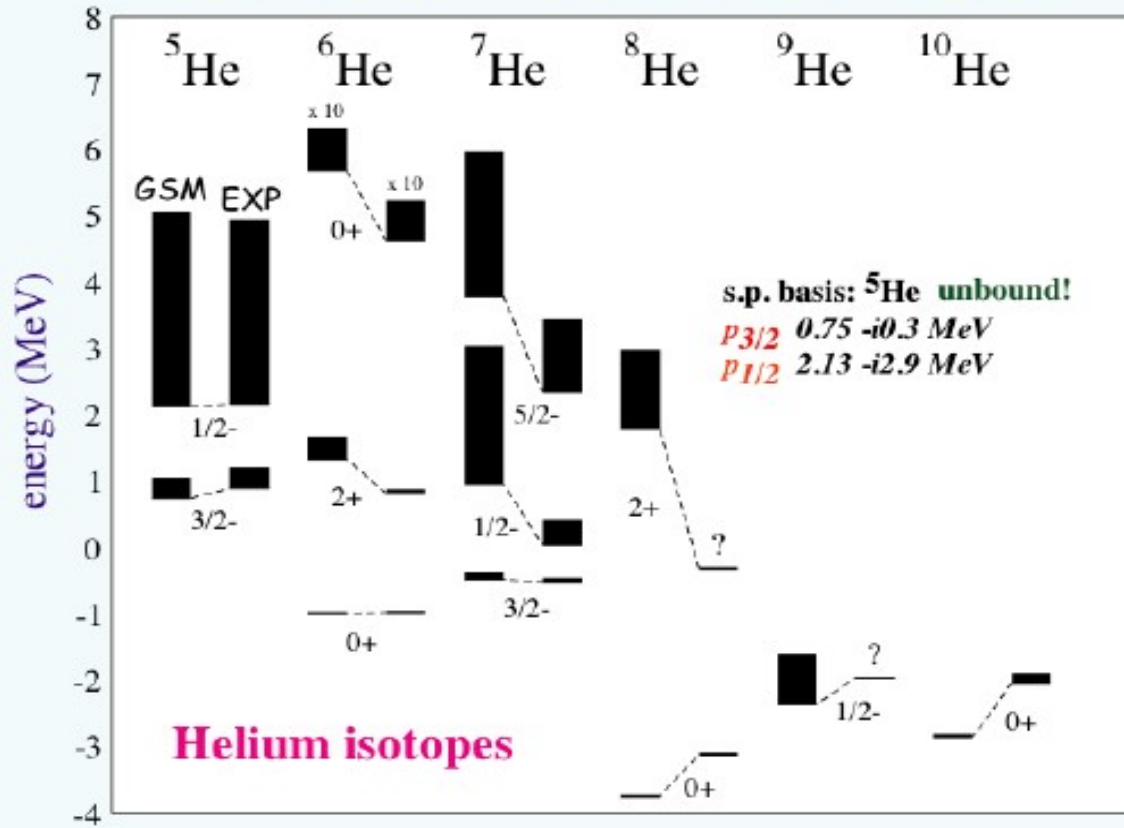


Many-body resonance states :

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

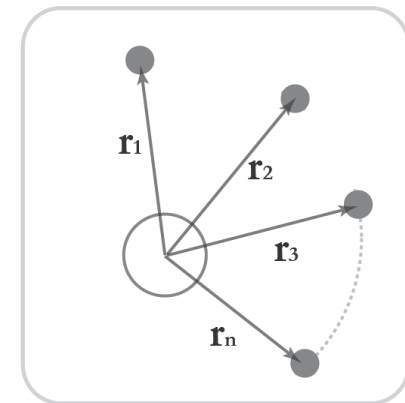
Helium chain (^4He core plus valence neutrons)

GSM: N. Michel et al., Phys.Rev.Lett. 89, 042502 (2002)



i) Woods-Saxon potential for (^4He -n)

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



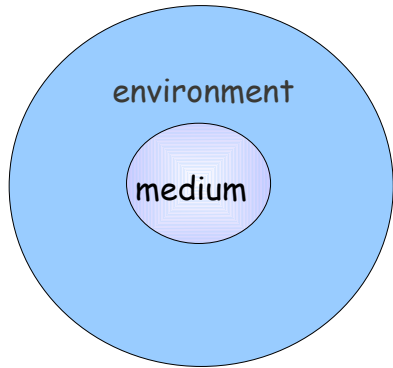
Pole approximation :

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

Density Matrix Renormalization Group (DMRG)

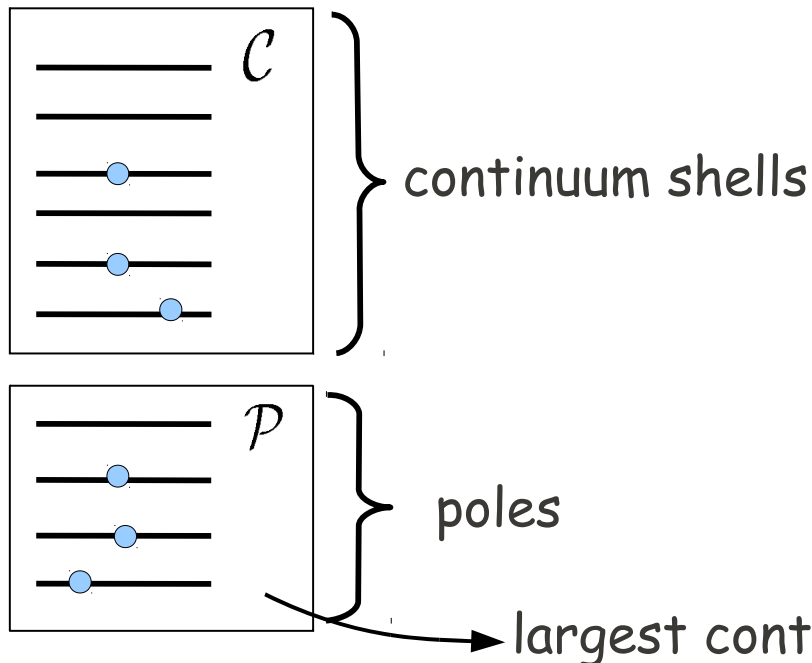
S. R. White, PRL. 69 (1992); PRB 48 (1993)
T.Papenbrock et al J.PG 31 (2005)
S.Pittel et al PRC 73 (2006)

quantum system



- * separation into a "medium" and "environment"
- * truncation of degrees of freedom in the environment

GSM-picture



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

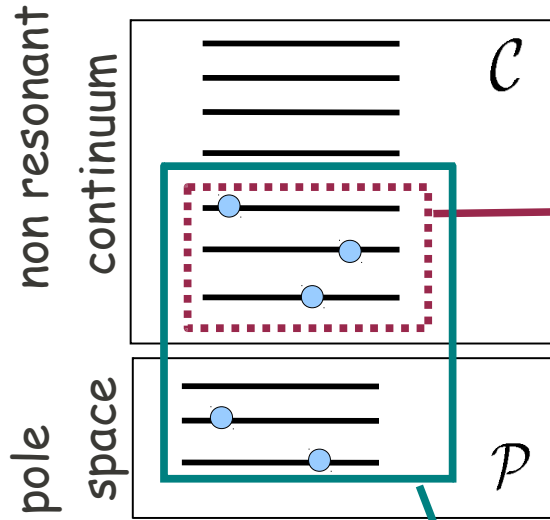
DMRG

truncation among states with nucleons in the continuum

largest contribution to the GSM wave function

Warm up phase

Construction of 2nd quantization operators and states in \mathcal{P} and \mathcal{C}



block

states with 0,1,...n nucleons

$$a_i^\dagger, (a_i^\dagger a_j^\dagger)^K, [(a_i^\dagger a_j^\dagger)^K \tilde{a}_k]^L \dots$$

states with 0,1,...n nucleons

$$a_i^\dagger, (a_i^\dagger a_j^\dagger)^K, [(a_i^\dagger a_j^\dagger)^K \tilde{a}_k]^L \dots$$

* diagonalization in the superblock $\longrightarrow |\Psi\rangle^J = \sum_{p,c} \Psi_{pc} (|p\rangle^{J_p} |c\rangle^{J_c})^J$

* singular value decomposition $\left\{ \begin{array}{l} |\Psi'\rangle^J = \sum_{p,\alpha} \Psi_{p\alpha} (|p\rangle^{J_p} |\alpha\rangle^{J_c})^J \\ |\Psi'\rangle^J \simeq |\Psi\rangle^J \end{array} \right.$

$|\alpha\rangle$: eigenvectors of density

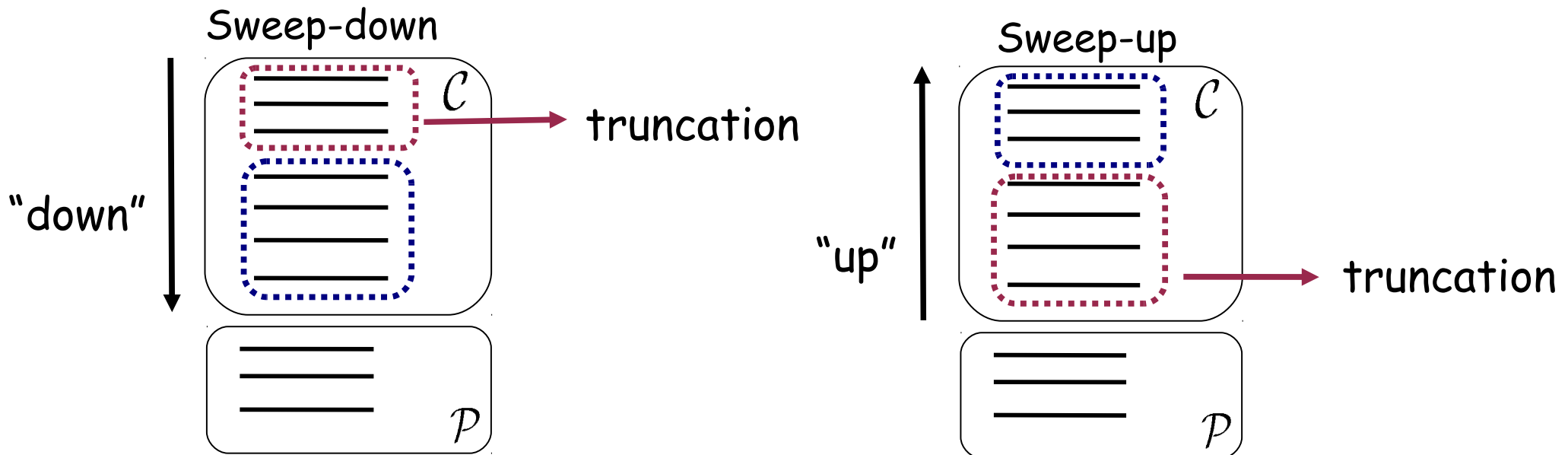
$$\rho_{c,c'}^{J_c} = \sum_p \Psi_{pc} \Psi_{pc'}$$

N_{opt} eigenstates of density with "largest" eigenvalues are kept:

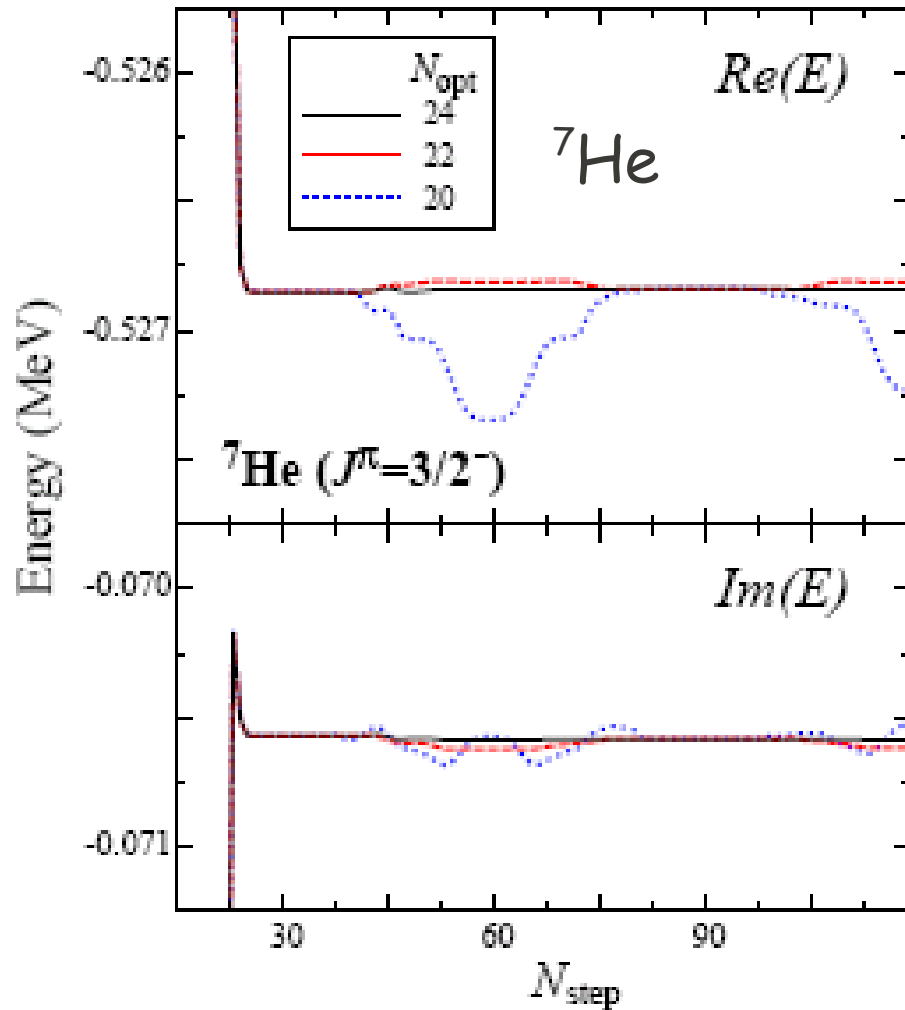
i) fixed N_{opt} or ii) $|1 - \text{Re} \left(\sum_{\alpha=1}^{N_{\text{opt}}} w_\alpha \right)| < \varepsilon$

In the warm up phase, continuum shells are added one by one until they all have been included.

sweeping phase



Convergence of the energy as a function of DMRG iteration



GSM description of ${}^7\text{He}$:

${}^4\text{He}$ core + 3 neutrons

*Woods-Saxon potential + Gaussian V_{nn}

*resonance : $0p_{3/2}$, $0p_{1/2}$

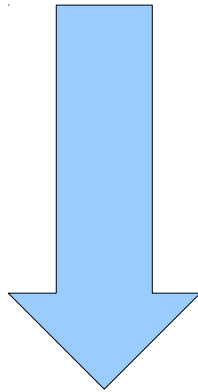
*complex-continuum shells: $p_{3/2}$, $p_{1/2}$

(62 shells)

Full GSM dimension = 83,948
DMRG dimension = 1,143

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

- * All nucleons are active
- * Expansion in the Berggren basis
- * Density Matrix Renormalization Group technique



Ab Initio description of light nuclear systems at and beyond the drip lines

"No Core Gamow Shell Model"

No Core Gamow Shell Model (NCGSM)

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

G. Papadimitriou *et al*,
arXiv:1301.7140

i) NN potential:

* AV18 (R.B. Wiringa *et al* PRC 51 (1995) 38)

* N³LO (D.R. Entem *et al* PRC(R) 68 (2003) 041001)

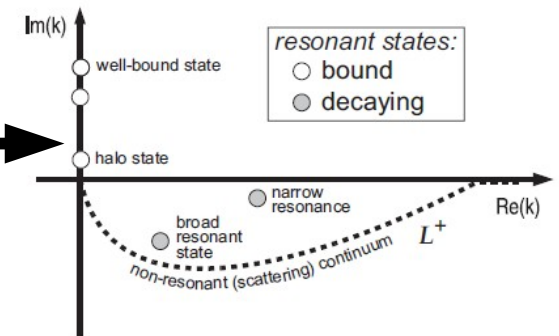
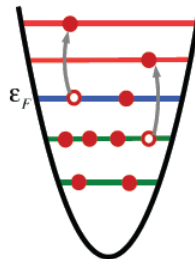
(For comparison with Faddeev, Faddeev-Yakubovsky and Coupled Cluster)

} softened by $v_{\text{low-k}}$ with $\Lambda = 1.9 \text{ fm}^{-1}$
(S. Bogner *et al*, Phys. Rep. 386 (2003) 1)

ii) single particle states:

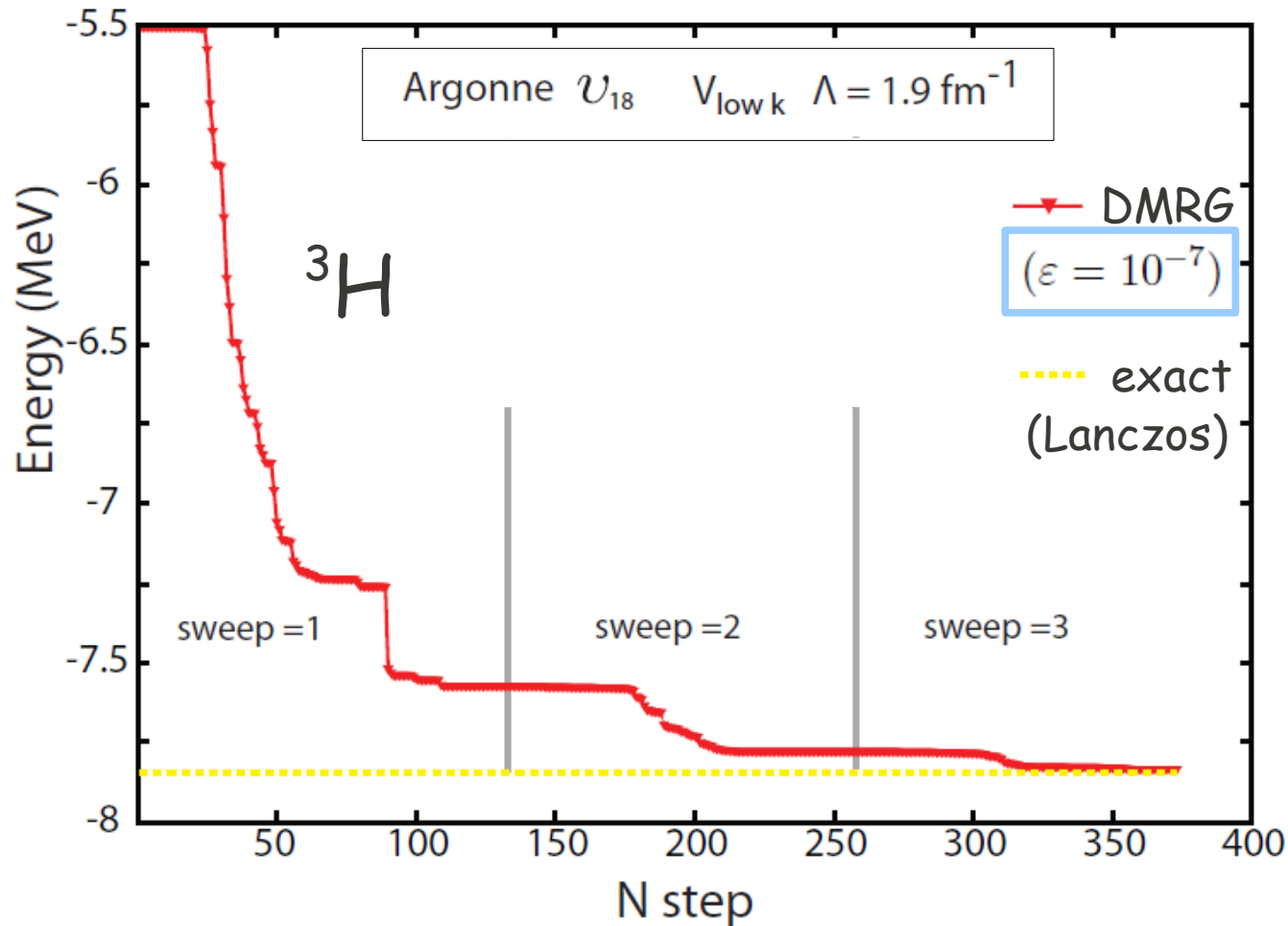
a) s- and p-shells from Hartree-Fock potential

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



iii) Numerical resolution with DMRG

Calculations of ³H, ⁴He and ⁵He



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

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

* $0s_{1/2}(p)$: $E = -10.417 \text{ MeV}$

* $0s_{1/2}(n)$: $E = -11.982 \text{ MeV}$

130 shells

J-scheme dimension

* Full NCGSM space: 96,883 $\longrightarrow E_{\text{exact}} = -7.840 \text{ MeV}$

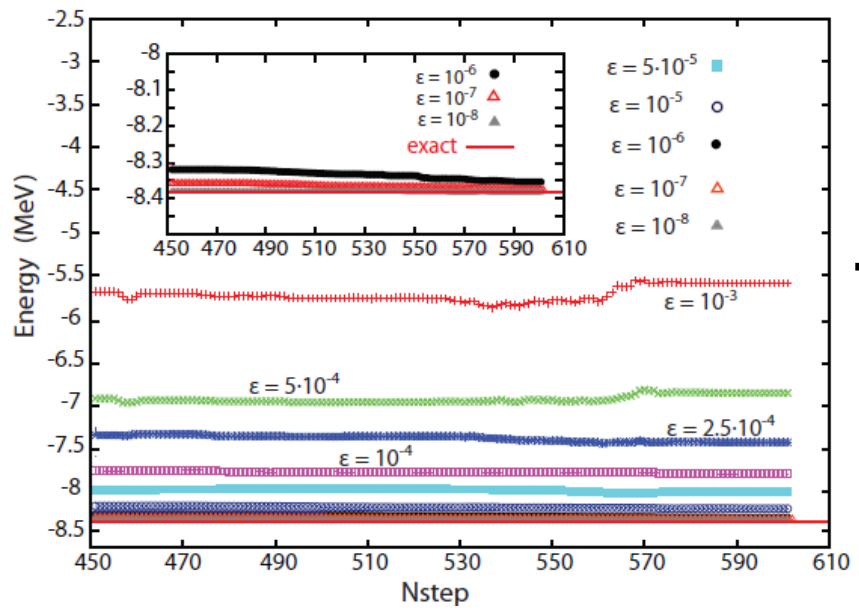
* DMRG $\sim 1,200$ $\longrightarrow E_{\text{DMRG}} = -7.832 \text{ MeV}$

G. Papadimitriou et al,
arXiv:1301.7140

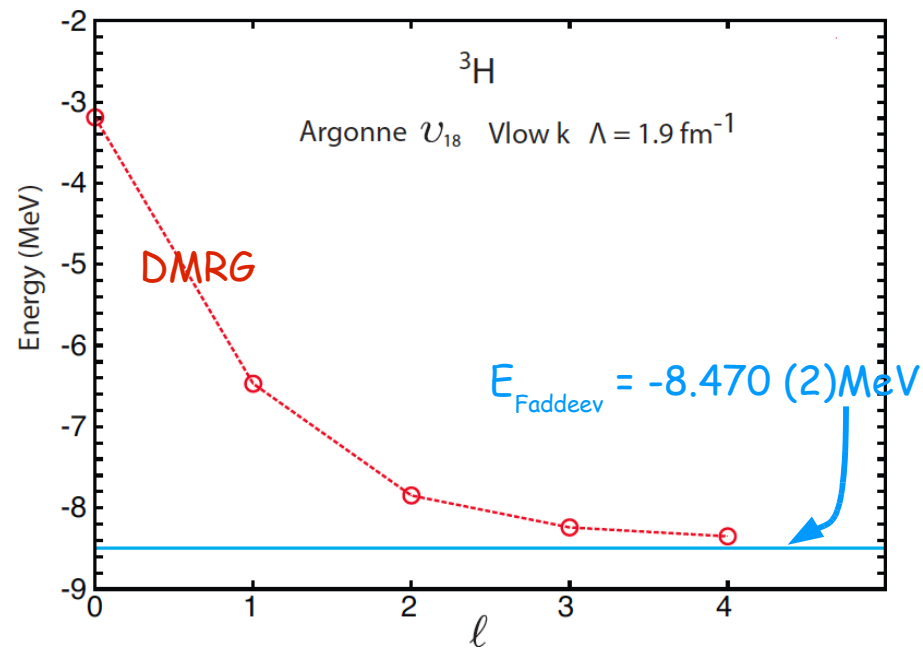
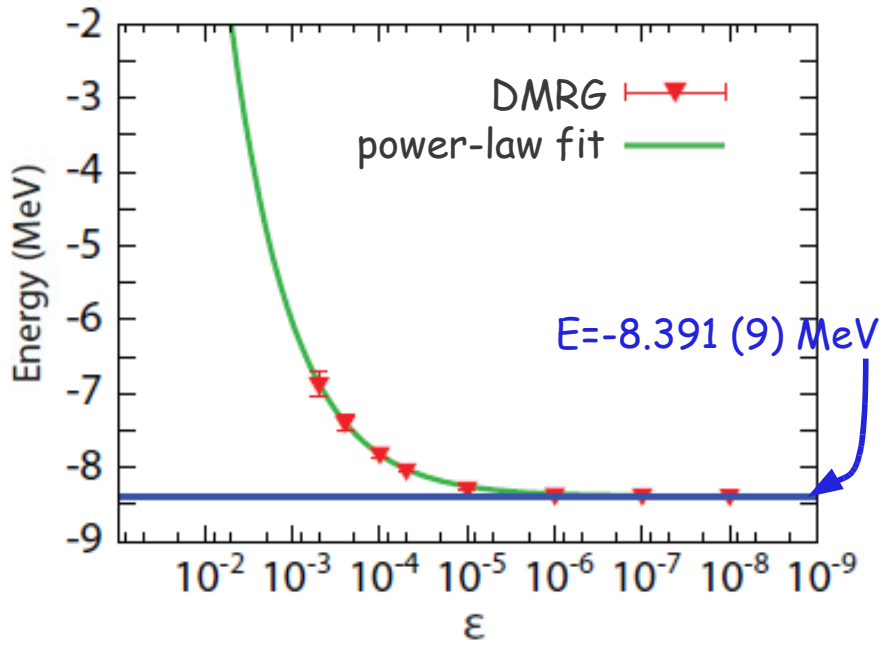
^3H binding energy

*spdfg shells
 *full NCGSM dim: 123,835

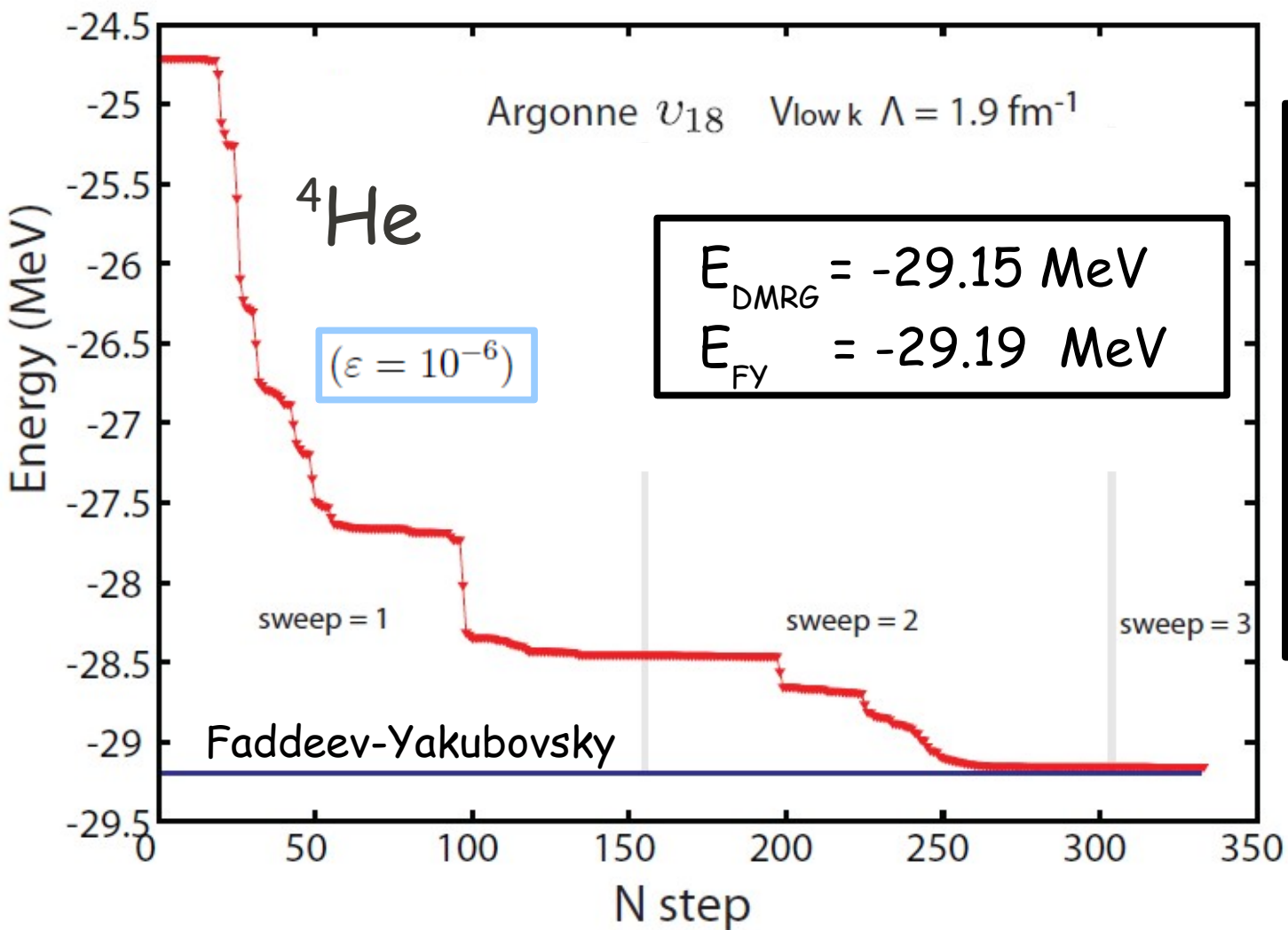
Evolution of energy with iteration



| ϵ | dimension | energy (MeV) |
|---------------------|-----------|--------------|
| $5.0 \cdot 10^{-4}$ | 99 | -6.878 |
| $2.5 \cdot 10^{-4}$ | 109 | -7.396 |
| 10^{-4} | 173 | -7.821 |
| $5.0 \cdot 10^{-5}$ | 308 | -8.042 |
| 10^{-5} | 600 | -8.287 |
| 10^{-6} | 1075 | -8.357 |
| 10^{-7} | 1909 | -8.381 |
| 10^{-8} | 2575 | -8.388 |



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



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

ii) dfg H.O states

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

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

156 Shells

G. Papadimitriou et al, arXiv:1301.7140

J-scheme dimension

* Full NCGSM space: 6,230,512

* DMRG ~ 6000

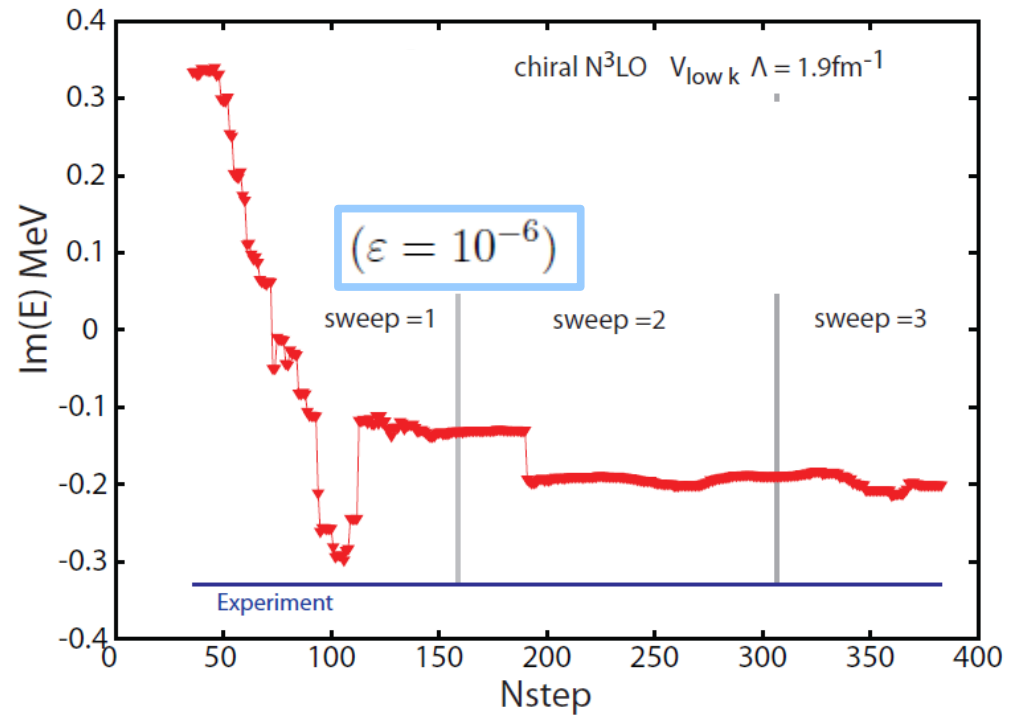
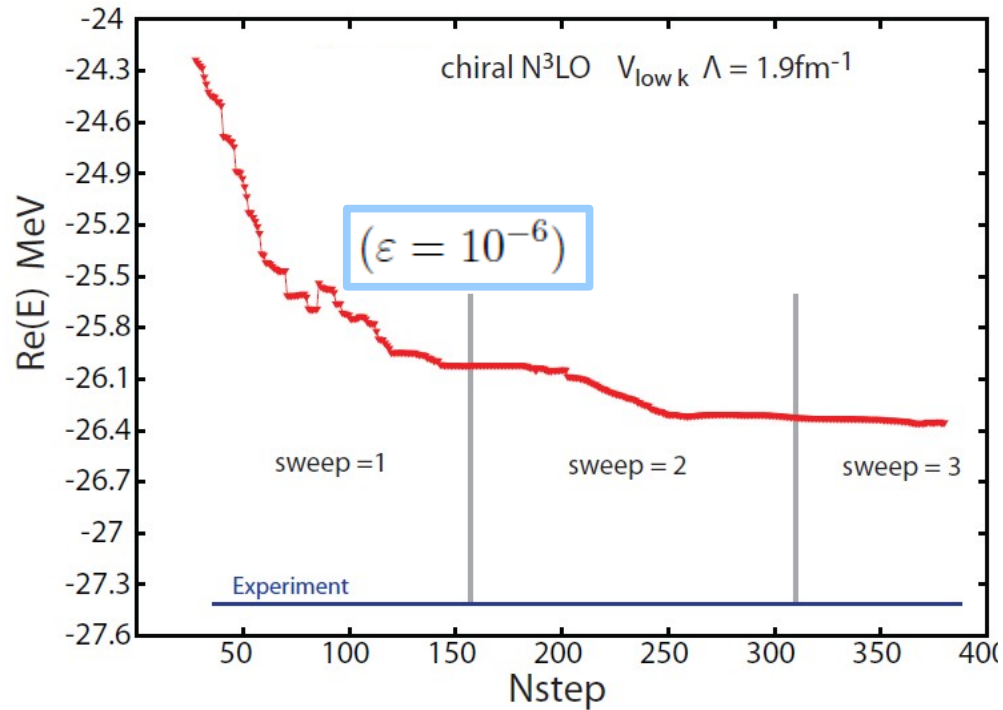
(FY result from Nogga et al, PRC 70 (2004))

${}^5\text{He}$

HF poles

- * $0p_{3/2}(n)$: $E = (1.194, -0.633)$ MeV
- * $0s_{1/2}(p)$: $E = -23.291$ MeV
- * $0s_{1/2}(n)$: $E = -23.999$ MeV

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



157 Shells

J-scheme dimension

- * Full NCGSM space: 1,379,196,439
- * DMRG $\sim 1.10^5$

DMRG

$(\epsilon = 10^{-6})$

$(-26.31, -0.20)$

Coupled Cluster

(CCSD)

$(-24.87, -0.16)$

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

Ab initio description of light nuclei in the Berggren basis

- ◆ coupling with the continuum states taken into account by expansion in the Berggren basis.
- ◆ application of the DMRG technique to the Gamow Shell Model and the No-Core Gamow Shell Model.

In development:

- * implementation of truncations
"N-particle N-hole" in DMRG
- * Monte Carlo technique to select continuum shells

Happy Birthday James !

