

Complex energy formalisms: Complex scaling with realistic interactions and The (No Core) Gamow Shell Model

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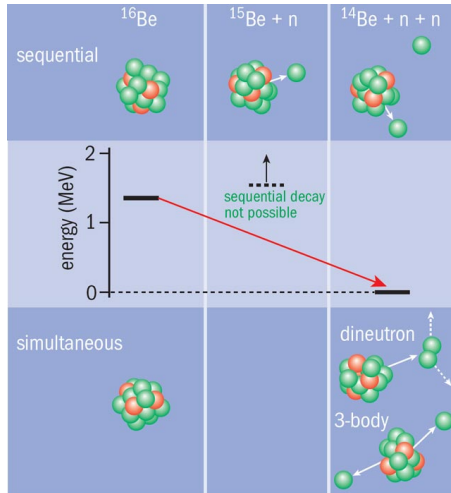
FUSTIPEN
French-U.S. Theory Institute for Physics with Exotic Nuclei

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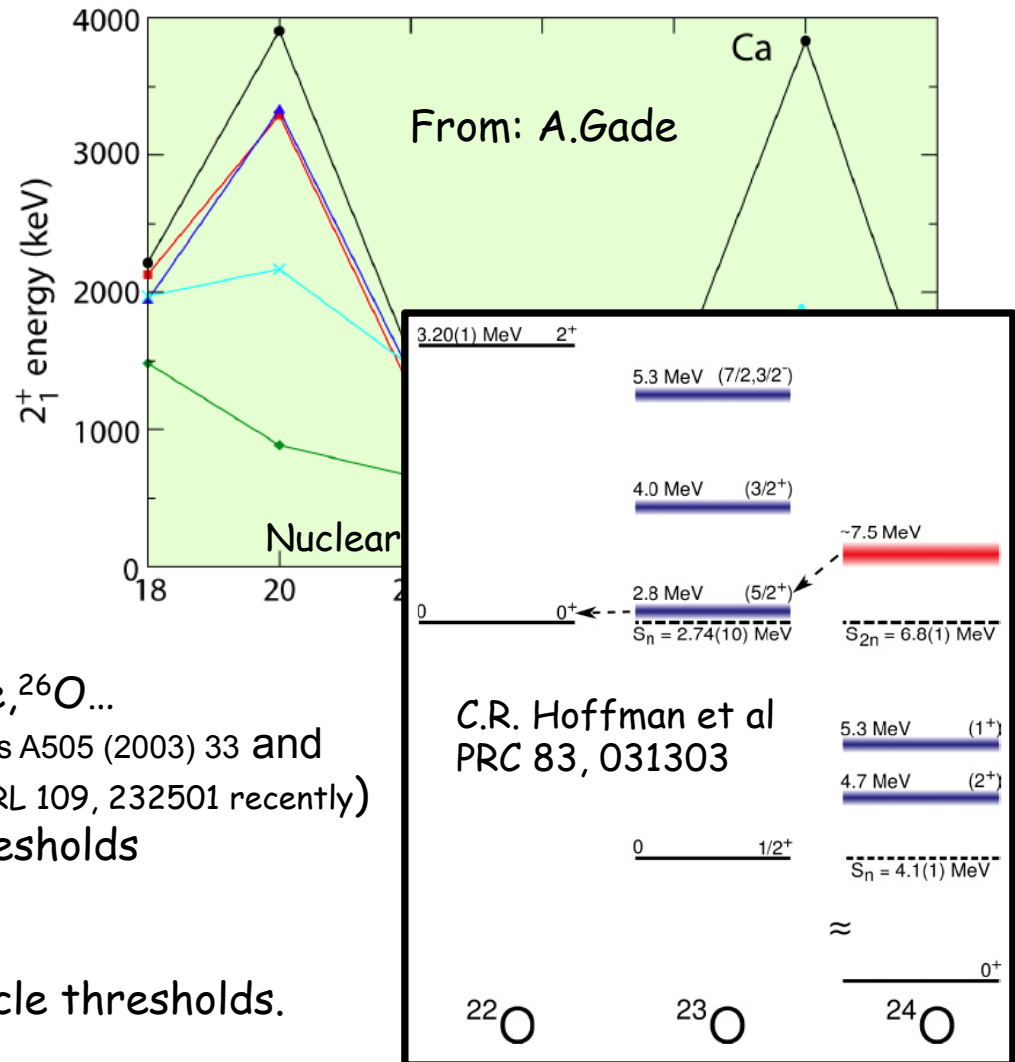
Life on the edge of nuclear stability: Experimental highlights

- New decay modes: 2n radioactivity



A.Spyrou et al

- Shell structure revisited: Magic numbers disappear, other arise.



- New exotic resonant states: ^{13}Li , ^{10}He , ^{26}O ...
(MoNA collaboration Nucl. Instr. and Methods A505 (2003) 33 and PRC 87, 011304, PRL 110 152501, PRL 108 142503, PRL 109, 232501 recently)
- Metastable states above particle thresholds are measured.
- Very dilute matter distribution
- Extreme clusterization close to particle thresholds.

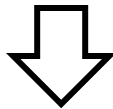
Provide stringent constraints to theory

But also: Theory is in need for predictions and supporting certain experimental aspects

Connections between structure and reactions

- They share many-common ideas and difficulties:
- Effective interactions/optical potentials
 - Many channels in CC equations/A lot of basis states (e.g in CI) => need for supercomputing/collaboration with Computer-Scientists
 - Approximations to make calculations easier: e.g Eikonal approximation/ basis truncations, MBPT, cluster expansions etc => How well are controlled? (Benchmarks are important)

The common denominator though it is that we (both) want to calculate observables.



observable $\sigma^{if} = \sum_{|J_f - J_i| \leq j \leq J_f + J_i} S_j^{if} \sigma_{s.p.}$

Spectroscopic factor

s.p cross section

From D. Bazin and R. Furnstahl

Spectroscopic factor

Another example: $\Gamma_{tot} = S \Gamma_{s.p}$

etc...

Avoid this route!!

Connections between structure and reactions

But we want to do it in a model independent way, so as to reduce uncontrollable errors by combining ingredients from different methods which are probably based on different assumptions.

- That is why the ultimate goal is to unify structure+reactions!
Calculate structure and reaction observables using the same assumptions and the same Hamiltonian.
- Try to depart from Spectroscopic factors and use, for example, ANCs
- Try to compute directly resonant parameters (resonances)
i.e. positions and total widths

Resonances

→ How to obtain them?

- On the real-energy axis from the phase-shift $\delta(E)$: Position → inflection point
Width → $2/(d\delta/dE)$ at inflection point. Basically it is an R-matrix formula (maybe not so reliable for broad resonances e.g. Thompson-Nunes book page 302)

In addition one needs $\delta(E)$, meaning that reaction coupled channel heavy calculation is unavoidable.

- “Stabilization” techniques on the real-axis
- Widths from ANCs and Integral relations
- On the complex energy axis, poles of complex S-matrix: unambiguous extraction
e.g. “Extended” R-matrix (Hale, Csoto) for broad ^5He , ^5Li resonances
 - Complex energy shell model
 - Complex Scaling

The complex scaling

Belongs to the category of:

- **Bound state** technique to calculate resonant parameters and/or states in the continuum
Prog. Part. Nucl. Phys. 74, 55 (2014) and 68, 158 (2013)
(reviews of bound state methods by Orlandini, Leidimann-Lazauskas, Carbonell)

Nuclear Physics

- Nuttall and Cohen PR 188, 1542 (1969)
- Lazauskas and Carbonell PRC 72 034003 (2005)
- Witala and Glöckle PRC 60 024002 (1999)
- Aoyama et al PTP 116, 1 (2006)
- Horiuchi, Suzuki, Arai PRC **85**, 054002 (2012)
- Myo, Kikuchi, Masui, Kato Prog. Part. Nucl. Phys. 79 1 (2014)

Chemistry

- Moiseyev Phys. Rep 302 212 (1998)
- Y. K. Ho Phys. Rep. 99 1, (1983)
- McCurdy, Rescigno PRL 41, 1364 (1978)

The complex scaling

Complex Scaling Method in a Slater basis

A.T.Kruppa, G.Papadimitriou, W.Nazarewicz, N. Michel PRC 89 014330 (2014)

1) Basic idea is to rotate coordinates and momenta i.e. $r \rightarrow re^{i\theta}$

Hamiltonian is transformed to $H(\theta) = U(\theta)H_{\text{original}}U(\theta)^{-1}$

$H(\theta)\Psi(\theta) = E\Psi(\theta)$ complex eigenvalue problem

- The spectrum of $H(\theta)$ contains bound, resonances and continuum states.

2) Slater basis or Slater Type Orbitals (STOs):

Basically, exponential decaying functions

$$\sum_{l_1, j_1} \sum_{l_2, j_2} \sum_{i, j=0}^N C_{l_1 j_1 l_2 j_2, ij} \mathcal{A} \left(r_1^{l_1+i} r_2^{l_2+j} \exp(-ar_1 - ar_2) [\mathcal{Y}_{l_1 j_1}(\hat{r}_1, s_{z1}) \otimes \mathcal{Y}_{l_2 j_2}(\hat{r}_2, s_{z2})]^{IM} \right)$$

→ CS: Powerful method to obtain resonance parameters in Quantum Chemistry

→ Involves L^2 square integrable functions. Resonance parameters are obtained without an implicit imposition of boundary conditions. Resonant states behave like bound states at large r .

→ Can (in general) be applied to available bound state methods techniques
(i.e. NCSM, Faddeev, CC etc)

Some results (${}^6\text{He}$)

- Comparison between Complex Scaling Slater and Gamow Shell Model

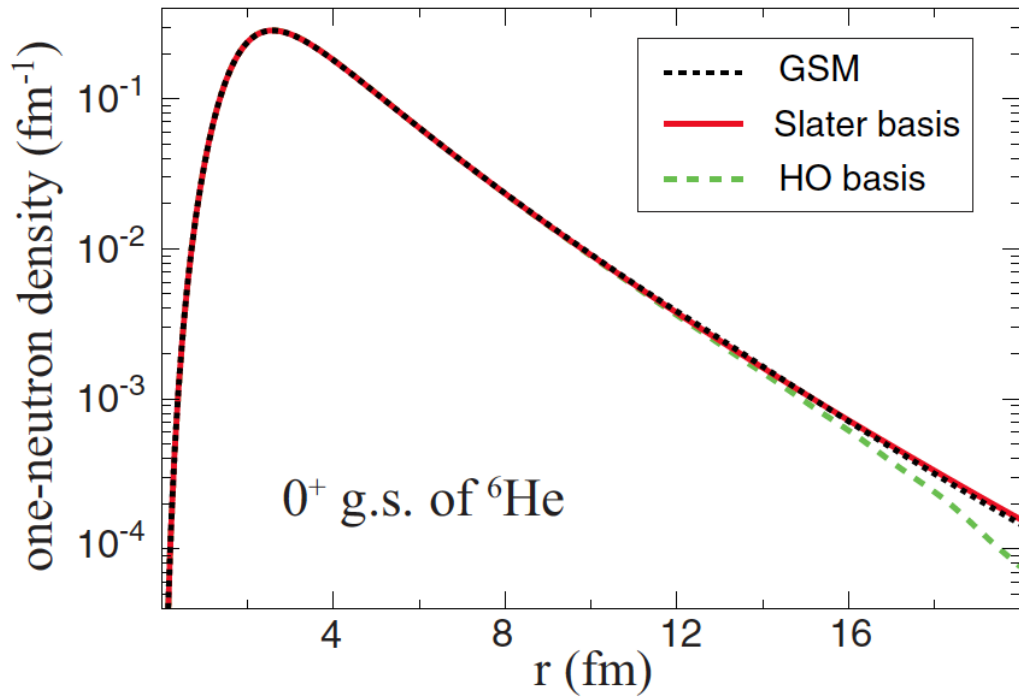
0^+ g.s, 2^+ 1^{st} excited Force Minnesota, α - n interaction KKNN

$\langle \hat{O} \rangle$	0^+	GSM	CS ($\vartheta = 0$)
$\langle \hat{H} \rangle$		-0.249	-0.247
$\langle \hat{T} \rangle$		24.729	24.731
$\langle V_{c-n} \rangle$		-21.642	-21.645
$\langle V_{nn} \rangle$		-2.711	-2.710
$\langle \frac{\vec{p}_1 \cdot \vec{p}_2}{m_3} \rangle$		-0.625	-0.623

$\langle \hat{O} \rangle$	2^+	CS ($\vartheta = \vartheta_{\text{opt}}$)	GSM _I
$\langle \hat{H} \rangle$		$1.239 - i0.291$	$1.239 - i0.292$
$\langle \hat{T} \rangle$		$17.340 - i7.949$	$17.311 - i7.825$
$\langle V_{c-n} \rangle$		$-15.831 + i7.408$	$-15.805 + i7.288$
$\langle V_{nn} \rangle$		$-0.270 + i0.250$	$-0.267 + i0.244$

→ Reliable calculation of widths of metastable states

Some results



${}^6\text{He } 0^+$ g.s.
Valence neutrons radial density

Phenomenological NN
Minnesota interaction

${}^6\text{He}$ is seen as a three body
problem.

Correct asymptotic behavior

Complex Scaling with a general non-local realistic force?

Has been tried with very strong core Reid and AV18 potentials (analytical/local)
(Lazauskas, Glöckle, Witala, Horiuchi...)

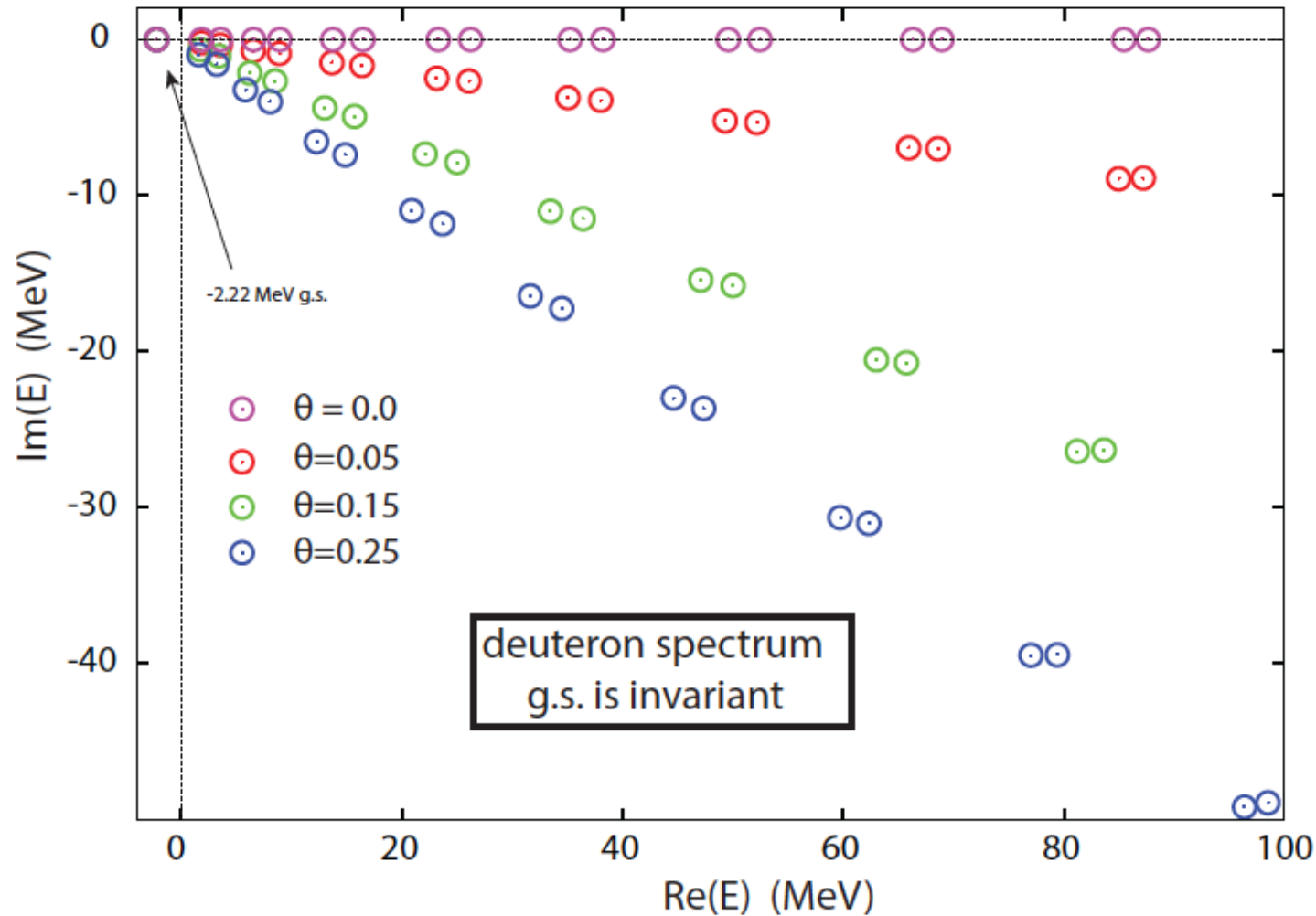
Apply CS in a chiral NN force:

- 2-body problem in relative coordinates.
- $H = T_{\text{rel}} + V_{\text{rel}}$ in HO basis
- Deuteron bound state (3S1-3D1 coupled channels)
- Compute complex scaled matrix elements of the interaction
- Simple implementation: Shift CS transformation to the basis for the TBME

$$H_{\theta} = e^{-2i\theta} T_{\text{rel}} + V_{\text{rel}}(\theta)$$

→ Diagonalize H_{θ} with your favorite diagonalization routine

Complex scaling with the NNLO_{opt} realistic potential



- Test is successful. Bound state position does not change after rotation.
- Probably the first application of CS on a chiral potential.
- That's all you need to create matrix elements in the lab system for other applications

Complex Scaling for scattering phase-shifts

(selected examples) G. Papadimitriou and J.P. Vary PRC(R) 91, 021001 2015

→ Connection with continuum level density (CLD)

$$\Delta(E) = -\frac{1}{\pi} \text{ImTr} \left[\frac{1}{E - H(\theta)} - \frac{1}{E - H_0(\theta)} \right] \quad \text{and} \quad \Delta(E) = \frac{1}{\pi} \frac{d\delta(E)}{dE}$$

$H(\theta)$ is the CS interacting Hamiltonian

$H_0(\theta)$ is the asymptotic Hamiltonian (kinetic energy + (Coulomb))

(Formulas based on work of Giraud, Kruppa, Arai, Kato...)

→ From the CLD one could also extract resonant parameters:

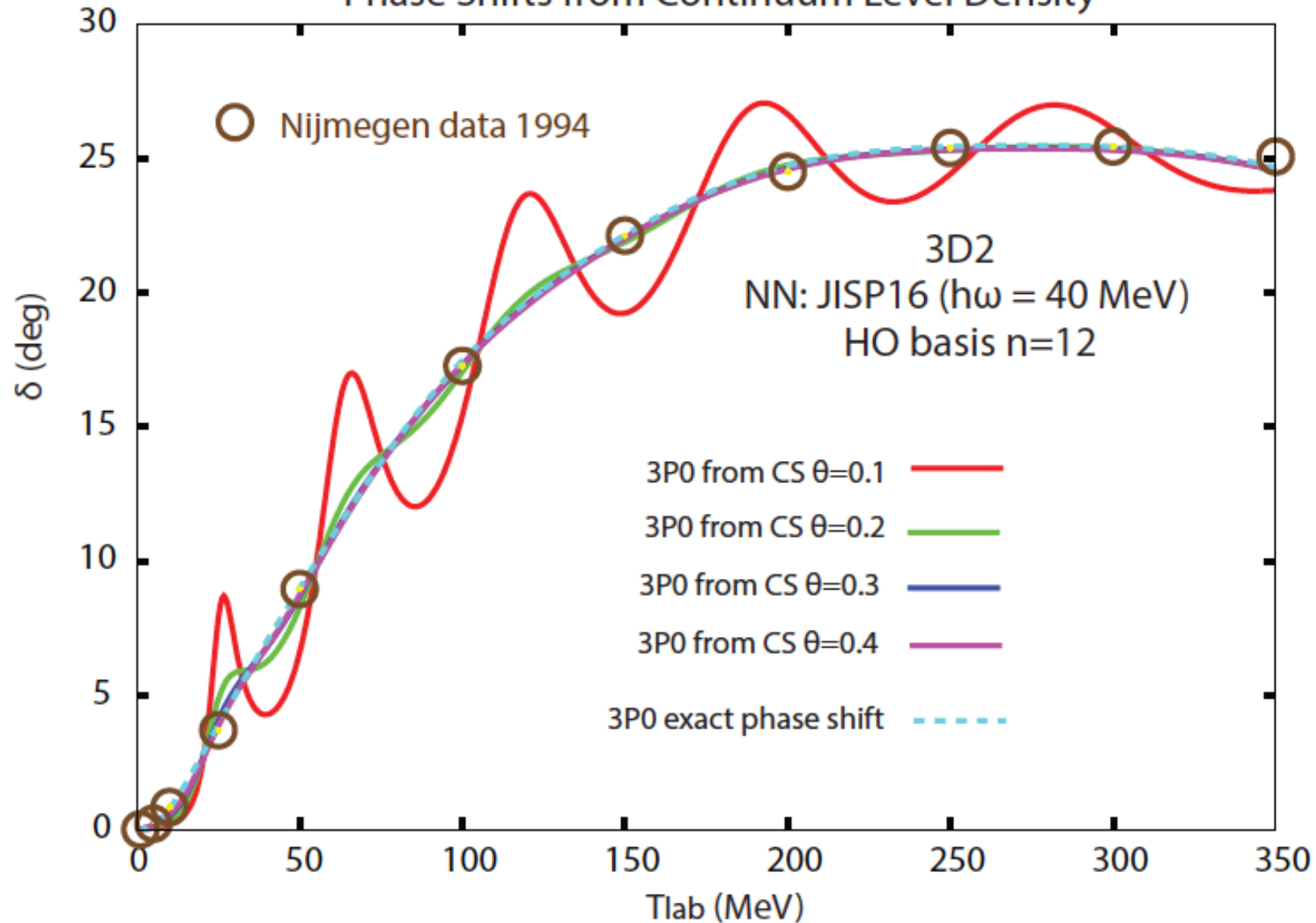
CLD has peaks in the vicinity of a resonance. Use a function to determine the resonant parameters

CS offers three different ways to obtain resonant parameters:

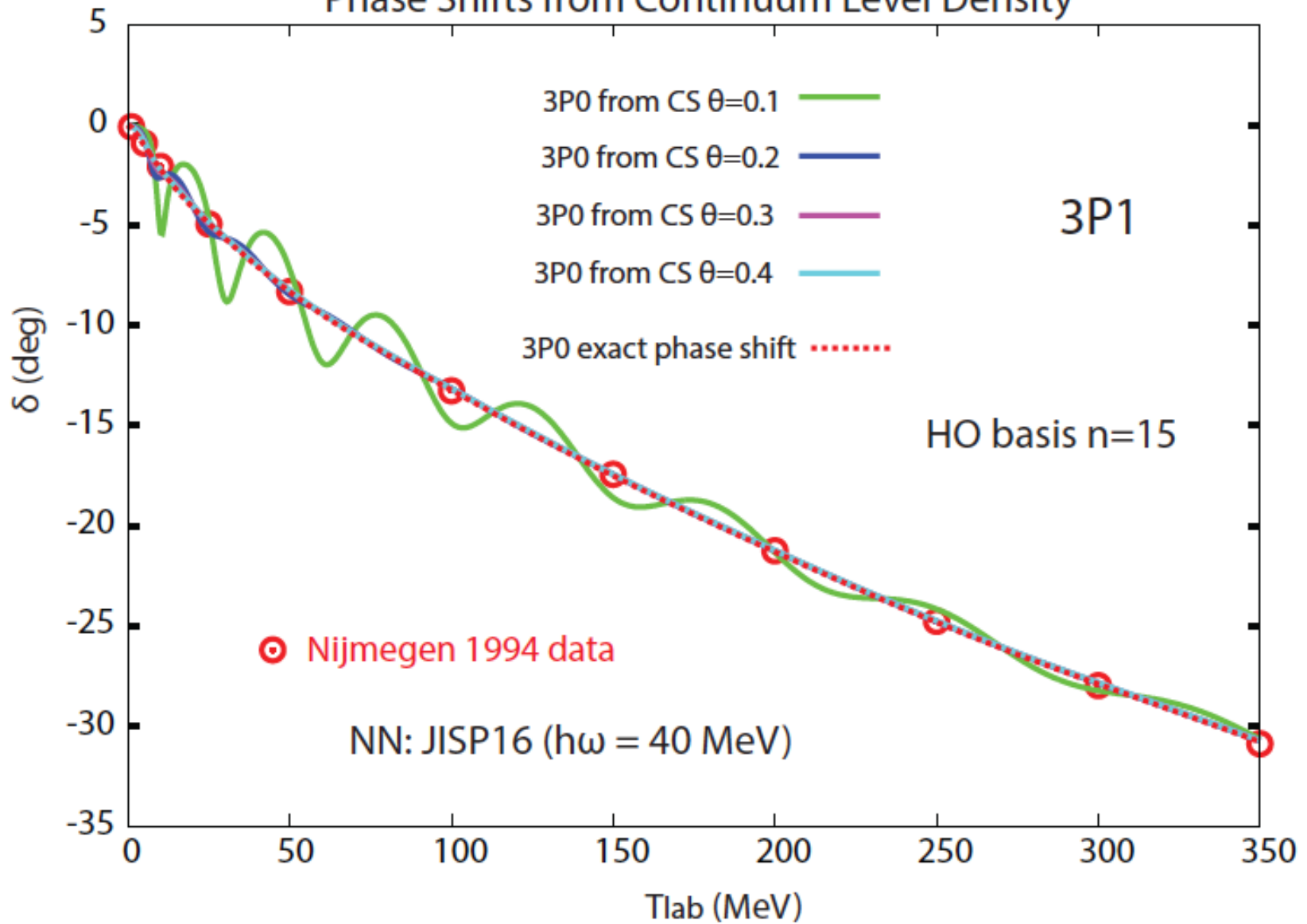
- 1) From eigenstates of Hamiltonian
- 2) From CLD (e.g. fit to Breit-Wigner)
- 3) From phase-shift via the inflection criterion

You could check with the same Hamiltonian what each 'method' gives

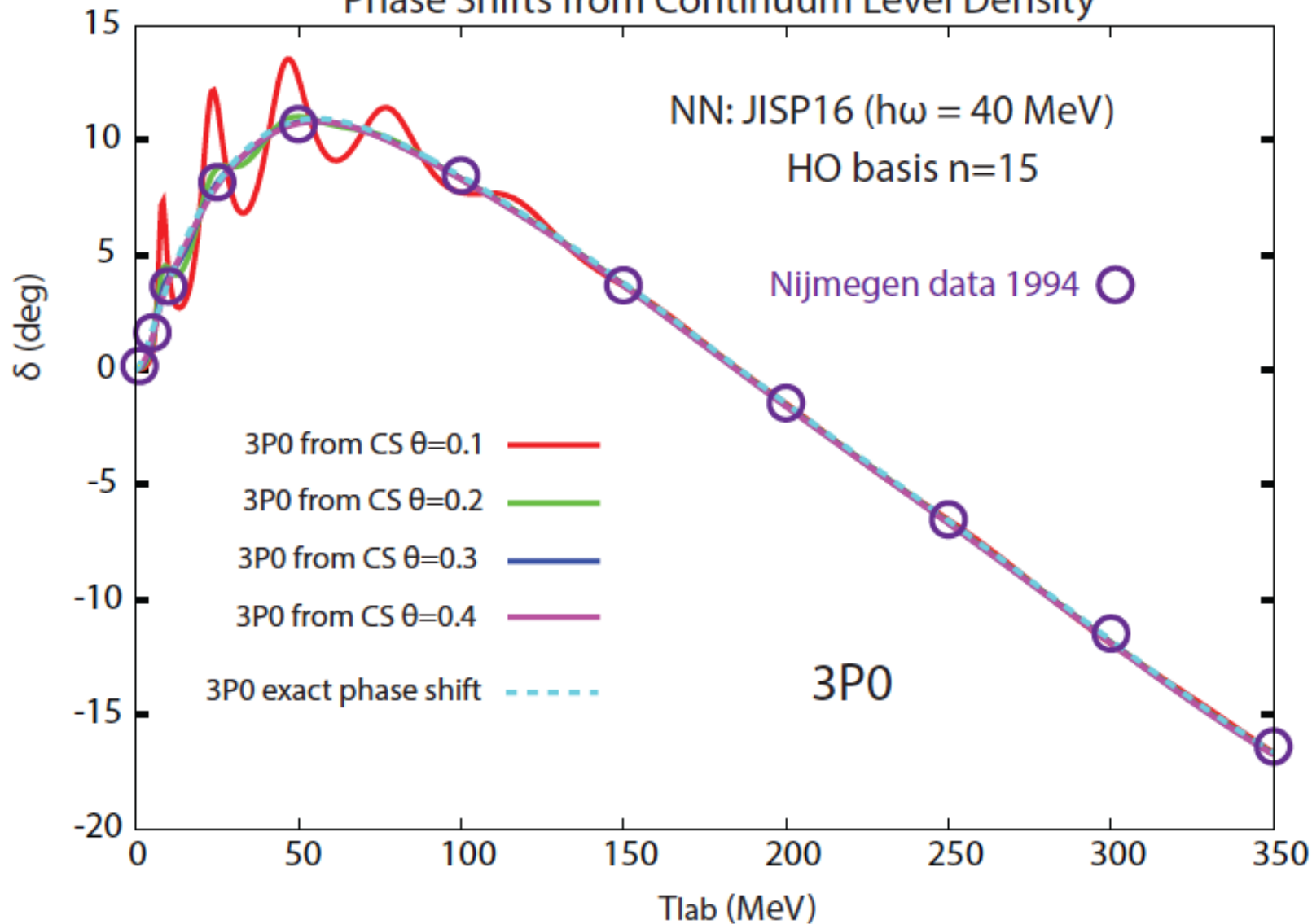
Complex Scaling for a realistic non-local potential
Phase Shifts from Continuum Level Density



Complex Scaling for a realistic non-local potential Phase Shifts from Continuum Level Density



Complex Scaling for a realistic non-local potential
Phase Shifts from Continuum Level Density



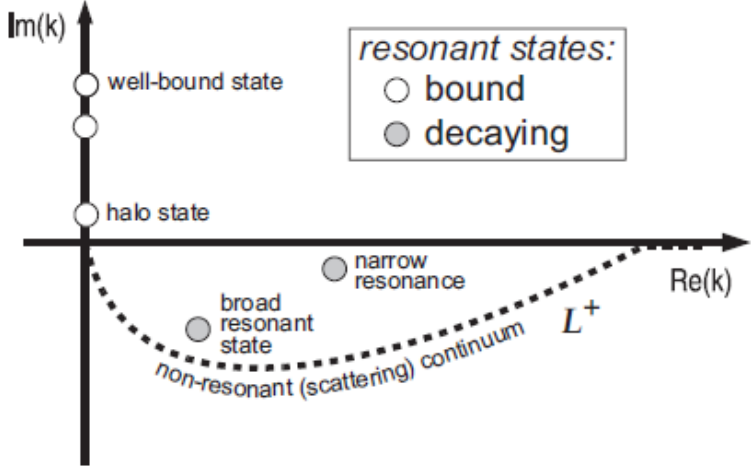
Complex Scaling for structure and reactions (some comments):

- Doable to use realistic, non-local chiral or phenomenological potentials.
- **Phase shifts** converge rapidly with increasing θ and they become independent of θ for values > 0.2 rad.
- **Phase shifts** are obtained by a **diagonalization** of a complex scaled Hamiltonian. No boundary condition is imposed to describe scattering. Bound state technique to obtain phase shifts and hence cross-sections.
- Method gives at the same time: widths, partial widths, position of resonances, (structure) and also reaction observables with a single diagonalization...
- Expected to work with any bound state technique, since it is built to use L^2 integrable functions (e.g. HO).
- The lack of boundary conditions may make the method suitable also for d,p reactions where the Coulomb treatment will not require any screening

Another Complex Energy Method: Gamow Shell Model

T.Berggren (1968)
NP A109, 265

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 **Non-resonant**
(bound, resonances...) **Continuum**
along the contour

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

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

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

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

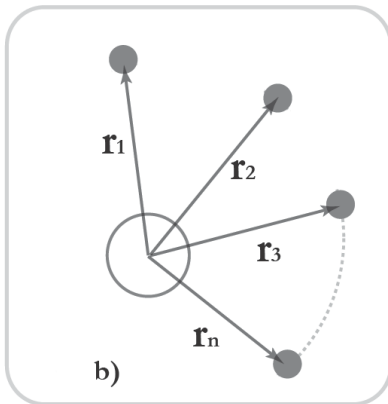
Many body correlations and coupling to continuum are taken into account simultaneously

GSM HAMILTONIAN

$$H = \sum_{i=1}^n \left[\frac{\mathbf{p}_i^2}{2\mu} + U_i \right] + \sum_{j>i=1}^n \left[V_{ij} + \frac{1}{A_c} \mathbf{p}_i \mathbf{p}_j \right]$$

→ We assume an alpha core in some of our calculations..

“recoil” term coming from the expression of H in relative coordinates.

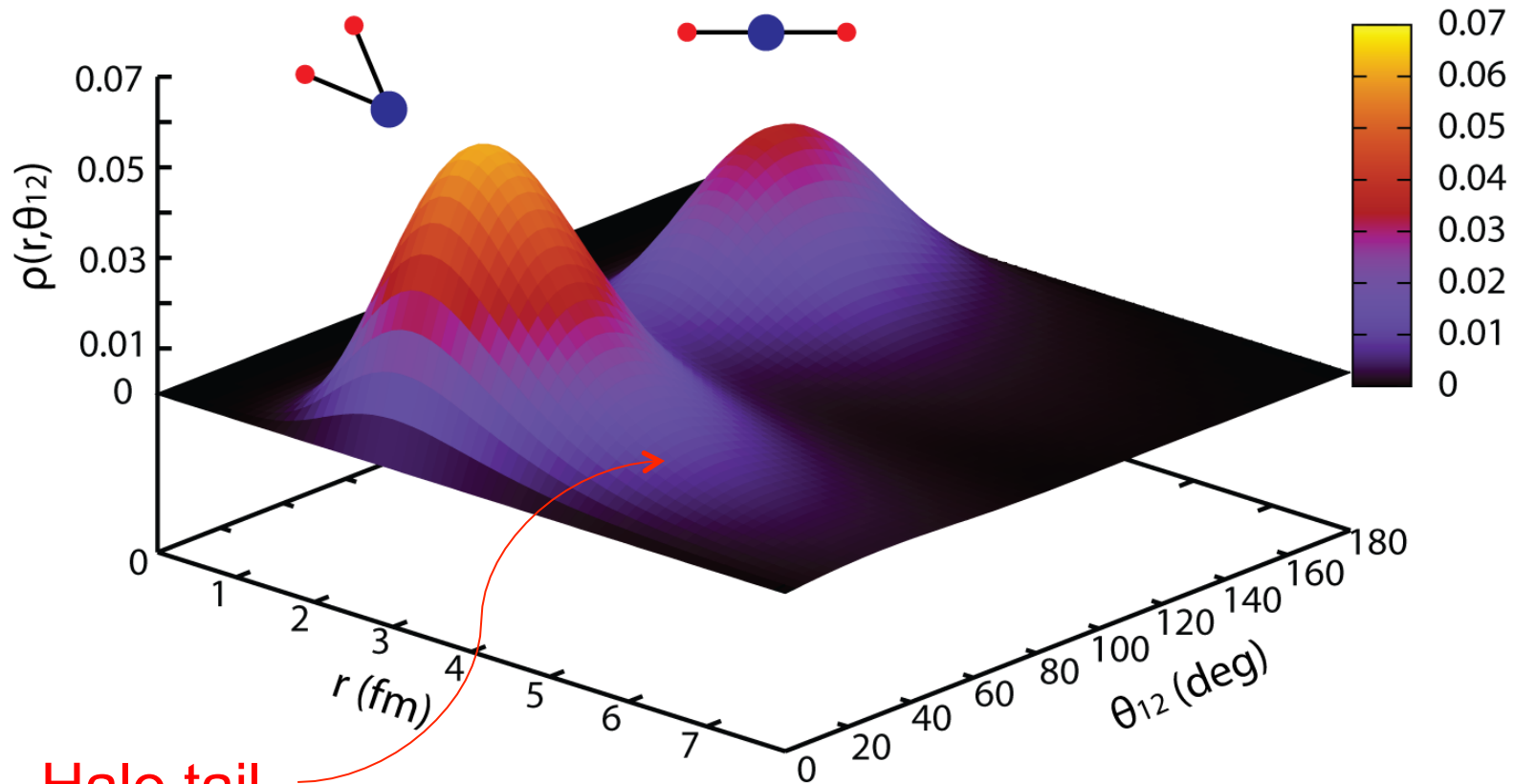


V_{ij} usually a phenomenological/schematic NN interaction, and fitted to spectra of nuclei:

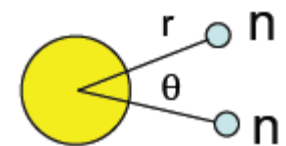
Minnesota force is used, unless otherwise indicated.

Examples: Neutron correlations in ${}^6\text{He}$ ground state (G. P et al PRC 84, 051304 2011)

$$\rho(r_1, r_2, \theta_{12}) = \langle \Psi | \delta(r_1 - r) \delta(r_2 - r') \delta(\theta_{12} - \theta) | \Psi \rangle$$



Halo tail



→ Probability of finding the particles at distance r from the core with an angle θ_{nn}

See also I. Brida and F. Nunes NPA 847,1 and Quaglioni, Redondo, Navratil PRC 88, 034320

Effective interactions in the (Gamow) Shell Model

→ Attempts to create an effective interaction are as old as nuclear physics

Two "schools" of thought:

1) Try to make a link with the microscopic NN interaction in free space by taking into account the in-medium effects.

Examples:

- Brueckner theory,
- Kuo-Brown MBPT,
- Density matrix expansion
- Effective interactions for shell model from CC, IM-SRG, NCSM with a core....

2) Assume an analytic form of the force consistent with symmetries of the nuclear Hamiltonian and make a global fit to nuclear properties and/or nuclear matter.

Examples:

- Skyrme-Gogny in nuclear DFT
- Shell Model Interactions à la Alex-Brown (USD etc)

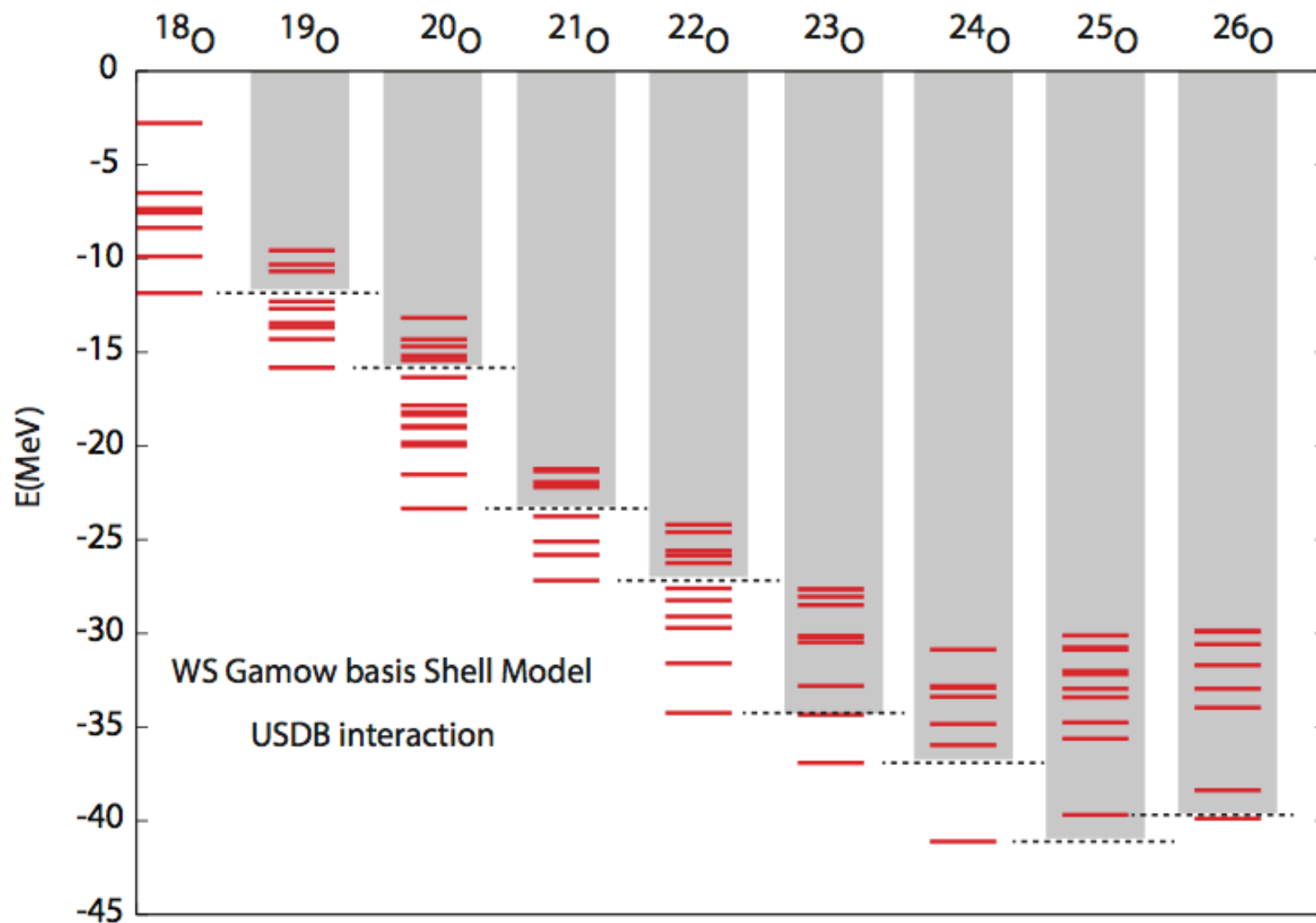
Of course even the free space NN interaction is also effective!
(Chiral EFT or meson exchange models)

Further approaches for renormalization include Vlowk, SRG, UCOM etc...

Oxygen isotopes: A playground for many-body methods.

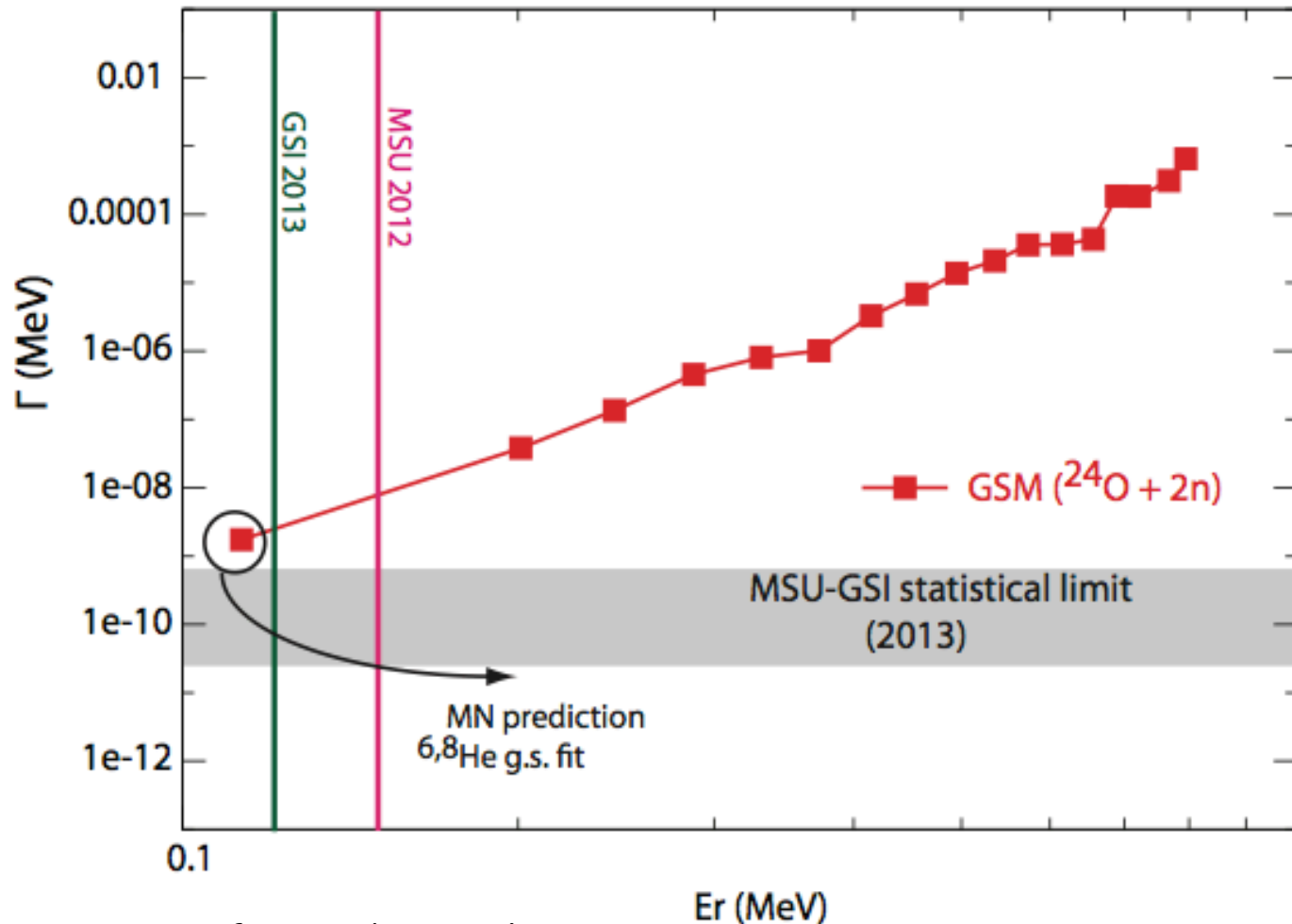
- $3N$ forces necessary, many states are unbound so you need a theory to obtain widths (continuum coupling)
- Most consistent calculation up to now ($3N + \text{continuum}$) by ORNL group (G. Hagen et al)
- Effective microscopic interaction plus continuum e.g. Q-box in Gamow basis for the sd interaction (^{24}O as a core Tsukiyama, Hagen, Jensen)
- IMSRG calculations, SCG(Gorkov)F etc

Preliminary (work in progress)



(work in progress) Phenomenology of ^{26}O

Using a ^{24}O core and a schematic interaction study S_{2n} -width correlation of ^{26}O



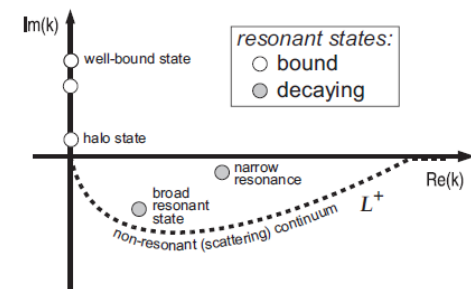
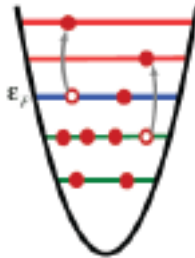
- Large Gamow basis for p-sd orbitals
- WS basis fitted to $^{24}\text{O}+n$ GSI experiment
- New experiments provide a very small width for ^{26}O g.s. Need precise calculation of S_{2n}

Gamow Shell Model in an ab-initio "no-core" framework

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

- Only NN forces at present
 - All particles active (No-Core). Solve the A-body Hamiltonian.
 - Argonne V18, (Wiringa, Stoks, Schiavilla PRC 51, 38, 1995)
 - N³LO (D.R.Entem and R. Machleidt PRC(R) 68, 041001, 2003)
 - V_{lowk} technique used to decouple high/low momentum nodes. $\Lambda_{Vlowk} = 1.9 \text{ fm}^{-1}$
(S. Bogner et al, Phys. Rep. 386, 1, 2003)
- Basis states
 - s- and p- states generated by the Gamow HF or WS potential

→ $l > 1$ H.O states



- Diagonalization of (1) → Applications to 4H,4Li,5H

When theorists agree!

- NN force: JISP16 (A. Shirokov et al PRC79, 014610) and NNLO_{opt} (A. Ekstrom et al PRL 110, 192502)
- Quality control: Verification/Validation, cross check of codes

Nucleus	MFDn	NCGSM	Difference
² H 1 ⁺ (N _{shell} = 4)	-1.6284	-1.6284	≤ 0.1 keV
² H 1 ⁺ (N _{shell} = 8)	-2.1419	-2.1419	≤ 0.1 keV
³ H 1/2 ⁺ (N _{shell} = 4)	-7.6016	-7.6016	≤ 0.1 keV
³ H 1/2 ⁺ (N _{shell} = 8)	-8.3203	-8.3203	≤ 0.1 keV
³ He 1/2 ⁺ (N _{shell} = 8)	-7.6084	-7.6084	≤ 0.1 keV
⁴ He 0 ⁺ (N _{shell} = 4)	-27.3685	-27.3684	0.1 keV
⁶ Li 1 ⁺ (N _{shell} = 4)	-24.9778	-24.9776	0.2 keV
⁶ Li 3 ⁺ (N _{shell} = 4)	-22.4959	-22.4957	0.2 keV

MFDn: Maris, Vary,...

NC-GSM:

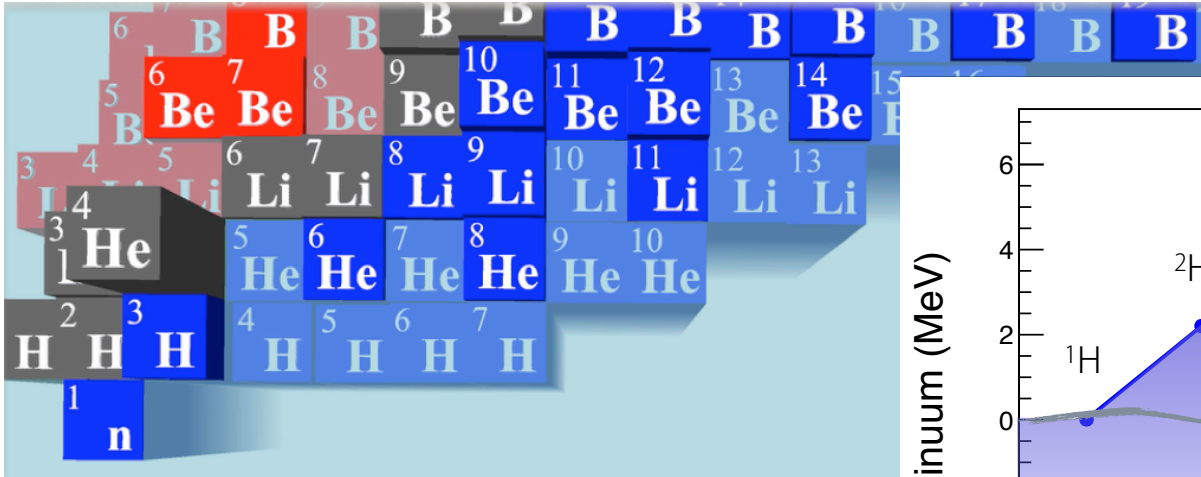
Papadimitriou...

Calculations are done a pure HO basis

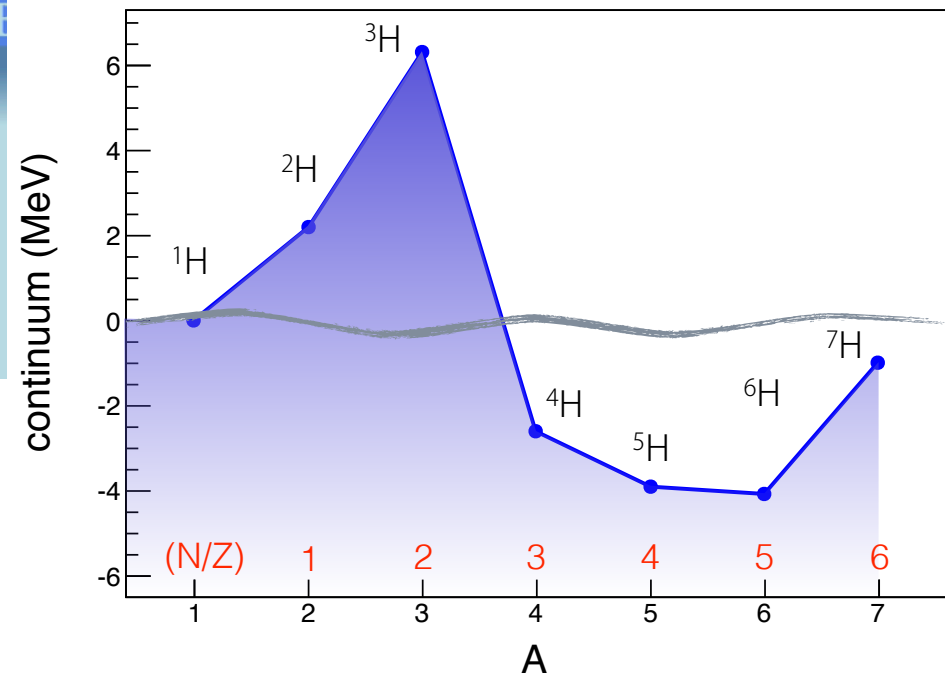
Nucleus	NCGSM	MFDn	Difference
³ H 1/2 ⁺ N ² LO _{opt} (N _{shell} = 4)	-5.9802	-5.9806	0.4 keV
³ H 1/2 ⁺ N ² LO _{opt} (N _{shell} = 8)	-8.1129	-8.1132	0.3 keV
³ H 1/2 ⁺ N ² LO _{opt} (N _{shell} = 10)	-8.2171	-8.2174	0.3 keV

Applications to ${}^4,5\text{H}$ and ${}^4\text{Li}$

- Towards the path to calculate super-heavy hydrogens
- Recent exciting experimental findings need theoretical support and guidance

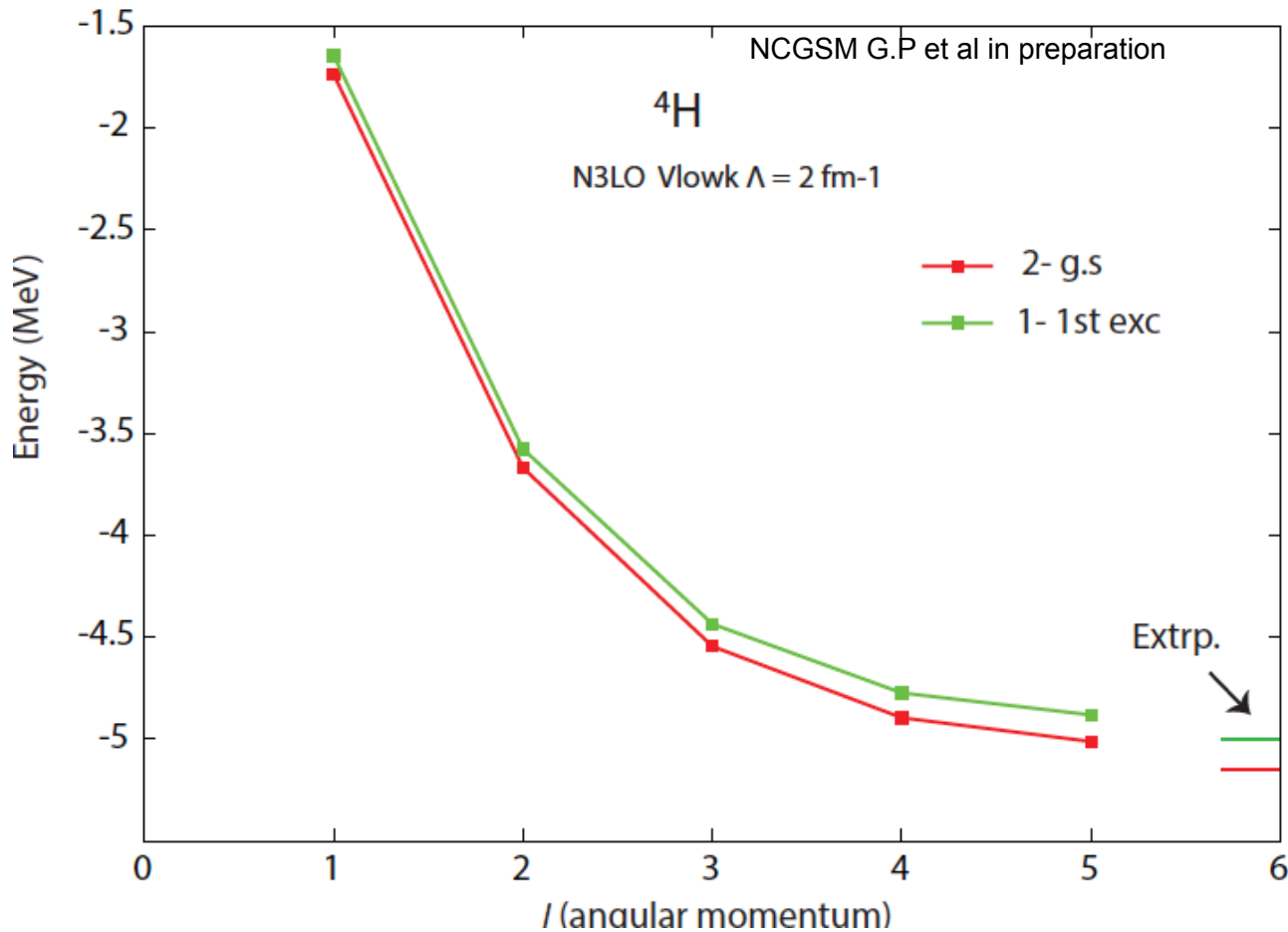


Schematic picture!
(Courtesy of M. Caamano)



- Extreme N/Z ratio
- Test ground for many-body methods and interactions
- Similar behavior to ${}^6,8\text{He}$ isotopic chain? It is believed that ${}^5\text{H} \sim {}^6\text{He}$, ${}^6\text{H} \sim {}^7\text{He}$, ${}^7\text{H} \sim {}^8\text{He}$...

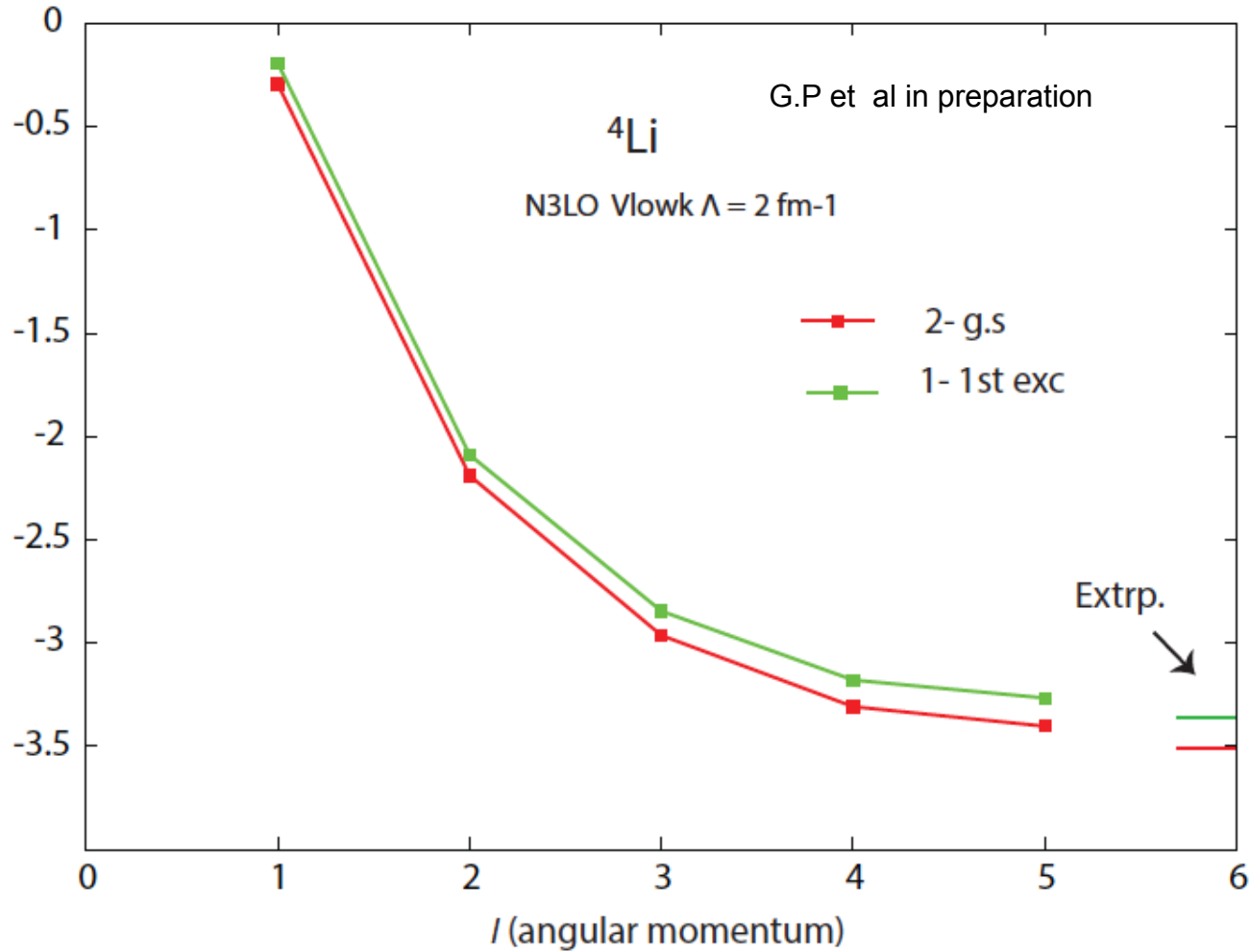
${}^4\text{H}, {}^4\text{Li}$:



Basis:
Gamow p3/2 neutron
states
(0p3/2 s.p. res) +
20 scattering continua.
Rest up to h-waves are H.O
States of $\hbar\omega = 20 \text{ MeV}$

- Extrapolated result has an uncertainty of about $\pm 20 \text{ keV}$
- Sensitivity tests to be completed

Results

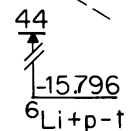
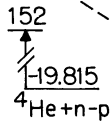
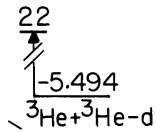
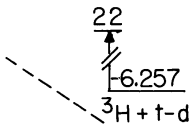
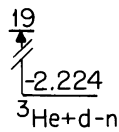
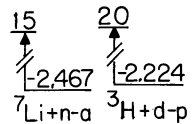
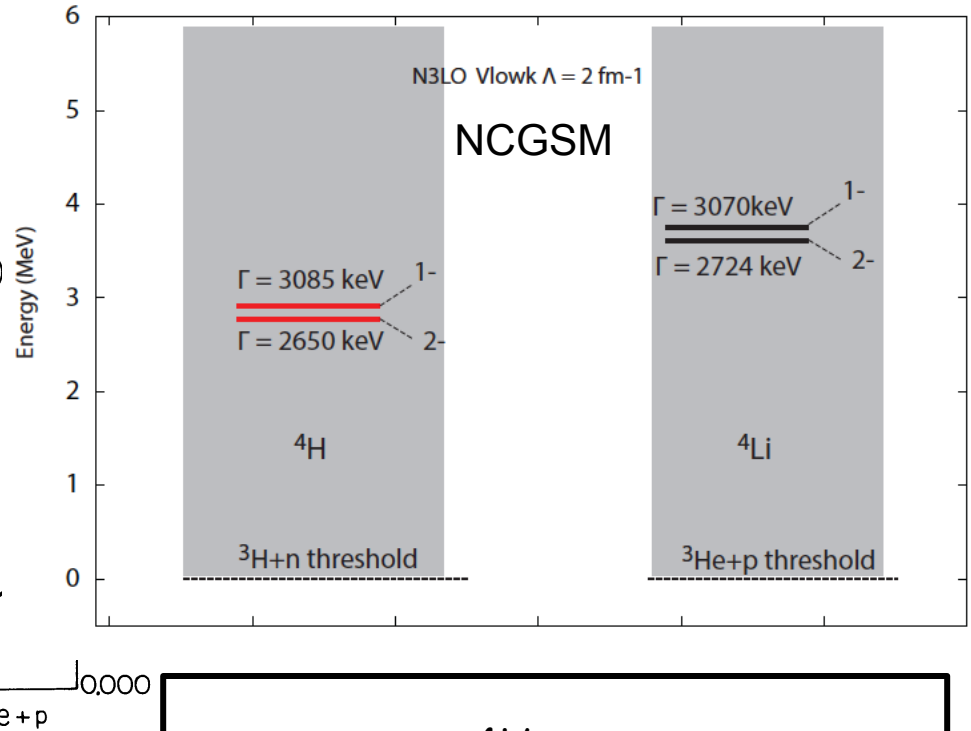
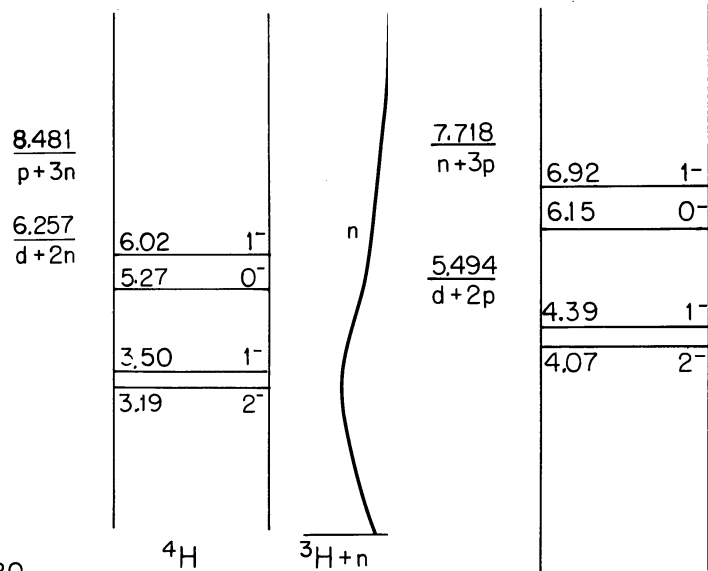


Basis:
Gamow p3/2 proton
states
(0p3/2 s.p. res) +
20 scattering continua.
Rest up to h-waves are H.O
States of hw= 20 MeV

➤ Similar trend with ${}^4\text{H}$

Results as compared to experiment

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

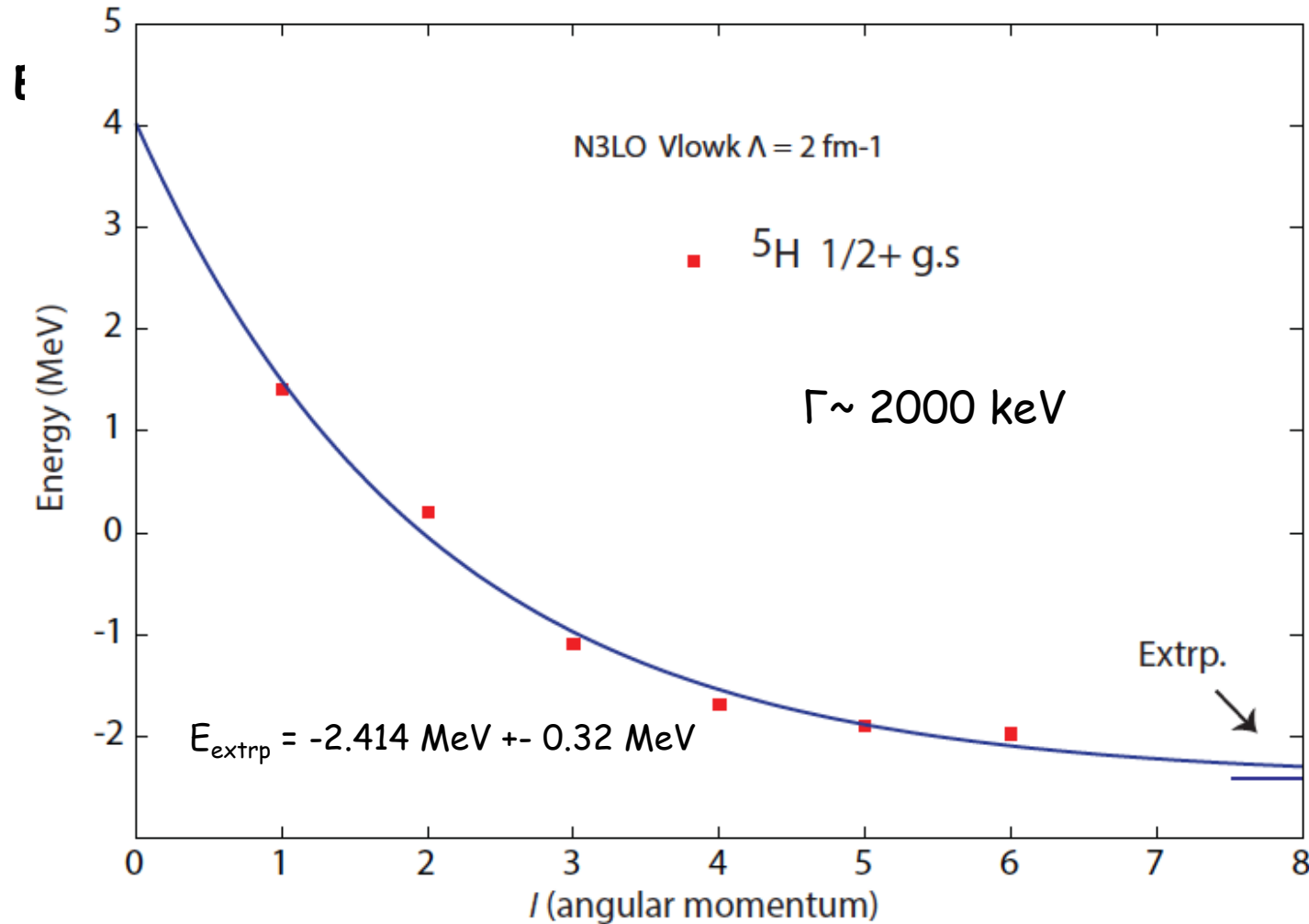


4H:
 2- g.s: 2.775 MeV $\Gamma = 2650$ keV
 1- 1st: 2.915 MeV $\Gamma = 3085$ keV

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

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

Results for ${}^5\text{H}$



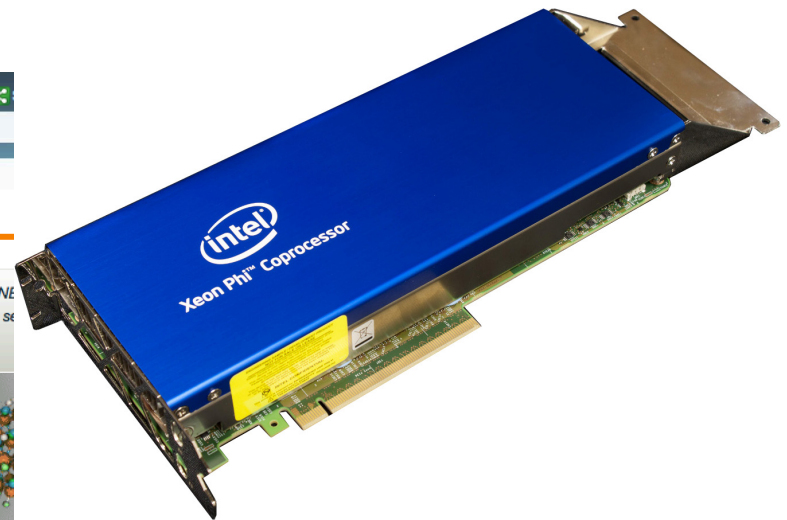
Smaller width than ${}^4\text{H}$, maybe an indication of a longer lifetime,
(Descouvemont made such an observation as well)
but... still sensitivity aspects to be investigated

What has just been described (and also other activities) was approved as a **NESAP** project for calculations of **weakly-bound** and **unbound resonant** states

(Iowa State University and Berkeley National Lab. Computer Scientists and **Intel staff**)

Cori Knights Landing

Next-generation Intel® Xeon Phi™ Knights Landing (KNL) product with improved single thread performance targeted for highly parallel computing



The screenshot shows the NERSC website interface. At the top, there is a navigation bar with the NERSC logo, a search bar, and links for Site Map and My NERSC. Below the navigation bar, there is a main content area with a sidebar on the left. The sidebar contains a 'FOR USERS' section with links to Live Status, My NERSC, Move to CRT, Getting Started, Computational Systems, NERSC-8: Cori, NERSC-8 Procurement, NESAP Projects, Application case studies, NESAP Description, Edison, Hopper, Carver, PDSF, Genepool, Testbeds, Retired Systems, Data & File Systems, Network Connections, Queues and Scheduling, Job Logs & Analytics, Training & Tutorials, Software, Accounts & Allocations, and Policies. The main content area features a header for 'NESAP PROJECTS' and 'NERSC Exascale Science Application Program Projects'. Below this, there is a paragraph stating that NERSC has accepted a selection of key DOE science projects into its NERSC Exascale Scientific Applications Program. A sidebar on the right contains a section titled 'Projects selected for NESAP' with a list of projects and three small images: a molecular structure, a grid pattern, and a landscape.

Complex Scaling for structure and reactions (some comments repeat):

- Doable to use realistic, non-local chiral or phenomenological potentials.
- **Phase shifts** converge rapidly with increasing θ and they become independent of θ for values > 0.2 rad.
- **Phase shifts** are obtained by a **diagonalization** of a complex scaled Hamiltonian. No boundary condition is imposed to describe scattering. Bound state technique to obtain phase shifts and hence cross-sections.
- Method gives at the same time: widths, partial widths, position of resonances, (structure) and also reaction observables with a single diagonalization...
- Expected to work with any bound state technique, since it is built to use L^2 integrable functions (e.g. HO).
- The lack of boundary conditions may make the method suitable also for d,p reactions where the Coulomb treatment will not require any screening

Conclusions/Future plans

- Complex scaling applied to non-local general realistic potentials
- Tests on p-n system successful. Phase-shifts calculated within an L^2 basis.

Explore CS more

- No boundary condition, HO basis (or other). Take advantage of model-independent extrapolations of the HO basis (UV/IR) for resonant states.

Additionally calculations were shown:

- Gamow basis, which is appropriate for calculations of weakly bound/unbound nuclei.
 - Calculations also naturally provide widths of resonances.
 - Realistic effective interactions for GSM → systematic improvement of method : (NN+3N + continuum) in a CI framework
 - Results with USDB + Gamow shell model (OK, but...)
 - For a more consistent study, manage to develop the microscopic effective interaction in a model space that also includes continuum states
- Gamow basis applied successfully in an ab-initio GSM framework
 - Realistic forces employed
 - Calculations of exotic superheavy hydrogens are in the pipeline

Back up

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

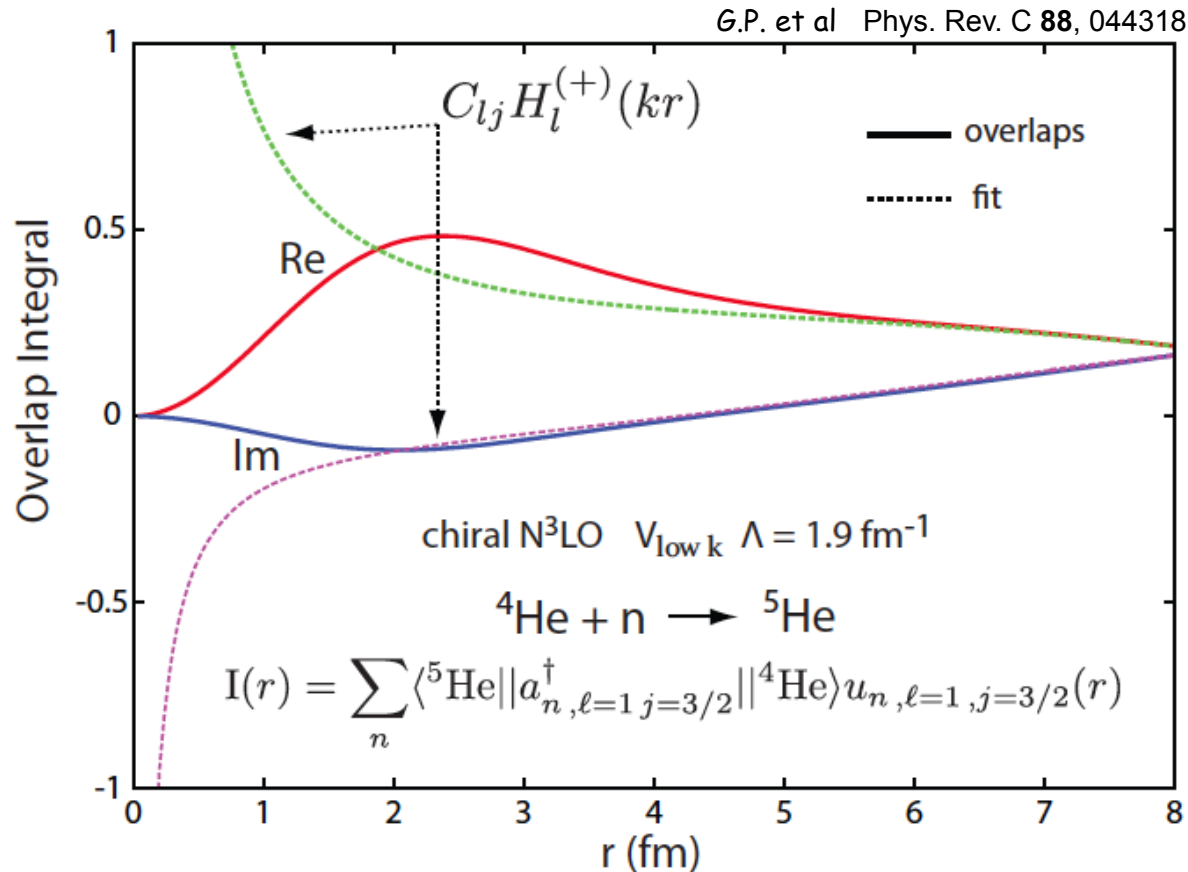
2) Sensitivity on S_{1n} ...

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

Results: Ab-initio overlaps in the NC-GSM

- Basic ingredients of the theory of direct reactions

Calculations at a Vlow k $\Lambda = 1.9 \text{ fm}^{-1}$



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

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

$$C = 0.197$$

and from (1)

$$\Gamma({}^5\text{He}) = 311 \text{ keV}$$

$$\Gamma({}^5\text{He}) = 400 \text{ keV (diagonalization of } H)$$

Two ways of calculating the width

a) many body diagonalization

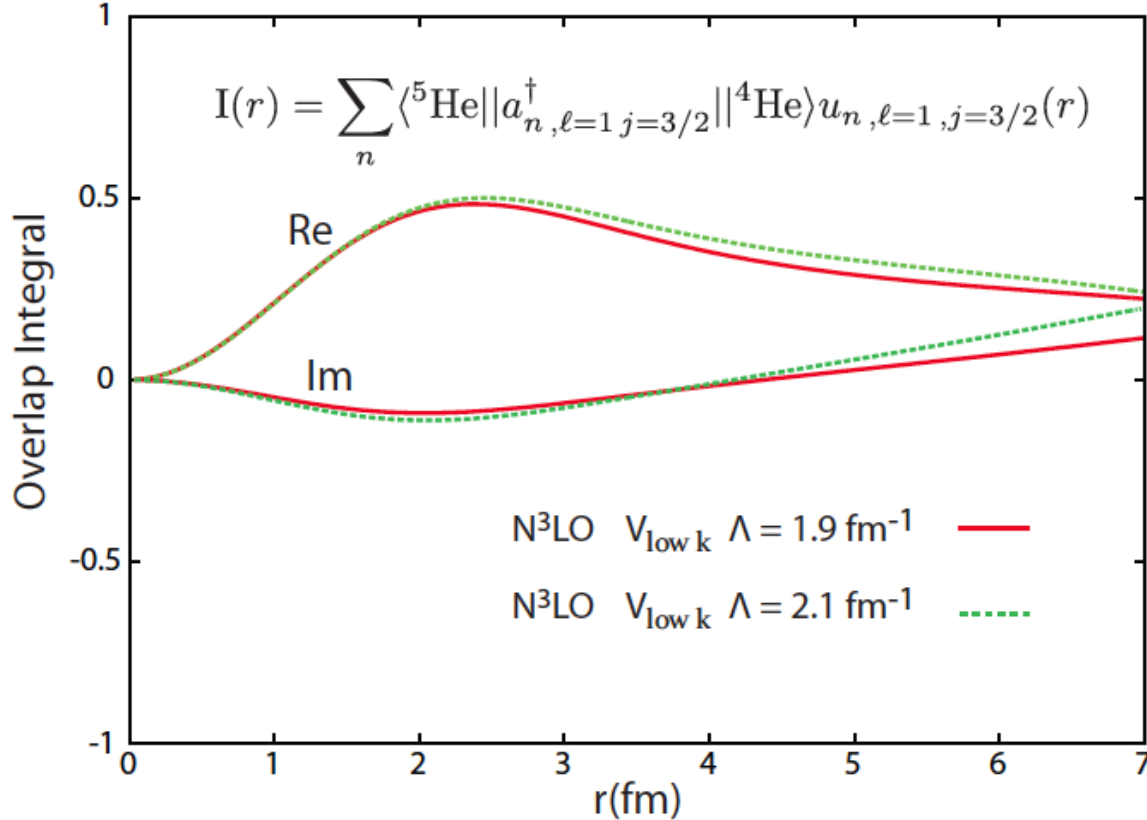
b) from overlap function

—————> Equivalent

Results: Ab-initio overlaps in the NC-GSM

Calculations at a Vlow k $\Lambda = 1.9 \text{ fm}^{-1}$ and 2.1 fm^{-1}

G.P. et al Phys. Rev. C **88**, 044318



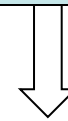
Overlap tail sensitive to S_{1n}

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

$$S_{1n} (\Lambda = 2.1 \text{ fm}^{-1}) = -2 \text{ MeV}$$

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

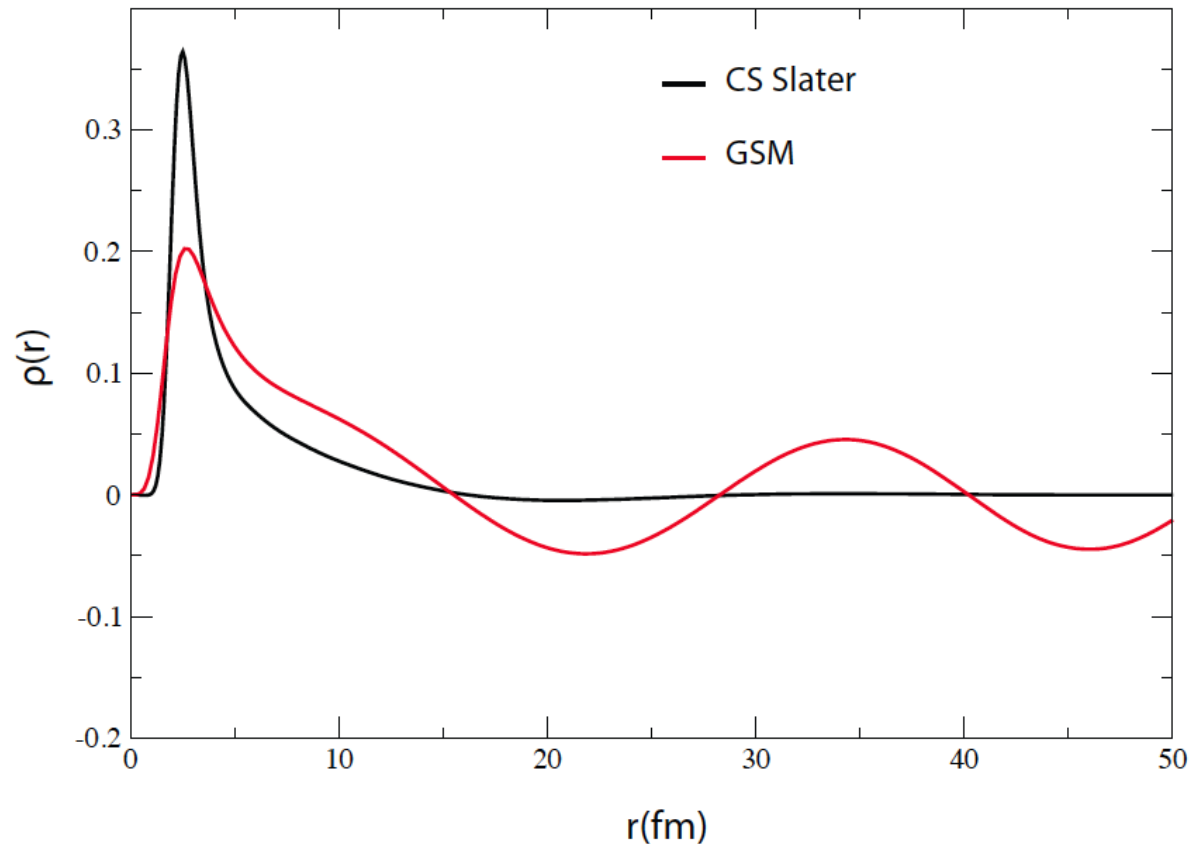
$$\Gamma_{\text{ANC}} = 570 \text{ keV}$$



The width exhibits the correct behavior

Some results

2^+ first excited state in ${}^6\text{He}$



The 2^+ state is a many-body resonance (outgoing wave)

☺ GSM exhibits naturally this behavior

☹ but CS is decaying for large distances, even for a resonance state

This is OK. The solution $\Psi(\theta)$ is known to "die" off (L^2 function)

Solution

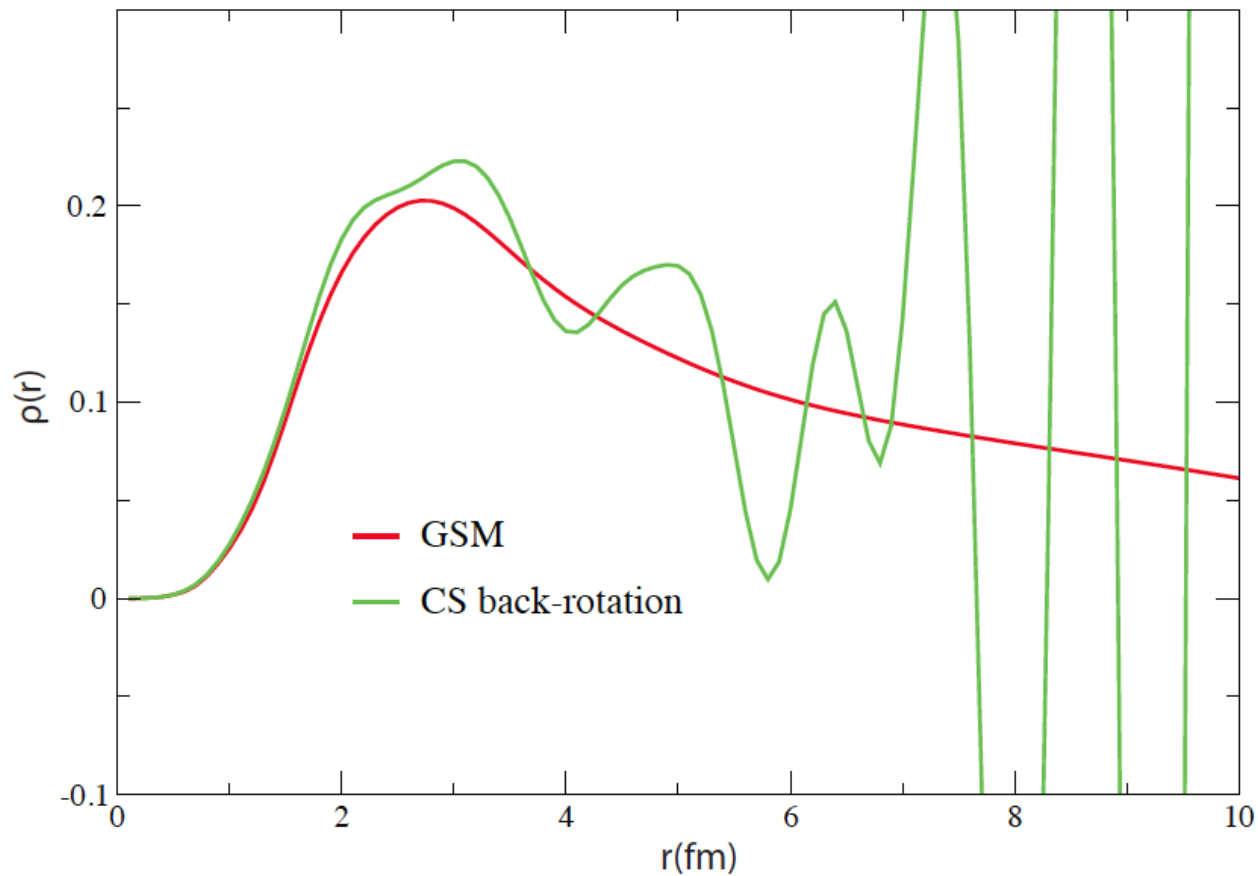
→ Perform a direct back-rotation. What is that?

$$\Psi_{\theta}(r_1, r_2) = e^{i3\theta} \Psi(e^{i\theta} r_1, e^{i\theta} r_2)$$

$$\Psi(r_1, r_2) = e^{-i3\theta} \Psi(e^{-i\theta} r_1, e^{-i\theta} r_2) \quad \text{Back-rotation}$$

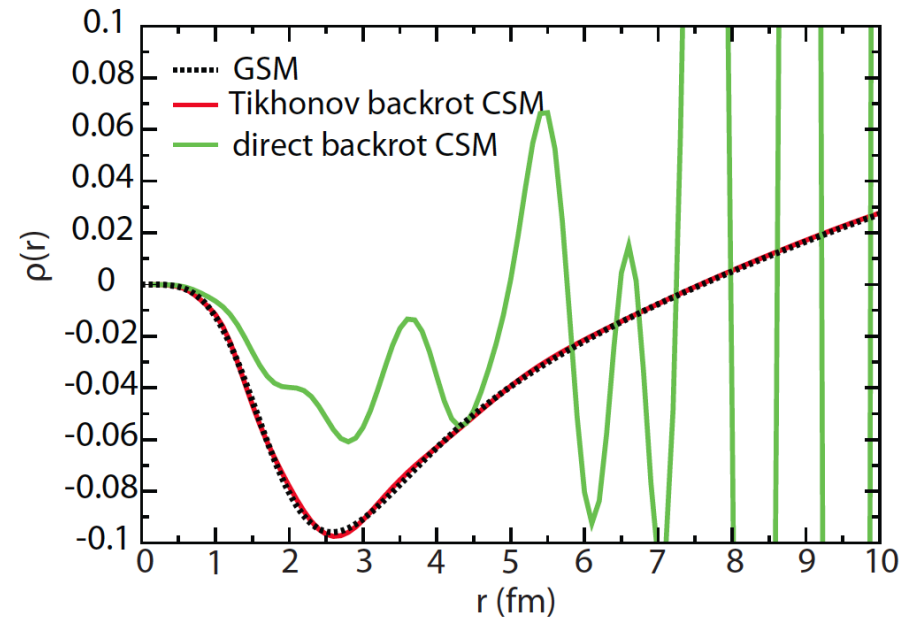
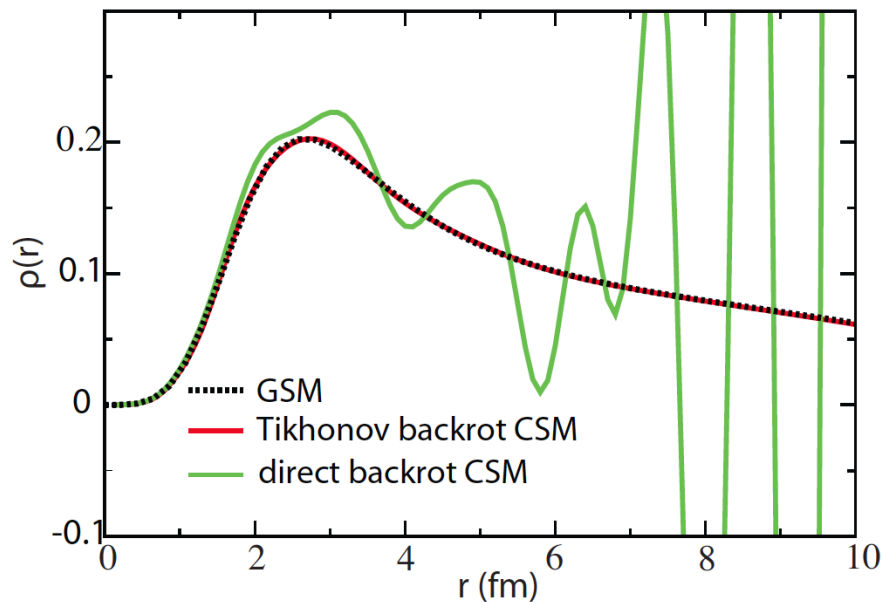
In the α

$\rho(r)$:



The CS density has the correct asymptotic behavior (outgoing wave)

- Back rotation is very unstable numerically.
Long standing problem in the CS community (in Quantum Chemistry as well)
- The problem lies in the analytical continuation of a square integrable function in the complex plane.
- We are using the theory of Fourier transformations and a regularization process (Tikhonov) to minimize the ultraviolet numerical noise of the inversion process.



$2+$ densities in ${}^6\text{He}$ (real and imaginary part)

Solution

Back rotation is very unstable numerically.

Unsolved problem in the CS community (in QC as well)

The problem lies in the analytical continuation of a square integrable function in the complex plane.

We are using the theory of Fourier transformations and Tikhonov regularization process to obtain the original (GSM) density

To apply theory of F.T to the density, it should be defined in $(-\infty, +\infty)$

$$f_{\theta}(x) = \rho_{\theta}(e^{-x}) \quad \rightarrow \text{Now defined from } (-\infty, +\infty)$$

$$f_{\theta}(\xi) = \frac{1}{2\pi} \int_{-\infty}^{\infty} e^{-ix\xi} f_{\theta}(x) dx \quad \rightarrow \text{F.T}$$

$$f(x + iy) = \frac{1}{2\pi} \int_{-\infty}^{\infty} e^{ix\xi} e^{-y\xi} f_{\theta}(\xi) d\xi \quad \rightarrow \text{Value of (1) for } x+iy \text{ (analytical continuation)}$$

$$f(x + iy) = \frac{1}{2\pi} \int_{-\infty}^{\infty} e^{ix\xi} e^{-y\xi} \frac{f_{\theta}(\xi)}{1 + \alpha e^{-2y\xi}} d\xi \quad \rightarrow \text{Tikhonov regularization}$$

$$x = -\ln r \quad , \quad y = \theta$$

The matrix elements of the interaction are calculated in practice by truncating the HO up to Nmax basis states ($N = 2n + 1$)

TBMEs in a Gamow basis

$$\langle ab|V_{\text{osc}}|cd\rangle \approx \sum_{\alpha \leq \beta}^N \sum_{\gamma \leq \delta}^N \langle ab|\alpha\beta\rangle \langle \alpha\beta|V_{\text{low-k}}|\gamma\delta\rangle \langle \gamma\delta|cd\rangle$$

Matrix elements between Gamow States

TBMEs in a HO basis → CD-Bonn, Av18, N3LO, Vlowk, SRG etc

In the end of the day we need to calculate overlaps between HO and Gamow states!

$$\langle ab|\alpha\beta\rangle = \frac{\langle a|\alpha\rangle\langle b|\beta\rangle - (-1)^{J-j_\alpha-j_\beta}\langle a|\beta\rangle\langle b|\alpha\rangle}{\sqrt{(1+\delta_{ab})(1+\delta_{\alpha\beta})}} \quad \text{Identical particles}$$

$$\langle ab|\alpha\beta\rangle = \langle a|\alpha\rangle\langle b|\beta\rangle \quad \text{protons-neutrons}$$

with

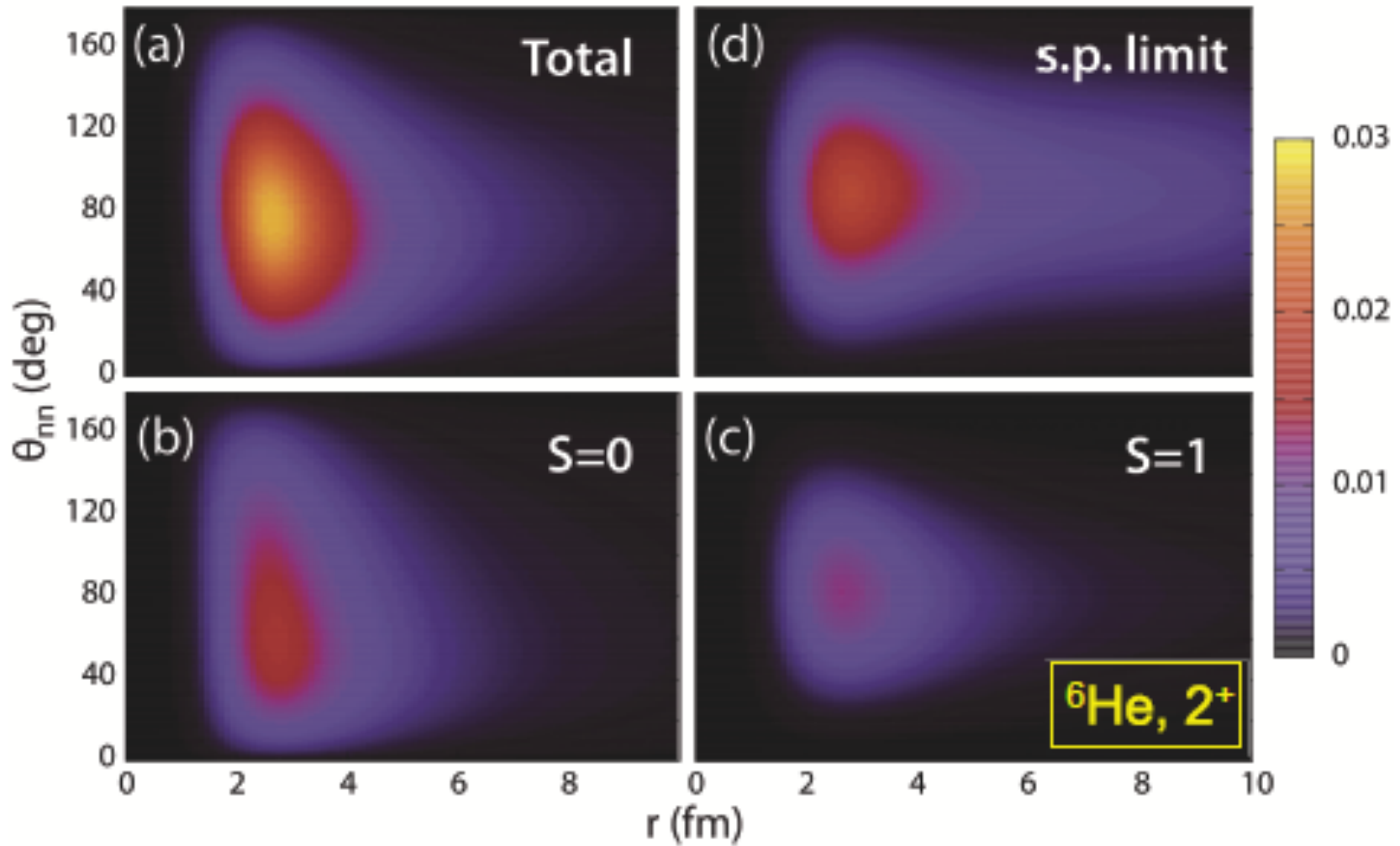
$$\langle a|\alpha\rangle = \int d\tau \tau^2 \varphi_a(\tau) R_\alpha(\tau) \delta_{l_a l_\alpha} \delta_{j_a j_\alpha} \delta_{t_a t_\alpha}$$

Neutron correlations in ${}^6\text{He}$ 2+ excited state

GSM: [0.851, 0.109] MeV

EXP: [0.822(25), 0.113(20)] MeV

G.P et al PRC(R) 84, 051304, 2011



→ 2+ neutrons almost uncorrelated...