Complex energy methods for structure and reactions

George Papadimitriou
papadimitrio1@llnl.gov

Lawrence Livermore National Laboratory

Nuclear & Chemical Sciences

YIPQS Long-term and Nishinomiya-Yukawa Memorial International workshop
Computational Advances in Nuclear and Hadron Physics (CANHP 2015)
21th September - 30th October, 2015
Yukawa Institute for Theoretical Physics, Kyoto, Japan

Outline

- Life on the edge stability, Experiment, Theory

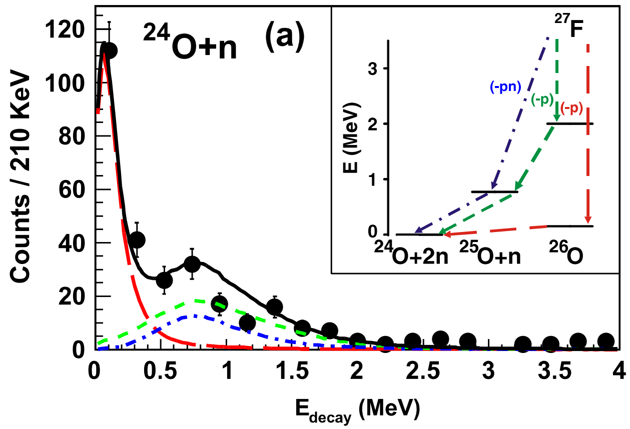
- Bound state techniques for scattering and Applications
  → Realistic interactions
  → Backrotation and applications on observables
  → R-matrix formulas for resonance parameters

- Selected applications of the complex energy Gamow Shell Model on weakly bound nuclei.

- Conclusions/Future plans

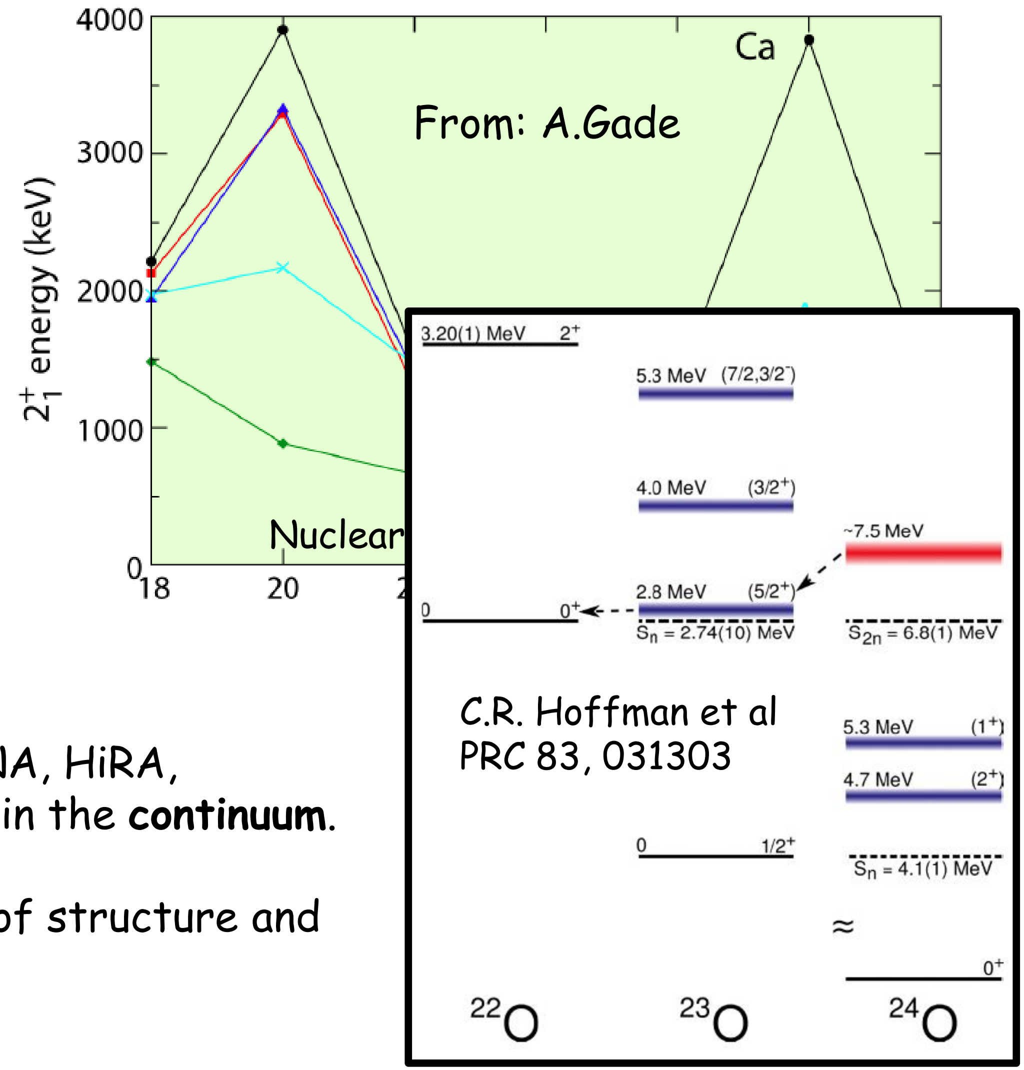
Life on the edge of nuclear stability: Experiment

- New decay modes: 2n radioactivity



^{26}O unbound by < 200 keV
Extremely narrow width

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



The list is getting bigger: Efforts in MoNA, HiRA, TexAT, STARLiTeR etc, all probe nuclei in the **continuum**.

Continuum: Positive energies, unification of structure and reaction aspects

Nuclear Landscape

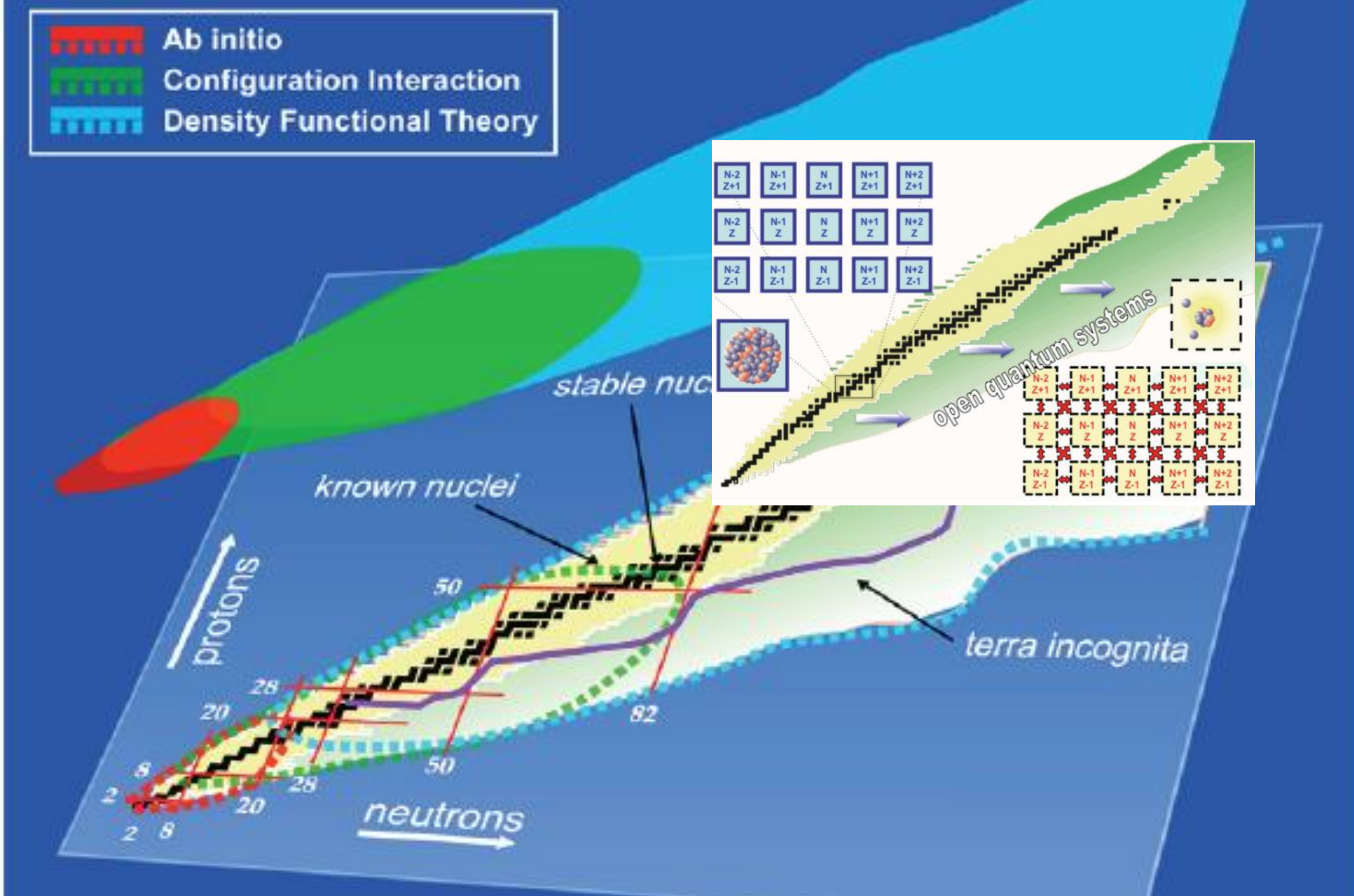


Fig: Bertsch,Dean,Nazarewicz, SciDAC review **2007**

Real and Complex energy methods for structure/reactions

Shell Model Embedded in Continuum (SMEC)
- K. Bennaceur *et al.*, Phys. Lett. **488B**, 75 (2000)
- J. Okolowicz.,*et al*, PR 374, 271 (2003)

NCSM/RGM-NCSMC
- S. Quaglioni, P. Navratil PRC 79, 044606 (2009)
- G. Hupin, S. Quaglioni, P. Navratil PRC 90, 061601 (2014)

Complex Energy Gamow Shell Model
- N. Michel *et al.*, Phys. Rev. C67, 054311 (2003)
- N. Michel *et al*, J.Phys. G: Nucl.Part.Phys 36, 013101 (2009)
- G.P. J. Rotureau, N. Michel, M. Ploszajczak, B. Barrett PRC 88, 044318 (2013)

Complex Energy GSM/Coupled Channels
- K. Fossez, N. Michel, M. Ploszajczak, Y. Jaganathen, R. Betan PRC 91, 034609 (2015)

Continuum Coupled Cluster (Coupled Cluster in Berggren basis)
- G. Hagen et al PRL 108, 242501 -109, 032502 (2012)

Complex Scaling Method
- T. Myo, Y. Kikuchi, H. Masui, K. Kato Prog. Part and Nucl Phys 79 (2014) 1-56
- R. Lazauskas Phys. Rev. C 91, 041001(R) (2015)
- A. Kruppa, G. Papadimitriou, W. Nazarewicz, N. Michel PRC 89 014330 (2014)

Other approaches: Calculable R-Matrix Baye, Descouvemont
Complex Energy in momentum space Deltuva, Fonseca

Bound states

- ✓ Localized wavefunctions
- ✓ Problem is being solved very precisely or with controllable precision

→ e.g. variational methods

Scattering

- Wavefunctions extend to infinity
- Complicated boundary conditions
- Singularities in momentum space

→ Having acquired so much experience in the bound-state problem solution, can we imagine solving the scattering problem as a bound state problem?

Examples: Bound state techniques for scattering

- Lorentz Inverse Transform

  Barnea, Efros, Orlandini, Leidemann, Quaglioni, Bacca

- Momentum Lattice

  Rubtsova, Kukulin

- L^2 Stabilization Techniques

  Arai, Kruppa, Hazi, Pei, Nazarewicz. Basically similar to Lattice QCD way of extracting scattering info

- 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

- Nuttal 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).

Recently: G. Papadimitriou and J.P. Vary PRC(R) 91,021001 (2015) and PLB 746, 121 (2015)

Chemistry

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

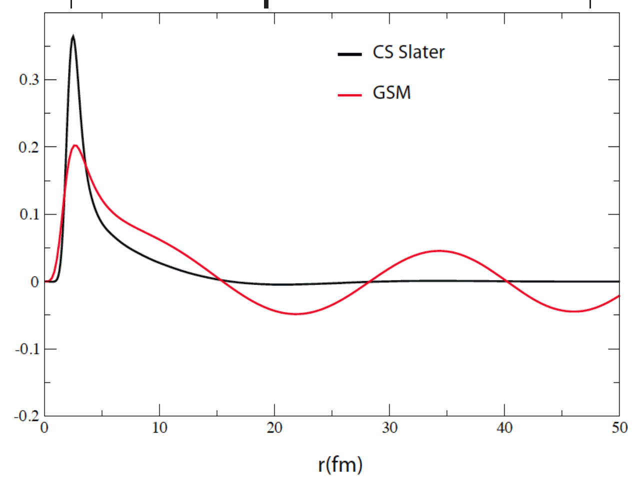
The complex scaling

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. $r \rightarrow re^{i\theta}$, $p \rightarrow pe^{-i\theta}$
   Hamiltonian is transformed to $H(\theta) = U(\theta)H_{original}U(\theta)^{-1}$
   $H(\theta)\Psi(\theta) = E\Psi(\theta)$ complex eigenvalue problem

- The spectrum of $H(\theta)$ contains bound, resonances and continuum states.
- It can be shown that a resonance wavefunction behaves asymptotically as a bound state:
  e.g:



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….)

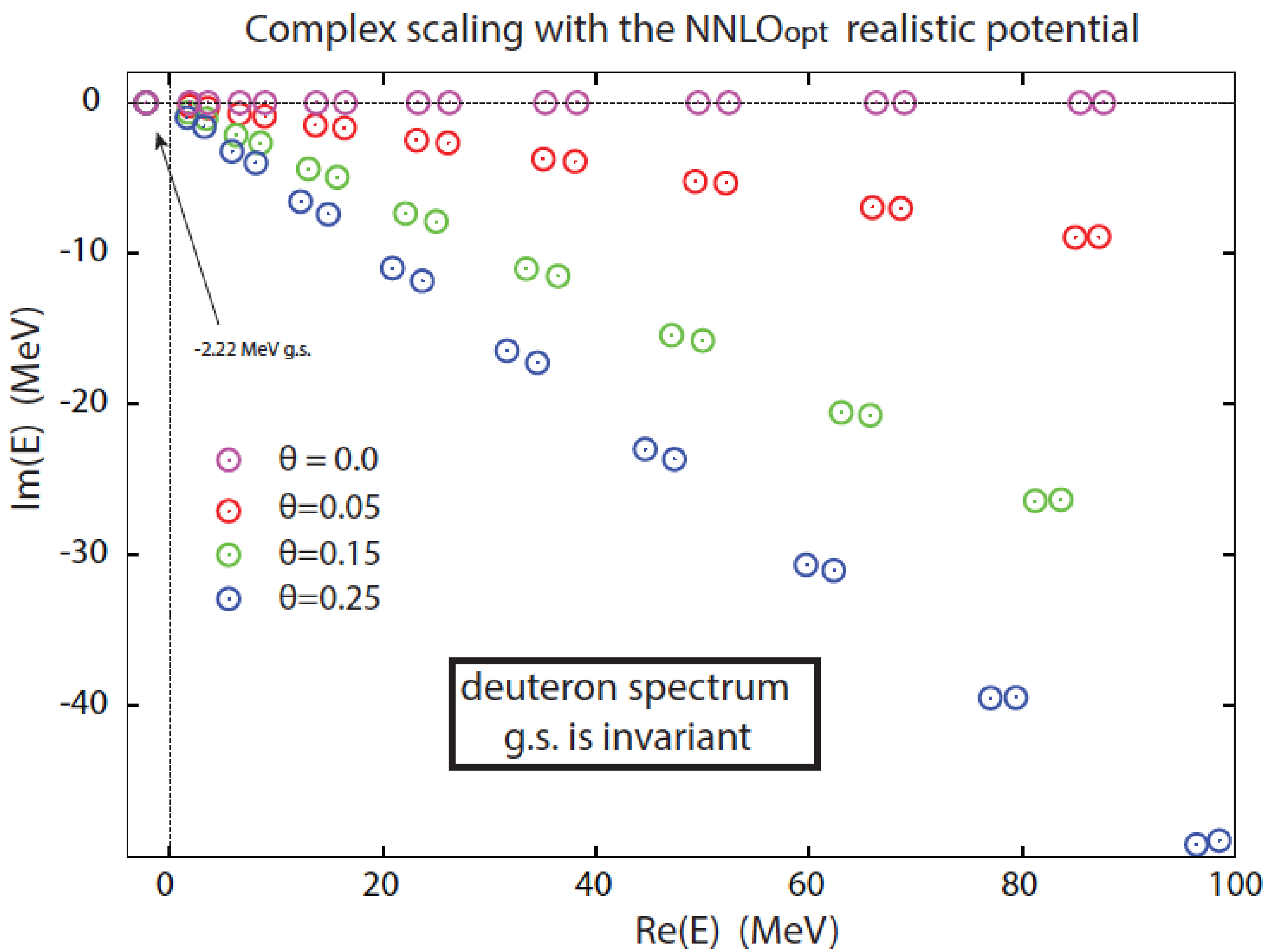
Apply CS in a chiral NN force:

- 2-body problem in relative coordinates.
- H = Trel + Vrel 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

$$H_\theta = e^{-2i\theta}\mathrm{Trel} + \mathrm{Vrel}(\theta)$$

→ Diagonalize H_θ with your favorite diagonalization routine

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



→ 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
G. P and J. P. Vary Phys. Lett. B 746, 121 (2015)

→ Connection with continuum level density (CLD)

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

H(θ) 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:

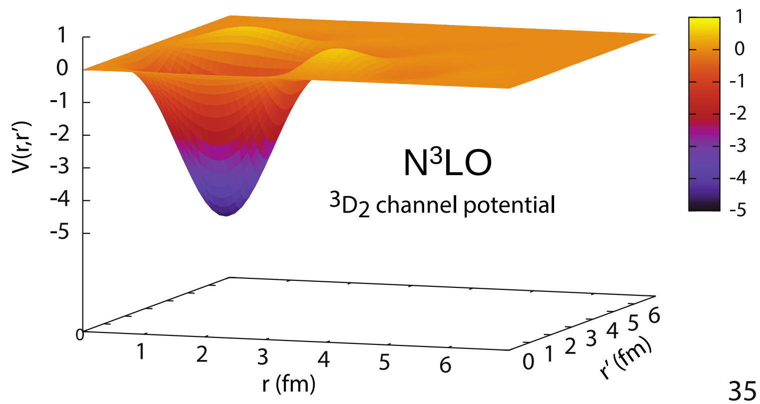
1) From eigenstates of Hamiltonian
2) From CLD (e.g. fit to Breit-Wigner)
3) From phase-shift via the inflection criterion

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

Input non-local realistic potential

$$V(r,r') = \sum_{n,n'} A_{nn'}\phi_n(r)\phi_{n'}(r')$$

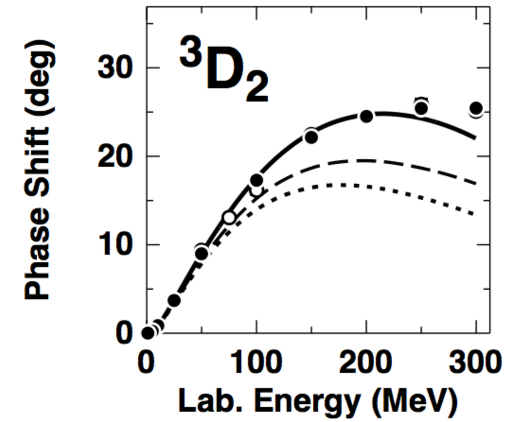
Ann' are HO basis matrix elements
φn(r) are radial HO basis



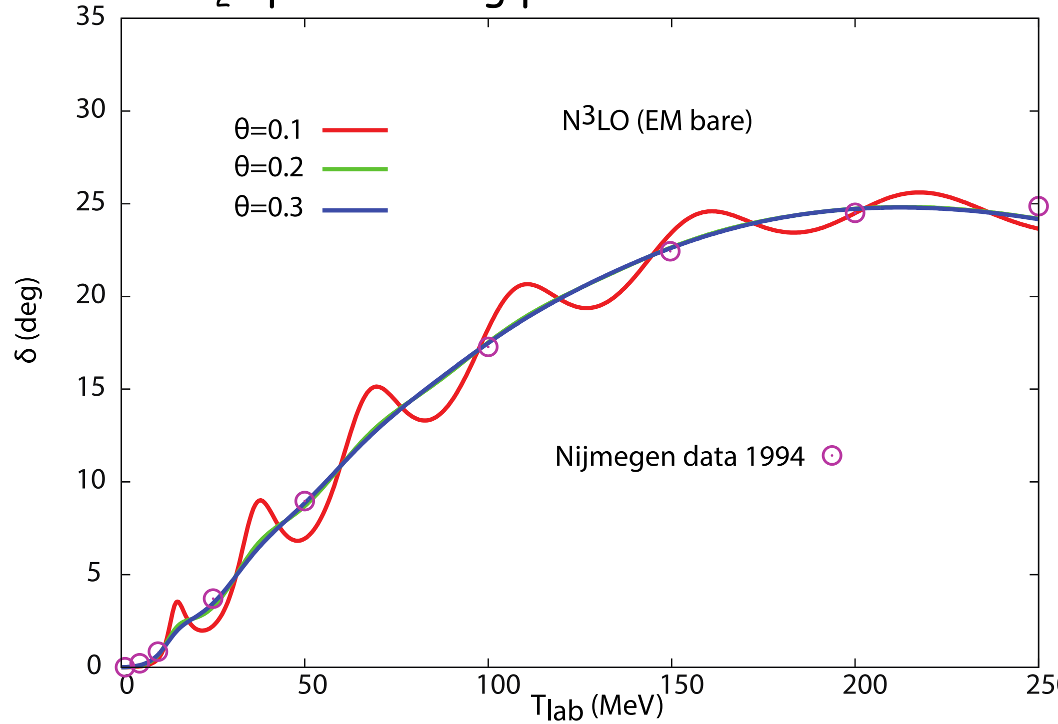
$$H_\theta \Psi_\theta = E_\theta \Psi_\theta$$

N=20 HO states
hw=30 MeV

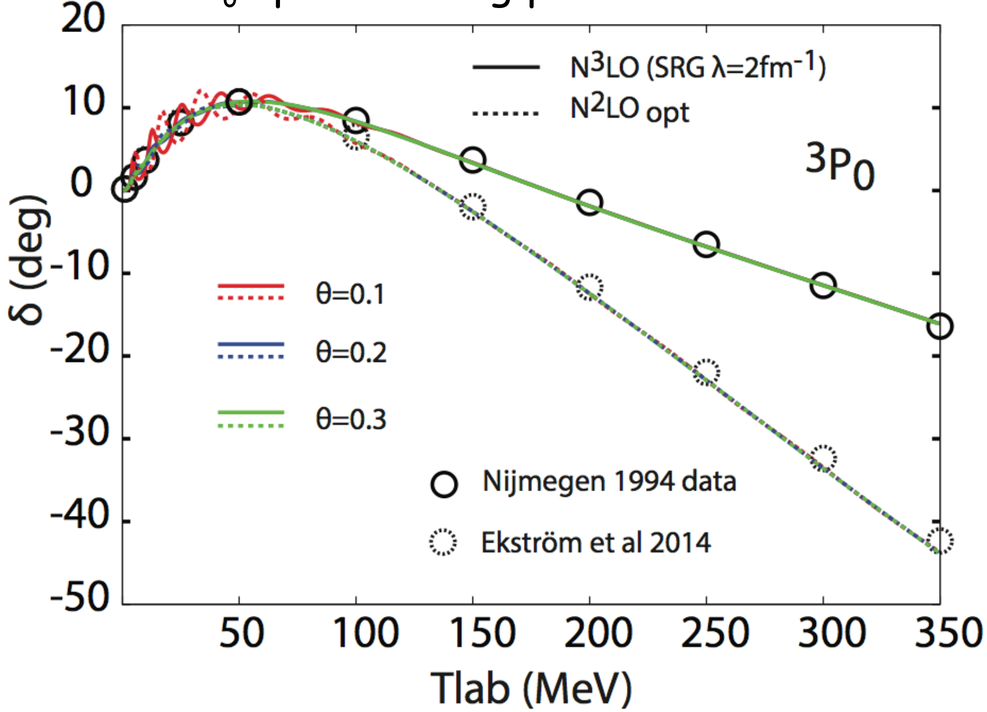
Entem-Machleidt (EM) fit



$^3D_2$ np scattering phase-shift

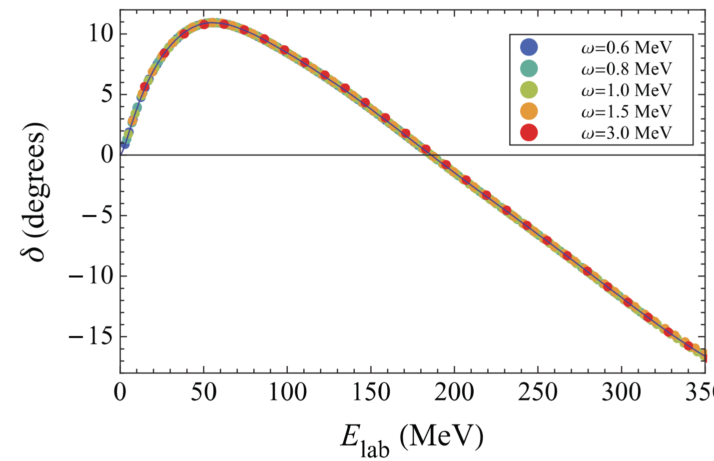


^3P_o np scattering phase-shift



Compare result with results obtained using the Busch formula for particles in a trap at hw → 0

T. Luu et al PRC 2010

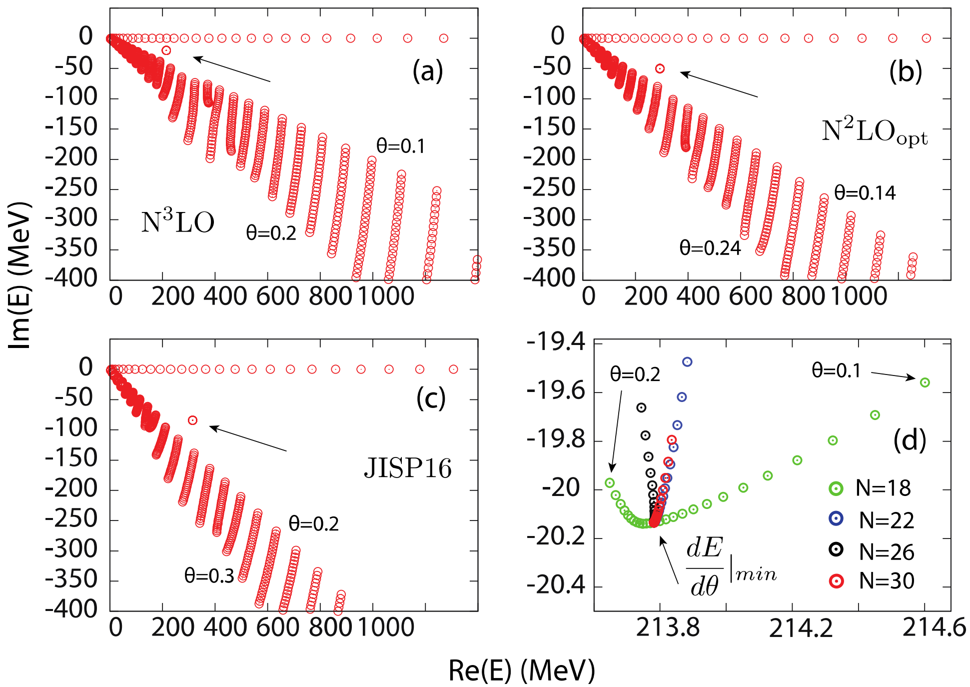


→ To extract phase shifts from nucleons in a HO trap one need **N=1800** HO basis states to have convergence as hw → 0

Resonant θ-trajectory with realistic interactions

G. P and J. P. Vary Phys. Lett. B 746, 121 (2015)

High energy, very model dependent poles in np scattering



N	N^3LO	N^2LO_{opt}	JISP16
14	(214.767 -i20.048)	(292.114 -i49.609)	(314.471 -i84.250)
18	(213.758 -i20.139)	(292.358 -i50.039)	(314.475 -i84.244)
22	(213.784 -i20.131)	(292.323 -i50.023)	(314.473 -i84.244)
26	(213.781 -i20.134)	(292.327 -i50.020)	(314.473 -i84.244)
30	(213.781 -i20.134)	(292.327 -i50.020)	(314.473 -i84.244)

Determination of resonant parameters through the θ-trajectory criterion

Back rotation in the CSM

→ Even though within CSM one is able to obtain resonant states, the radial dependence of the resonant state is not proper.

→ The wavefunction being constructed as a linear superposition of L^2 integrable basis decays asymptotically

$$u_\theta(r) = \sum_{n=1}^{N} C_n^\theta \phi_n(r)$$

→ Observables are calculated as: $\langle O \rangle = \langle \widetilde{u_\theta} | O_\theta | u_\theta \rangle$

where $O_\theta = U_\theta O U_\theta^{-1}$ For example: $\langle r^2 \rangle = \langle \widetilde{u_\theta} | e^{2i\theta} r^2 | u_\theta \rangle$

→ It is known that once the wavefunction is backrotated then
i) the Gamow character can be retrieved
ii) observables can be calculated in the usual way: $\langle O \rangle = \langle \widetilde{u(r)} | O | u(r) \rangle$

where $$u(r) = e^{-\frac{3}{2}i\theta} \sum_{n=1}^{N} C_n^\theta \phi_n(re^{-i\theta})$$

→ We will apply the backrotation for calculations of observables starting with a schematic model

Schematic model for backrotation

Model: Two particles interacting via a local potential in 3D:

$$V(r) = -8.0e^{-0.16r^2} + 4.0e^{-0.04r^2} \qquad H = T + V(r)$$

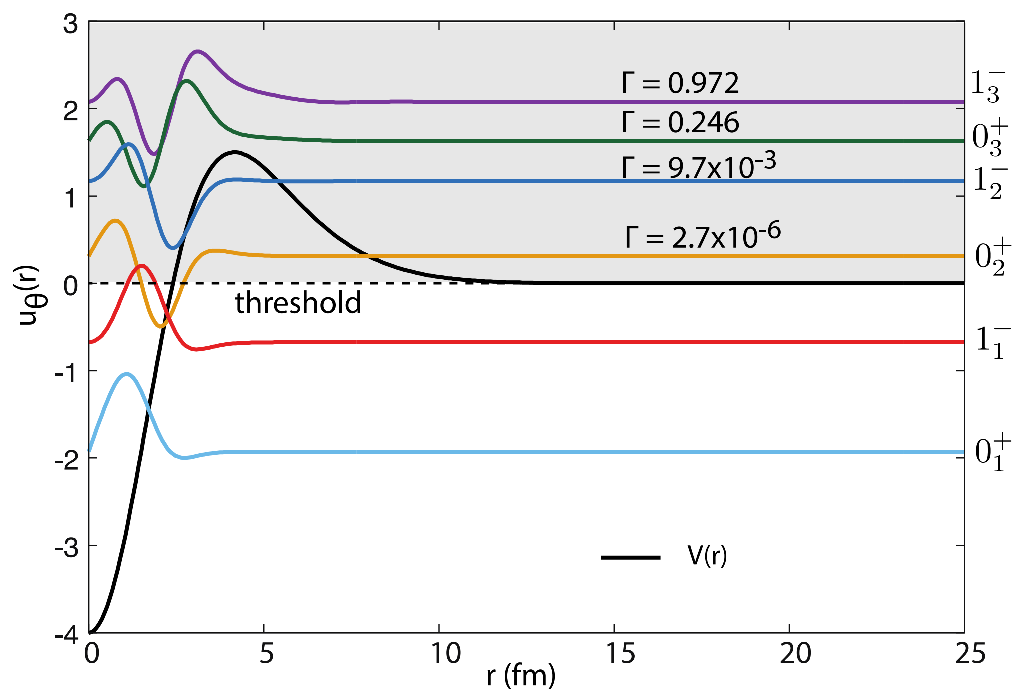
Introduced by Csótó et al PRA 71, 1990
Also used by T. Myo et al in PTP 99, 1998 and recently by D. Baye Phys.Rep 1 2015

→ It supports bound states and resonances above threshold and provides a playground for testing purposes (and learning)

CSM diagonalization in a HO basis

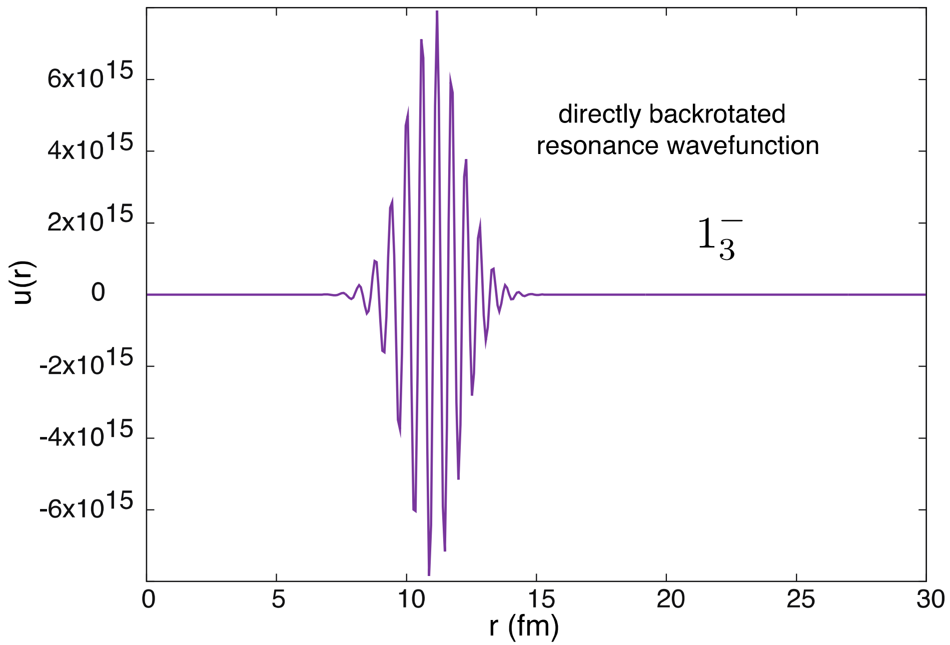
$H(\theta) = e^{-2i\theta}T + V(re^{i\theta})$

N = 30
θ = 0.35
h = c = b = 1



Schematic model for backrotation

→ Back rotate the 1_3 broad resonant state to obtain the Gamow character of the state



Not good

Schematic model for backrotation

The problem of backrotation is a known problem in CSM

The solution lies in the Tikhonov regularization method

The recipe that is followed is:

$$f_\theta(x) = u_\theta(e^{-x})$$ → Now defined from (-∞,+∞)

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

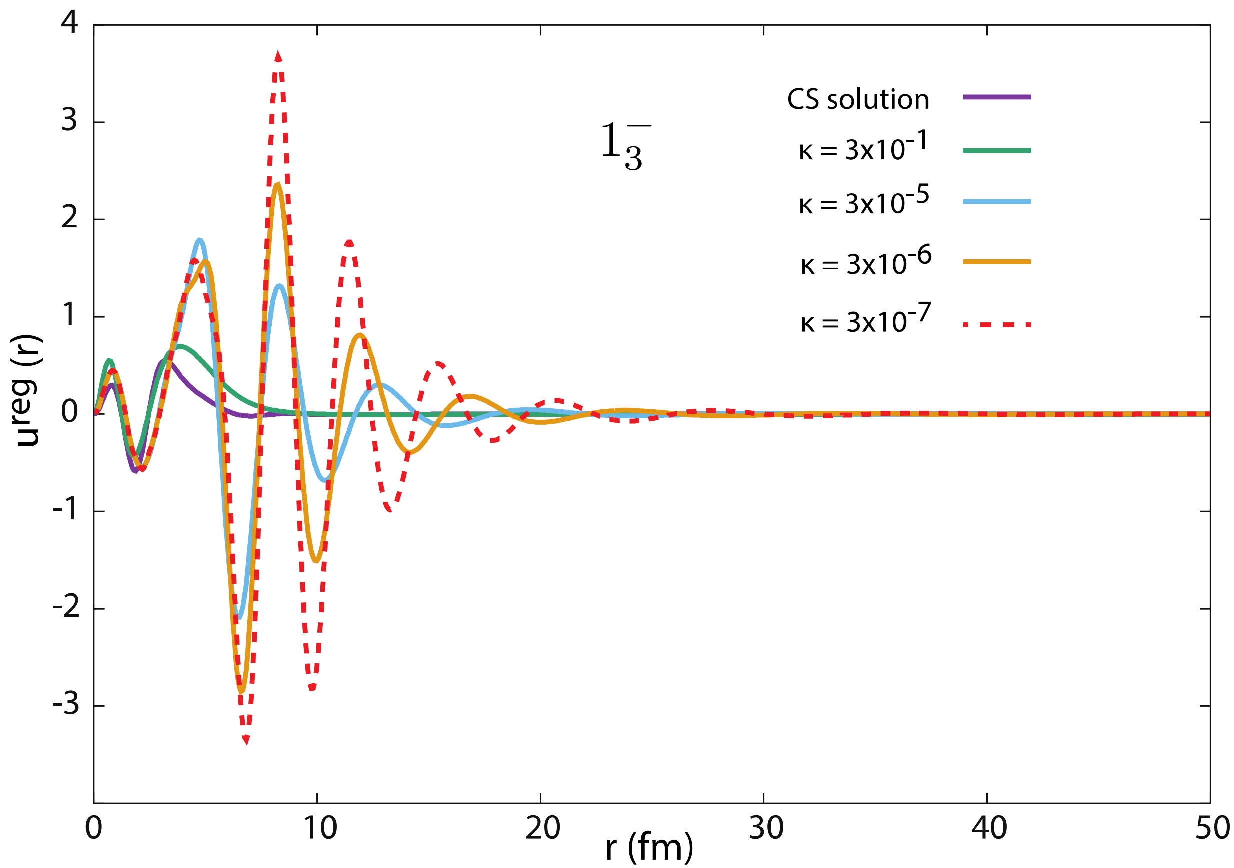
$$f(x+iy) = \frac{1}{2\pi}\int_{-\infty}^{\infty} e^{ix\xi} e^{-y\xi} f_\theta(\xi)d\xi$$

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

x = -lnr , y = θ

Parameter κ controls the regularization

Schematic model for backrotation



For several κ the long-range behavior is different, showing an outgoing behavior initially
The state however dies-off for large r.

→ We will calculate observables with this state

Schematic model for backrotation

rms radius

κ	$\widetilde{\langle u^{reg}(r)}\|r^2\|u^{reg}(r)\rangle^{\frac{1}{2}}$ (fm)
3×10^{-1}	(4.36348, 0.80081)
3×10^{-3}	(3.24315, 1.34967)
3×10^{-4}	(3.21818, 1.39037)
3×10^{-5}	(3.22016, 1.39346)
3×10^{-6}	(3.22010, 1.39341)
3×10^{-7}	(3.22009, 1.39345)
3×10^{-8}	(3.22005, 1.39359)
3×10^{-9}	(3.22018, 1.39323)
3×10^{-10}	(3.22003, 1.39456)
$\widetilde{\langle u_\theta(r)}\|e^{2i\theta}r^2\|u_\theta(r)\rangle^{\frac{1}{2}}$	(3.22008, 1.39351)

The complex rotated operator calculation (typical in CSM) serves as benchmark
Converged results for N=30 (θ-independence for θ > 0.25)

Schematic model for backrotation

Dipole transition 0+ → 1-

In CSM based on the extended or Berggren completeness of the many-body spectrum

$$\mathcal{S}(E) = -\frac{1}{\pi}\sum_{\nu=1}^{N} Im \frac{\langle \widetilde{u_\theta^i(r)}|\hat{O}(\theta)|u_\theta^\nu(r)\rangle\langle \widetilde{u_\theta^\nu(r)}|\hat{O}^\dagger(\theta)|u_\theta^i(r)\rangle}{E - E_\nu^\theta}$$

✓ i is the initial state (e.g. 0+), v are the final CSM continuum states (e.g. 1-)

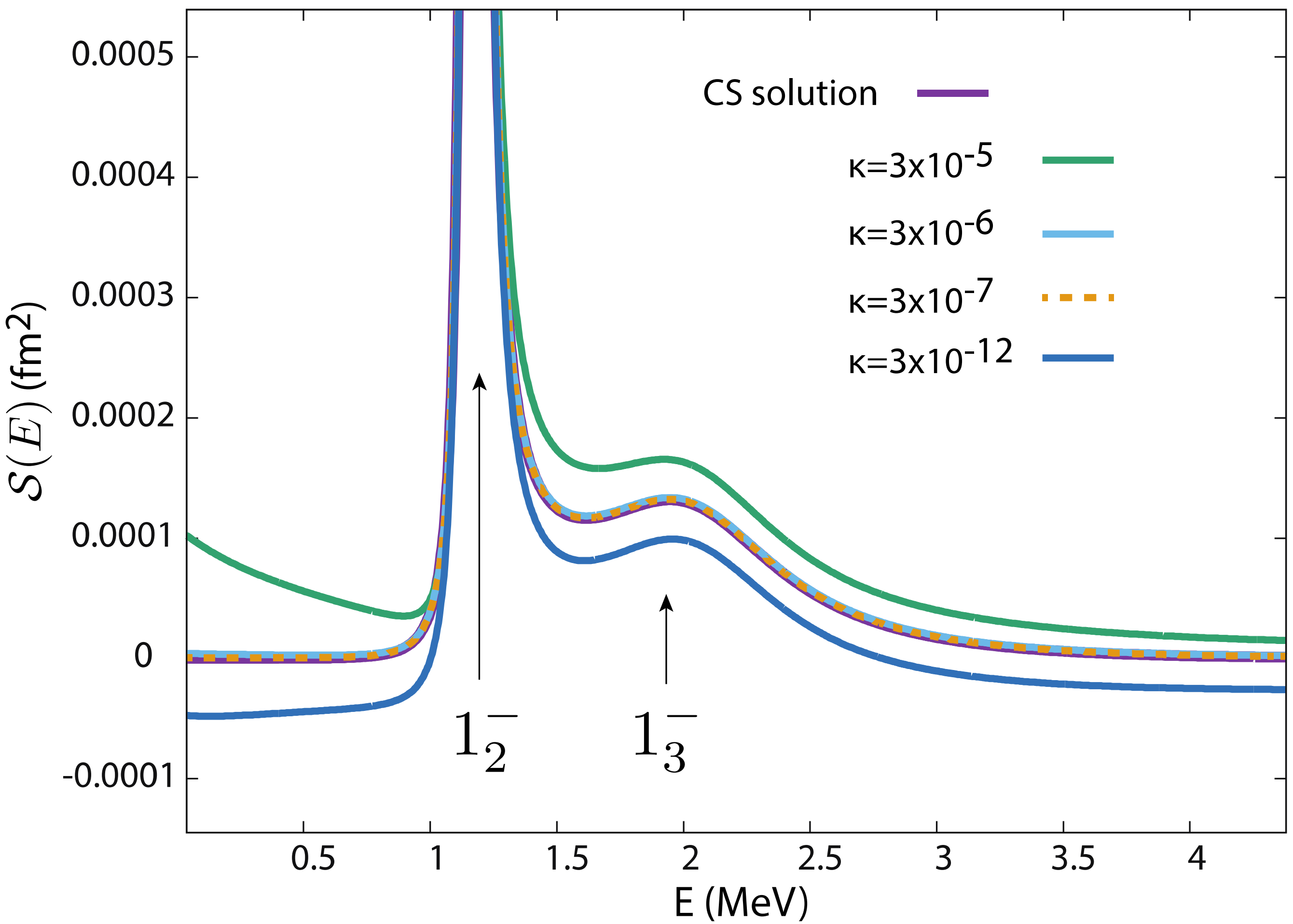
and $\hat{O}(\theta) = re^{i\theta}Y_0^1$

→ We calculate the following:

$$\mathcal{S}(E) = -\frac{1}{\pi}\sum_{\nu=1}^{N} Im \frac{\langle \widetilde{u_{reg}^i(r)}|\hat{O}|u_{reg}^\nu(r)\rangle\langle \widetilde{u_{reg}^\nu(r)}|\hat{O}^\dagger|u_{reg}^i(r)\rangle}{E - E_\nu^\theta}$$

→ More stringent test on the back rotation since we back rotate an ensemble of states

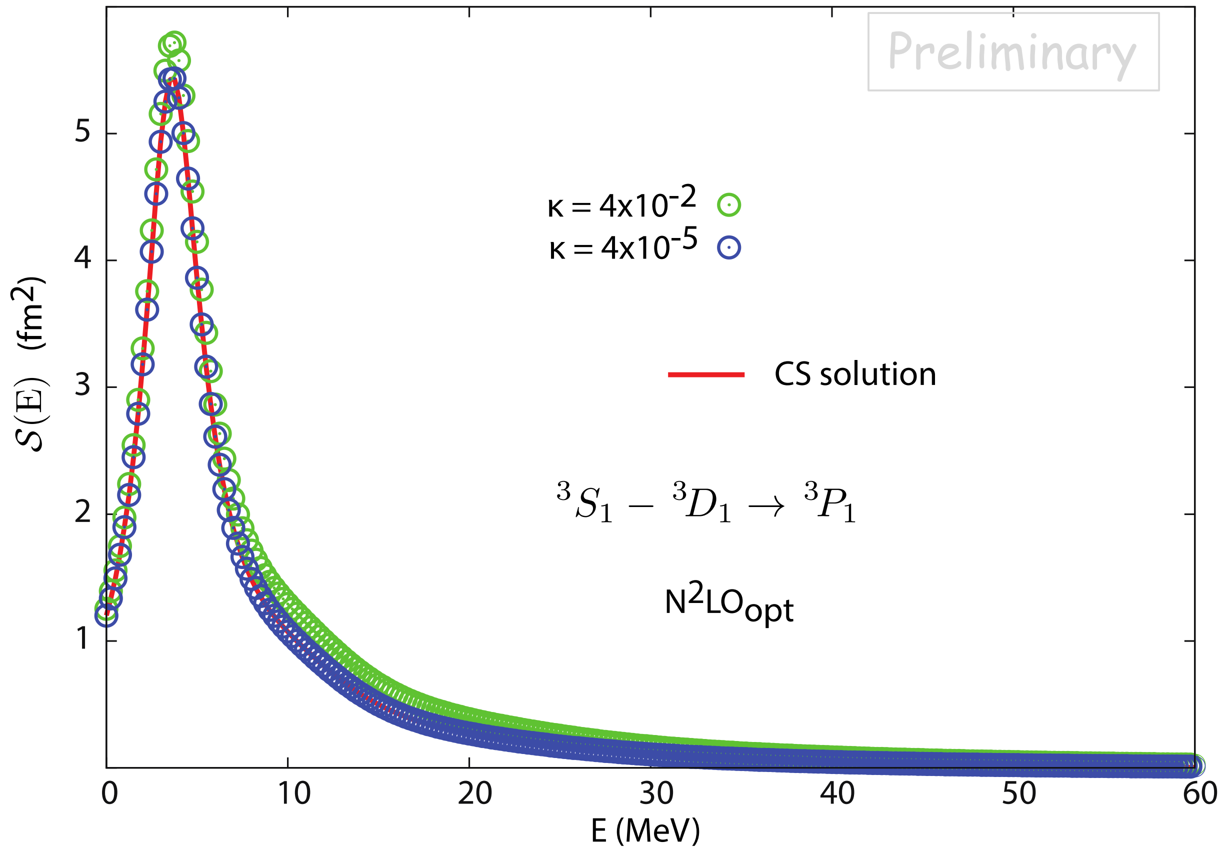
Schematic model for backrotation



Results are indistinguishable which also implies that the back rotated solutions form a complete set

Realistic case for backrotation

- Dipole transition from the 3S1-3D1 channel to the continuum 3P1 channel.

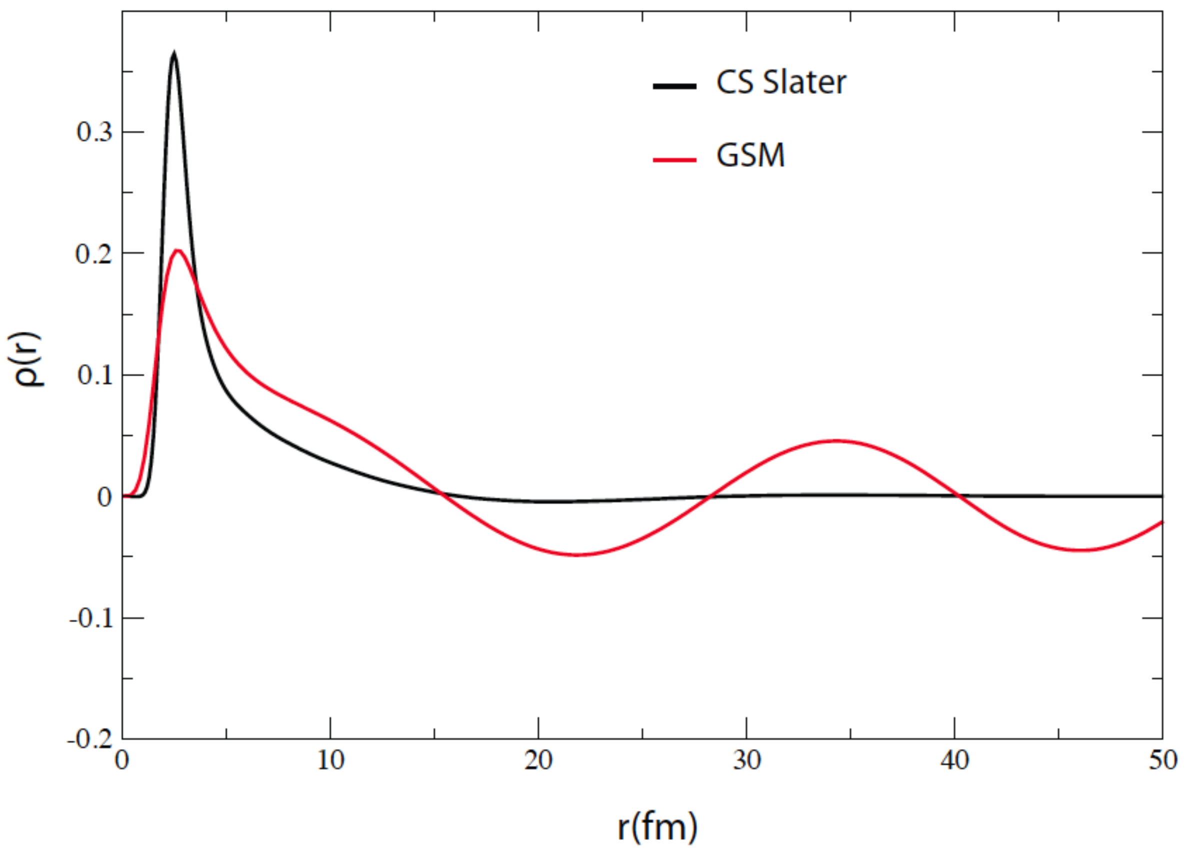


Successful test of back rotation with a realistic interaction

Backrotation in ^{6}He 2+ resonant state density (CSM in a Slater basis)

Kruppa, Papadimitriou, Nazarewicz, Michel (PRC 89 (2014))

2^{+} first excited state in ^{6}He



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

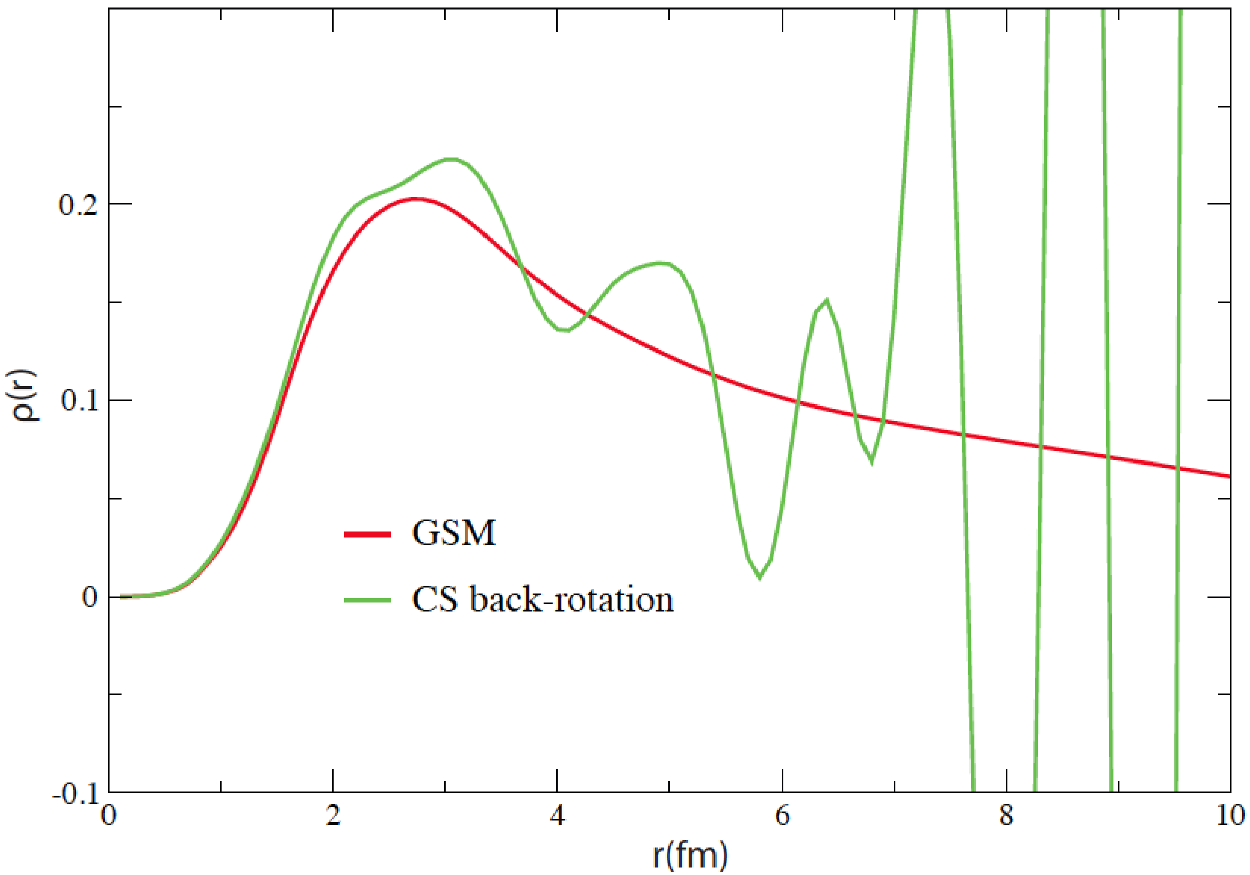
☺ GSM exhibits naturally this behavior

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

This is OK. The solution Ψ(θ) is known to “die” off (L^2 function)

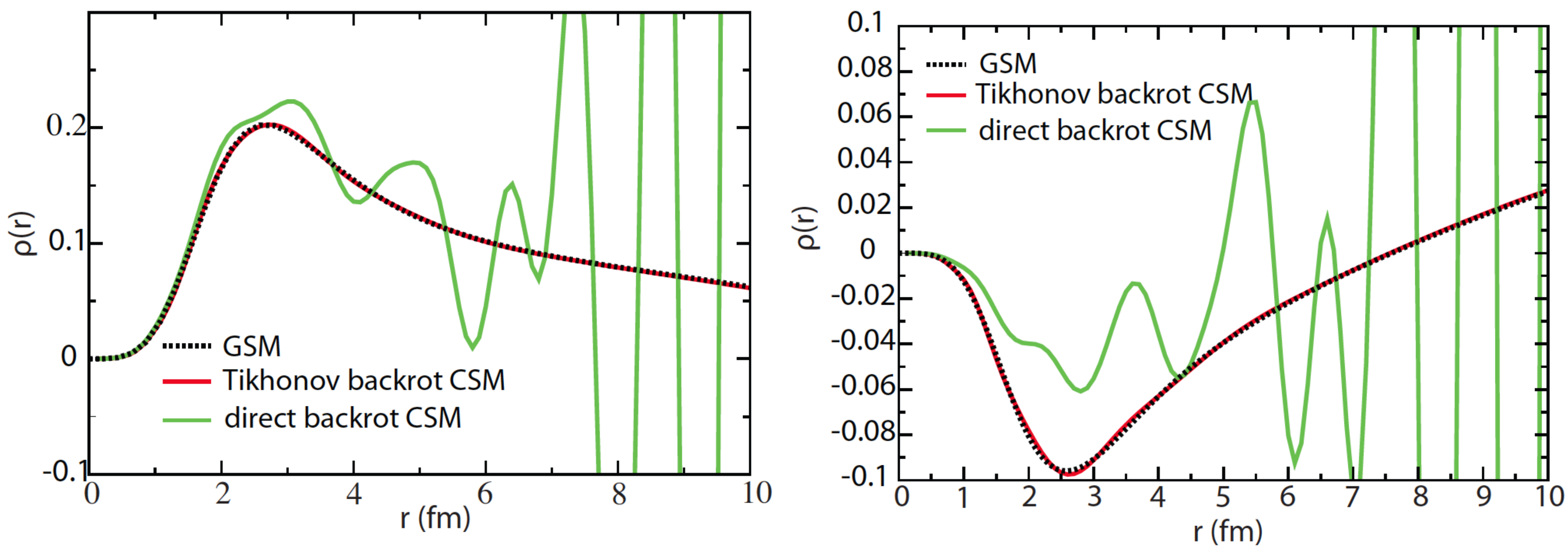
Solution

→ Perform a direct back-rotation.



The CS density regains the correct asymptotic behavior

→ Regularization via Tikhonov method



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

Widths using (phenomenolodgical) R-matrix formulas

- Scattering takes place on the real-axis. Cross sections, phase-shifts are all real energy quantities.
- With CSM we can obtain the resonant state as the complex eigenvalue of the CS Hamiltonian but at the same time with the same method we can compute real energy phase-shifts through the CS CLD.

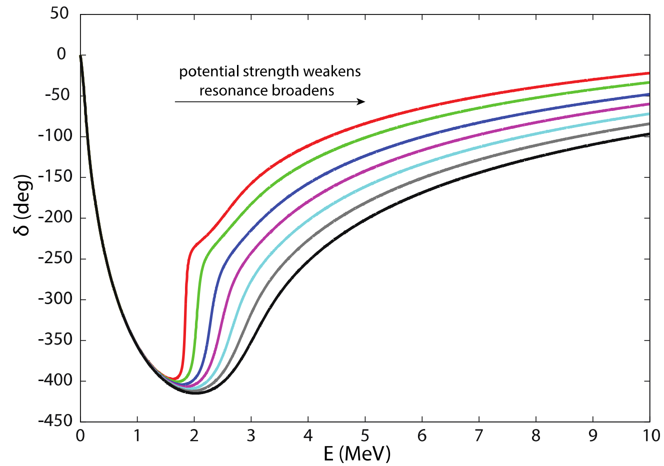
→ The formulas one employs for the determination of resonance parameters through the phase-shift are based on the inflection criterion:

$$\left.\frac{d\delta(E)}{dE}\right|_{E=E_r} \rightarrow \text{Max} \qquad \Gamma = \frac{2}{\left.\frac{d\delta(E)}{dE}\right|_{E=E_r}}$$

$$V(r) = -V_0 e^{-0.16r^2} + 4.0e^{-0.04r^2}$$

V_0 is reduced gradually

V_0	(E_r, Γ) diagonalization	(E_r, Γ) inflection
4.1	$(1.843,\ 5.343\times10^{-2})$	$(1.843,\ 5.422\times10^{-2})$
3.7	(2.042, 0.118)	(2.046, 0.117)
3.2	(2.279, 0.251)	(2.282, 0.240)
2.8	(2.463, 0.402)	(2.471, 0.370)
2.4	(2.644, 0.596)	(2.660, 0.522)
2.0	(2.825, 0.834)	(2.857, 0.696)
1.6	(3.009, 1.211)	(3.064, 0.886)



→ R-matrix inflection point formula works well for widths up to Γ~600 keV. Position in good agreement
→ Going to complex energy provides an unambiguous determination of resonance parameters.

Complex Energy Method: Gamow Shell Model

Why use different basis sets for nuclei:

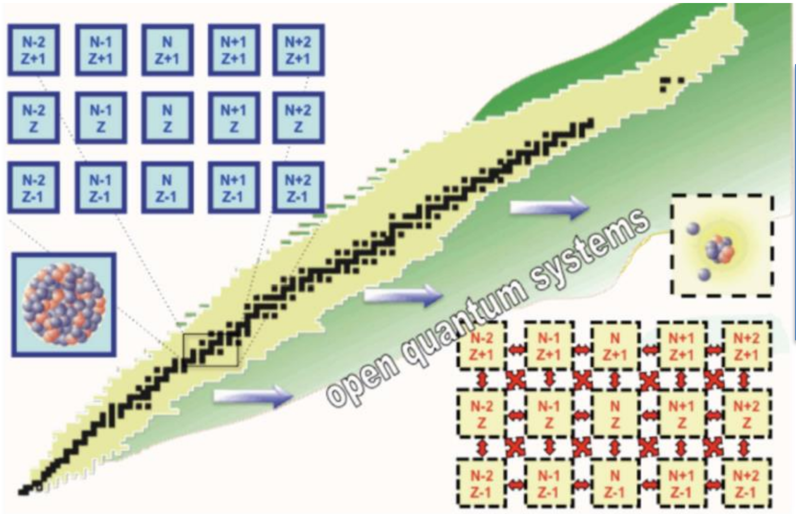
→ Describe nucleus of radius R with an interaction Λ using a basis

→ One would need a number of basis states $n = \propto (R\Lambda)^3$

→ Proportionality depends on the underlying basis and efficiencies could be gained by using Berggren basis, Sturmian, Discrete Variable Representation

→ In the case of the Berggren basis one has access to an automatic description of resonant and non-resonant continuum states

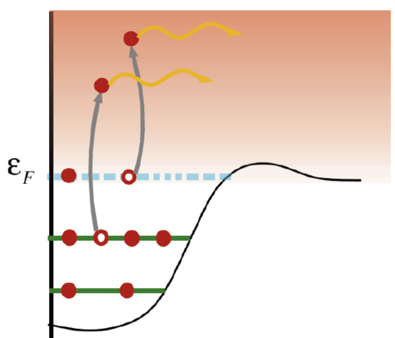
The Gamow Shell Model

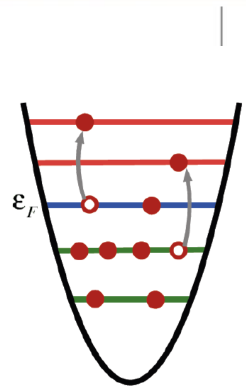


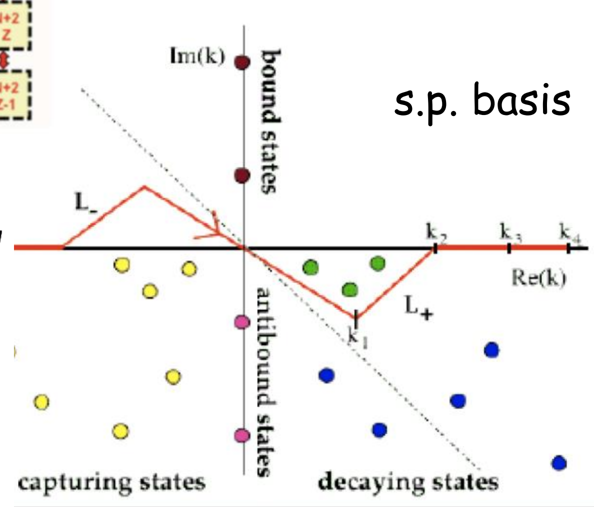
The Berggren completeness treats bound, resonant and scattering states on equal footing.

Has been successfully applied in the shell model in the complex energy plane to light nuclei. For a review see

N. Michel et al J. Phys. G 36, 013101 (2009).





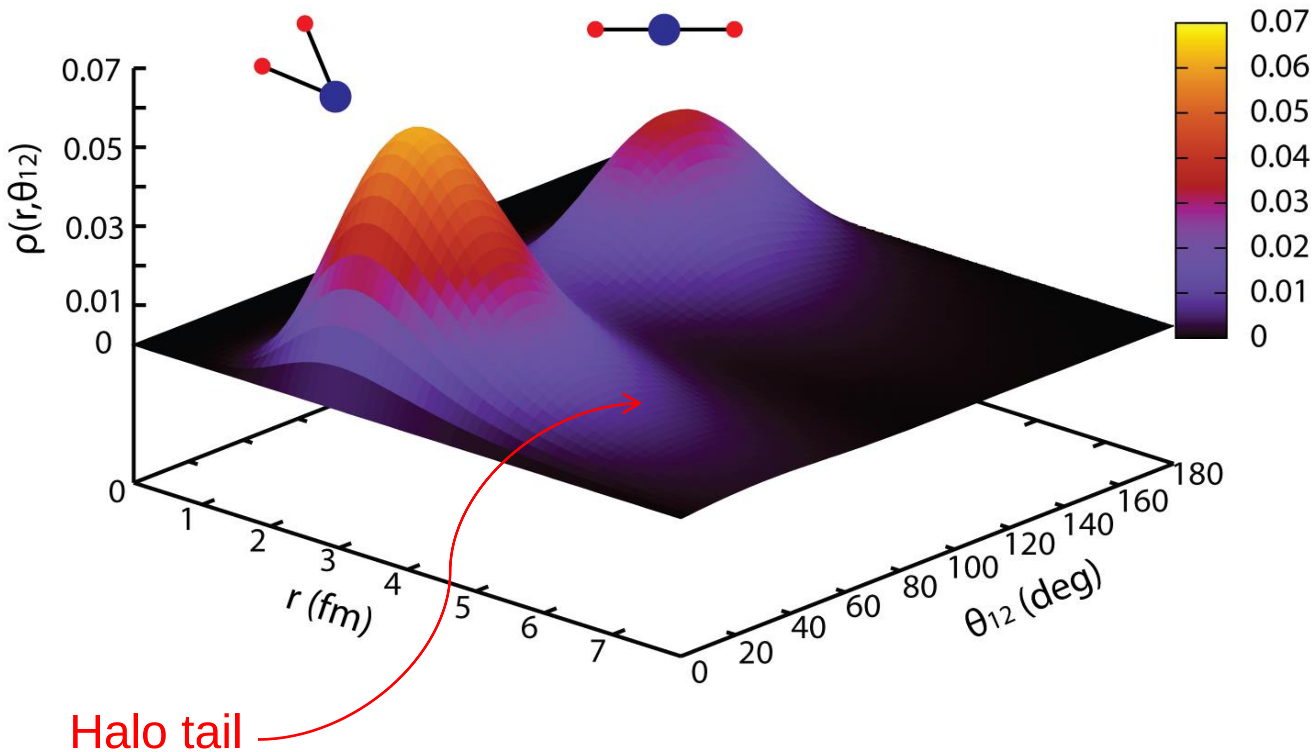


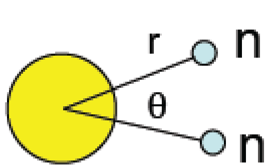
Adopted from G. Hagen

- Complete orthonormal basis
- Hamiltonian expressed in COSM coordinates keeping Fock space tractable
- Complex Symmetric standard eigenvalue problem $AX = \lambda X$
- Any kind of interaction applicable

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

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





→ Probability of finding the particles at distance **r** from the core with an angle $\boldsymbol{\theta_{nn}}$

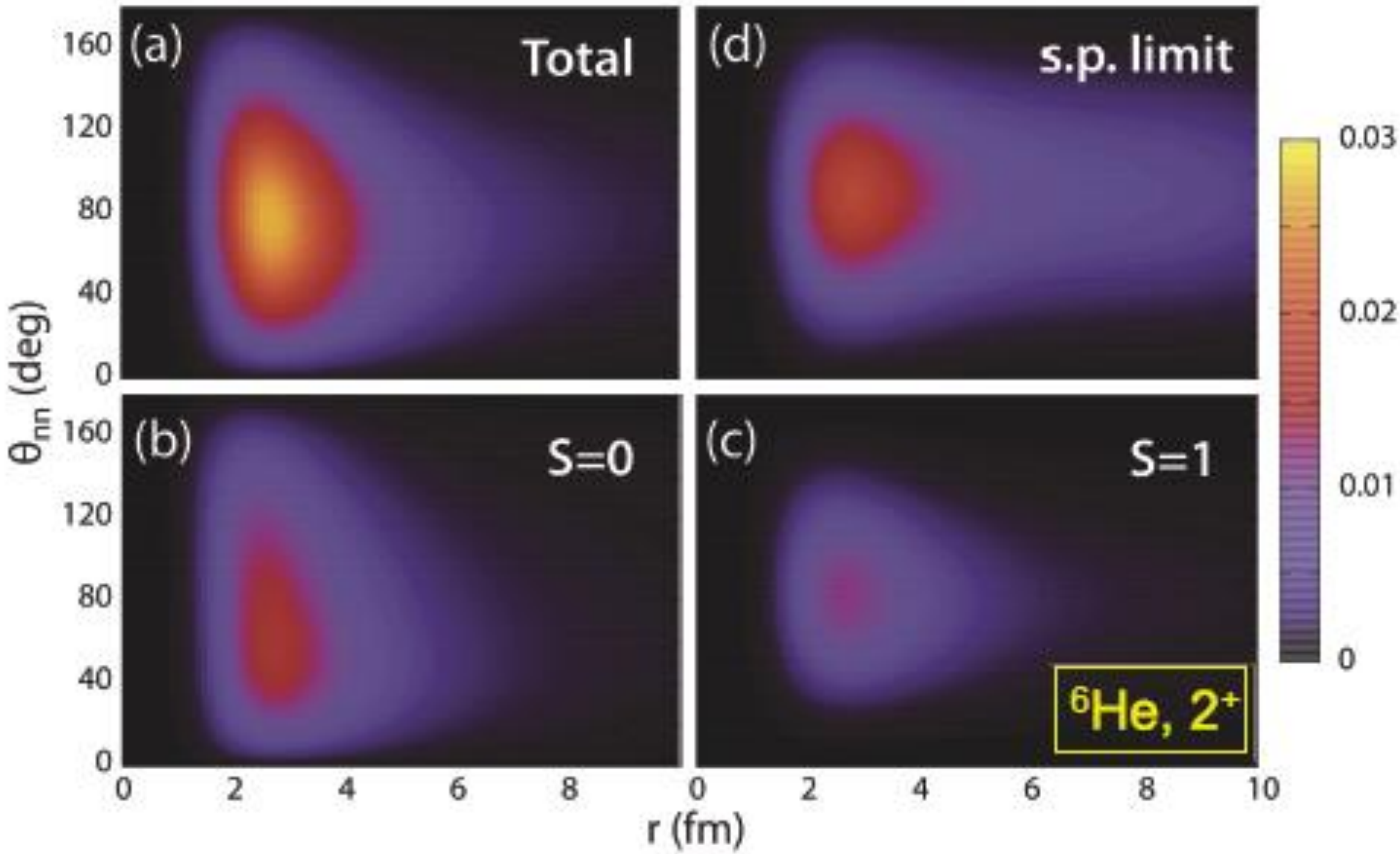
It contains a lot of info. Manifests the strong dineutron correlation, Implies that s.p. basis may not be able to capture the clusterization physics. "Infinite COSM basis" S2n ~ 500keV Jacobi basis S2n ~ 900 keV for the same interaction
(see also Descouvemont, Daniel, Baye PRC 67 (2003), Aoyama et al PTP 93 (1995))

→ It is an interesting mathematical/technical problem
→ Effective interactions eventually cure the "missing" physics.

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

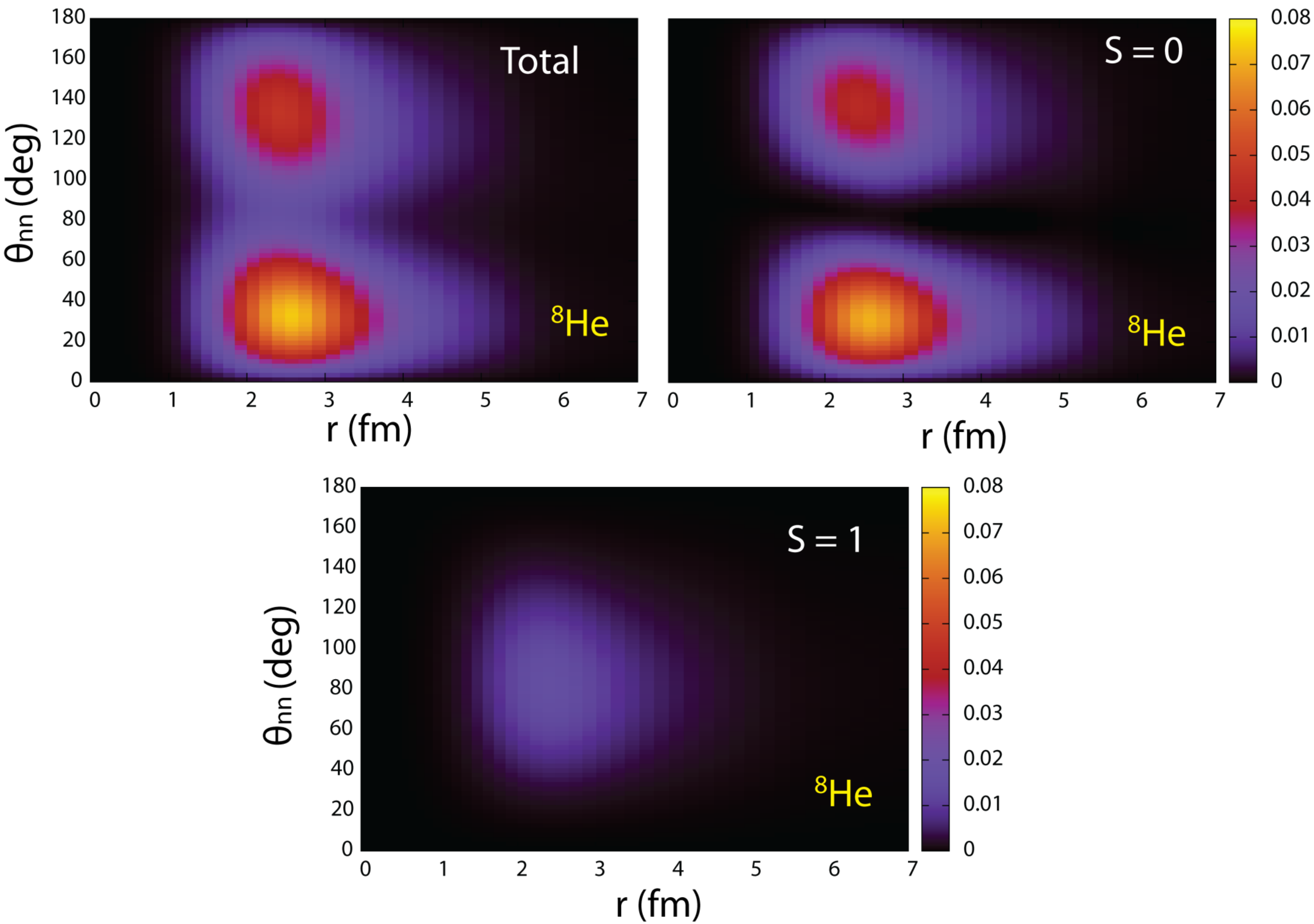
GSM: [0.851, 0.109] MeV
EXP: [0.822(25), 0.113(20)] MeV

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

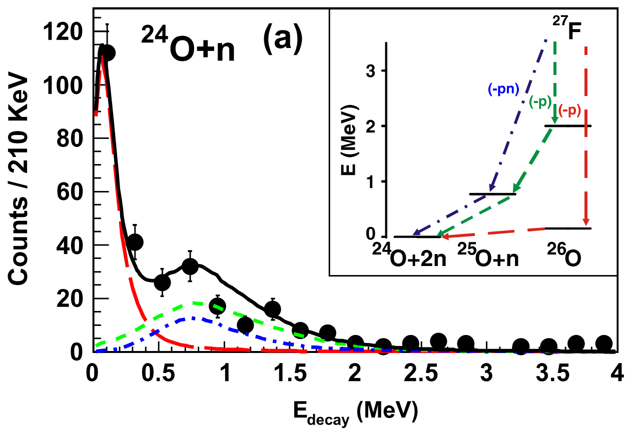


→ 2+ neutrons almost uncorrelated…

Neutron correlations in ^{8}He ground state



^{26}O: Experimental and Theoretical situation



- Different theory predictions: Trace the discrepancy in either the many-body technique or the Hamiltonian

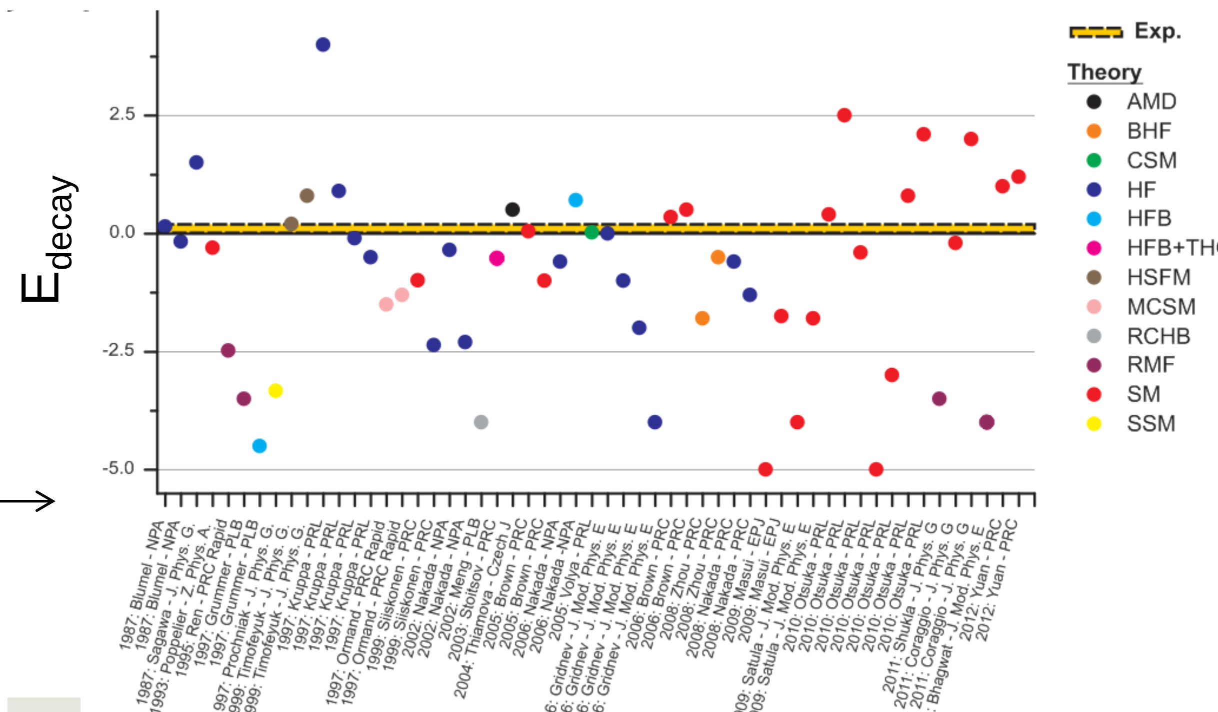
→ Prediction ⟺ observation
→ Many body methods ⟺ nuclear Hamiltonian

^{26}O unbound by < 200 keV
Extremely narrow width

Experiment

Theory

From Z. Kohley ICNT 2015 talk



Chronological time

Radioactivity

Pfutzner et al. (2012): $T_{1/2} > 10^{-14}$ s (10 fs)

- K-shell vacancy half-life of carbon atom 2×10^{-14} s

From Z. Kohley ICNT talk

Cerny & Hardy (1977): $T_{1/2} > 10^{-12}$ s (1ps)

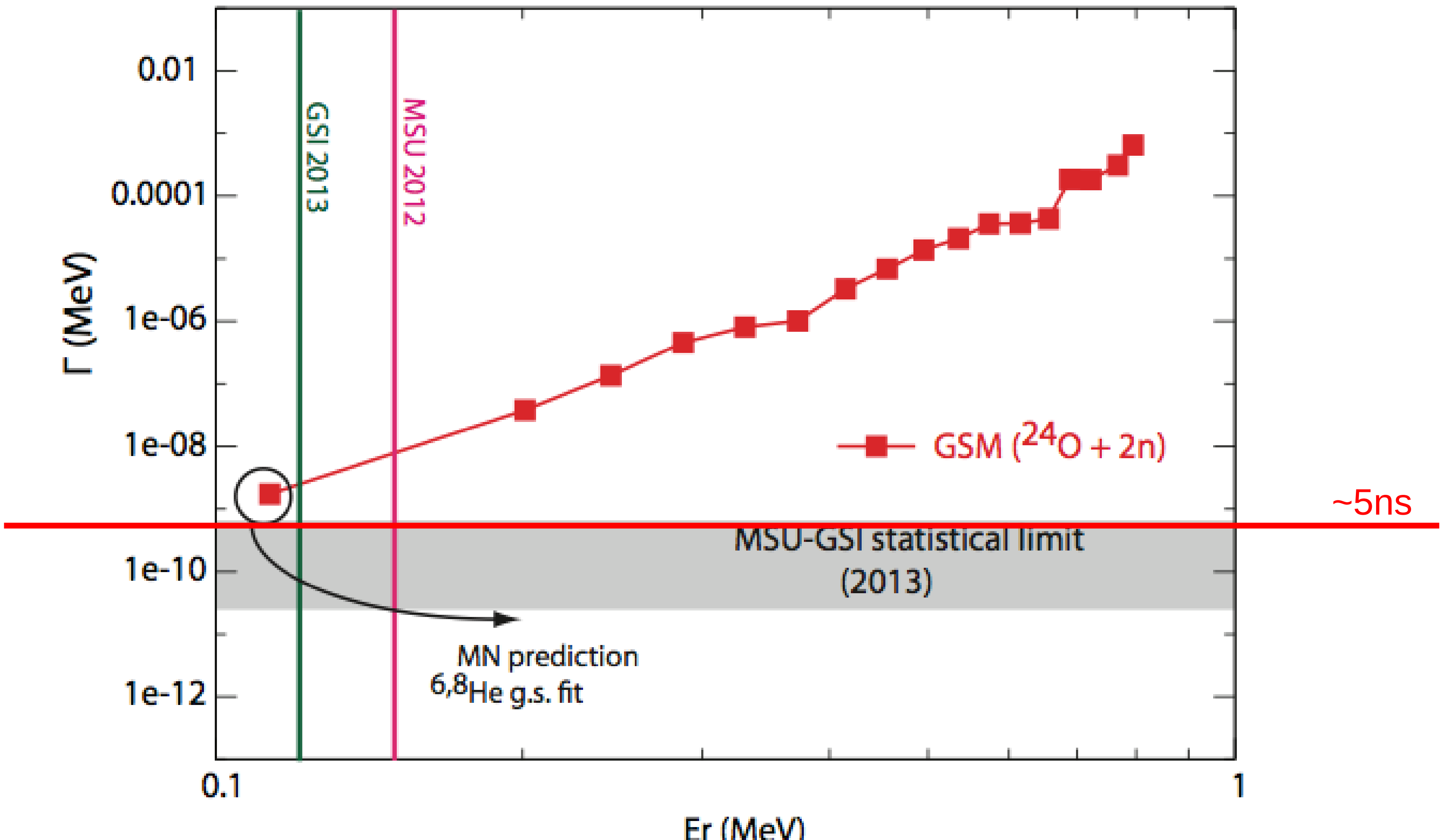
IUPAC, discovery of element: $T_{1/2} > 10^{-14}$s (10 fs)

- Around the time for nucleus to acquire outer electrons

→ ^{26}O may qualify as a two-neutron emitter

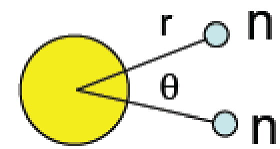
Phenomenology of ^{26}O

Using a ^{24}O core and a schematic interaction study S2n-width correlation of ^{26}O

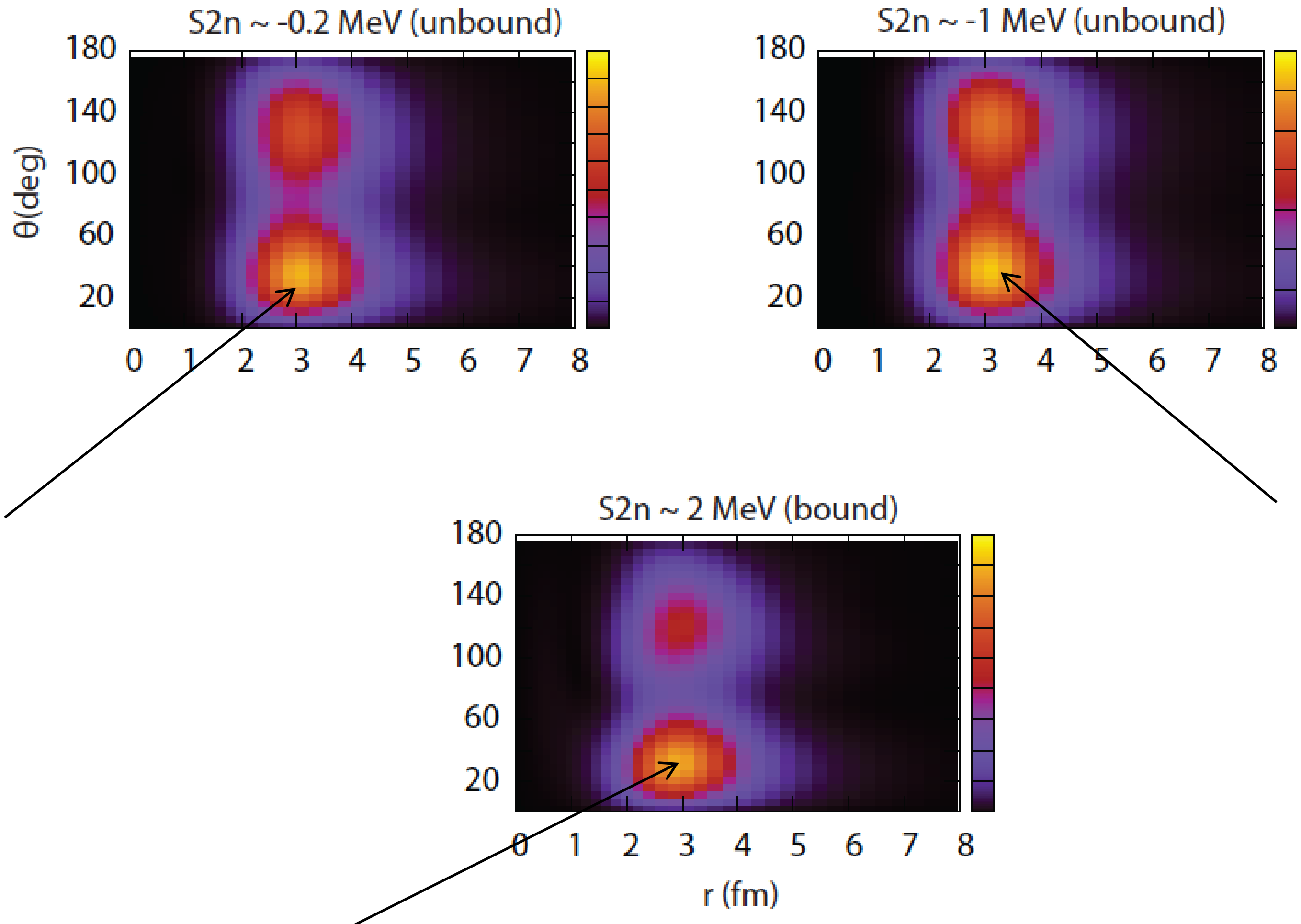


- Large Gamow basis for p-sd orbitals
- WS basis fitted to ^{24}O+n GSI experiment
- New experiments provide a very small width for ^{26}O g.s. Need precise calculation of S2n

Correlations in ^{26}O



→ Study of correlations as a function of the S2n

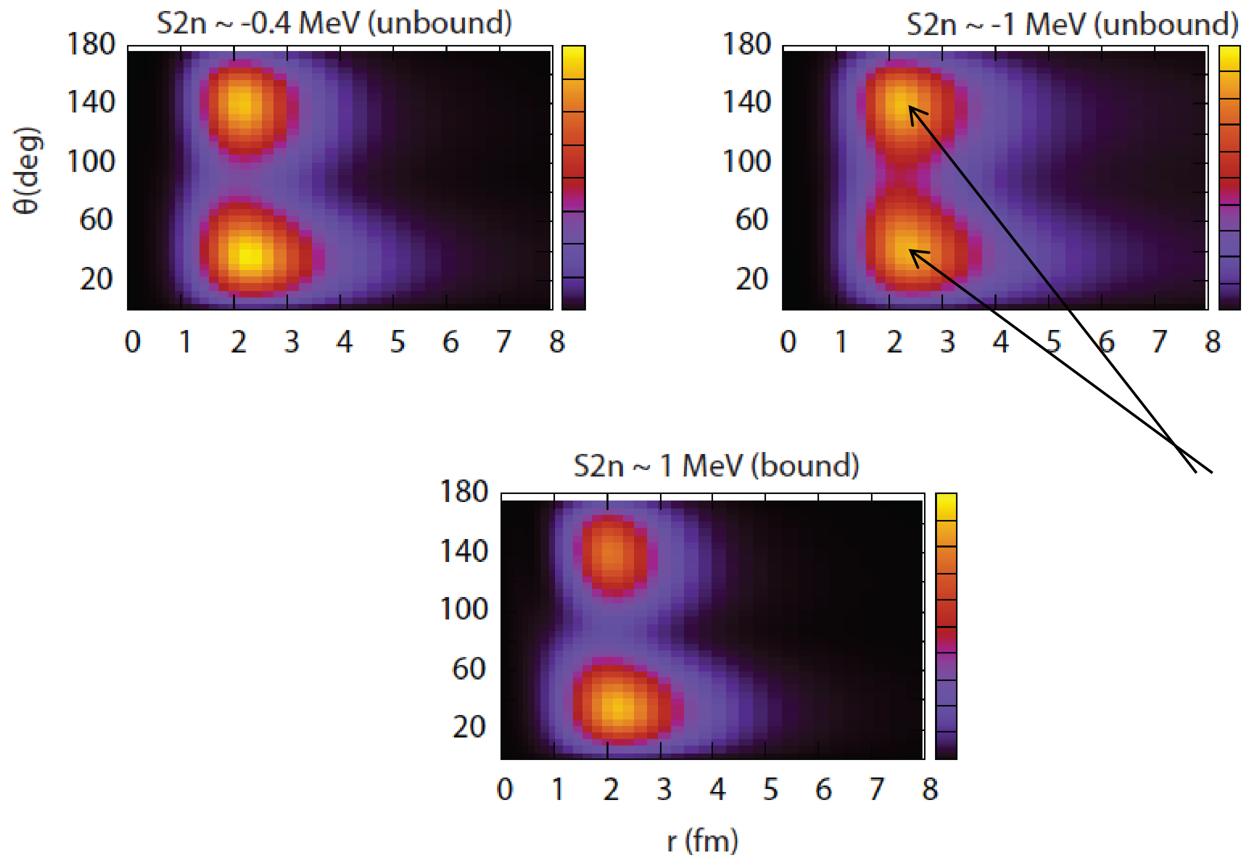


- Asymmetry in the distributions
- Even when the system is very unbound, neutrons show preference to be close to each other

→ Hint of correlated **emission** of neutrons

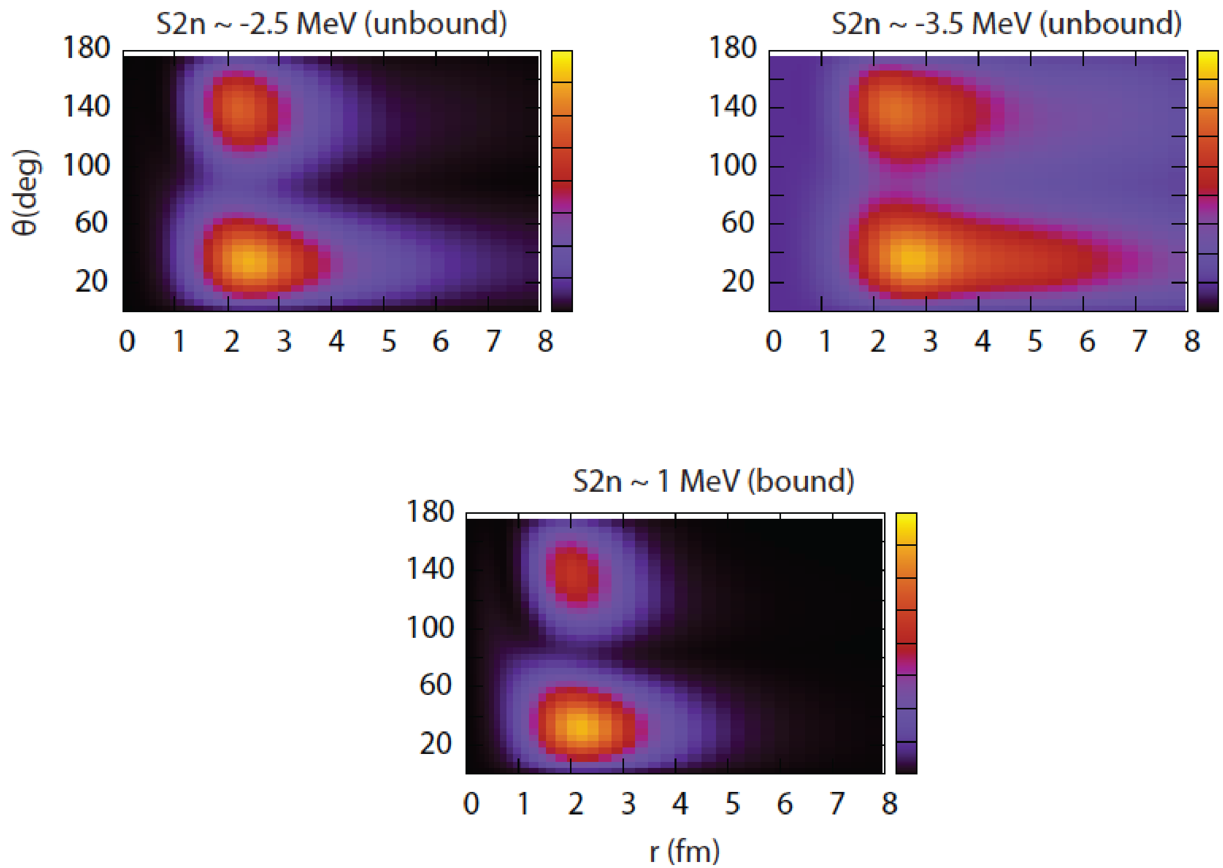
^{6}He

→ Study of correlations as a function of the S2n



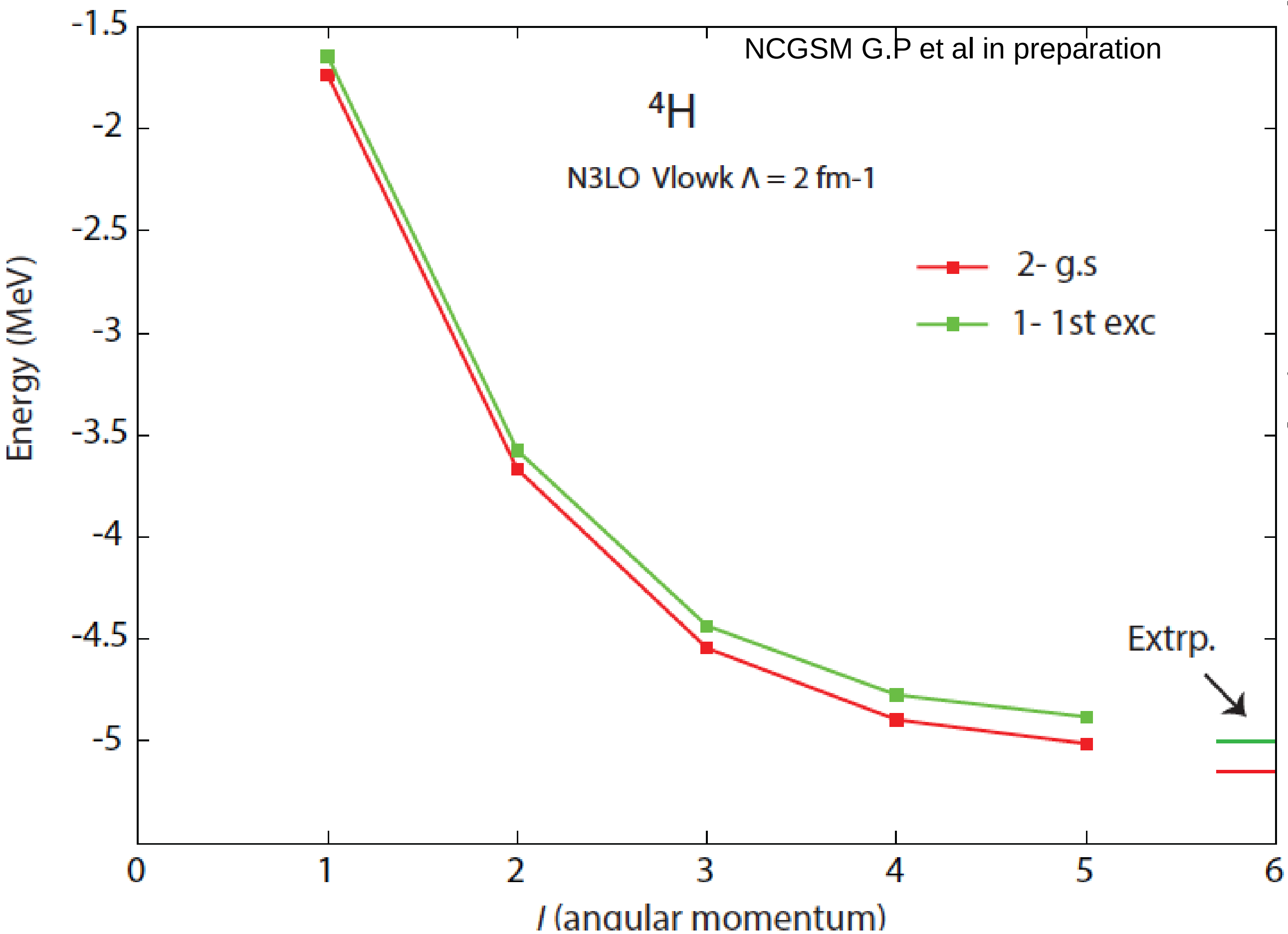
→ ^{6}He is not a neutron emitter and in the unbound regime there is a democratic distribution of neutrons around the core.
Different situation as compared to ^{26}O

^{6}Be



Substitute 2 neutrons with 2 protons. Bound state regime similar to ^{6}He
Very extended proton distribution in the continuum. Protons still well correlated.

^4H,^4Li:



to each other

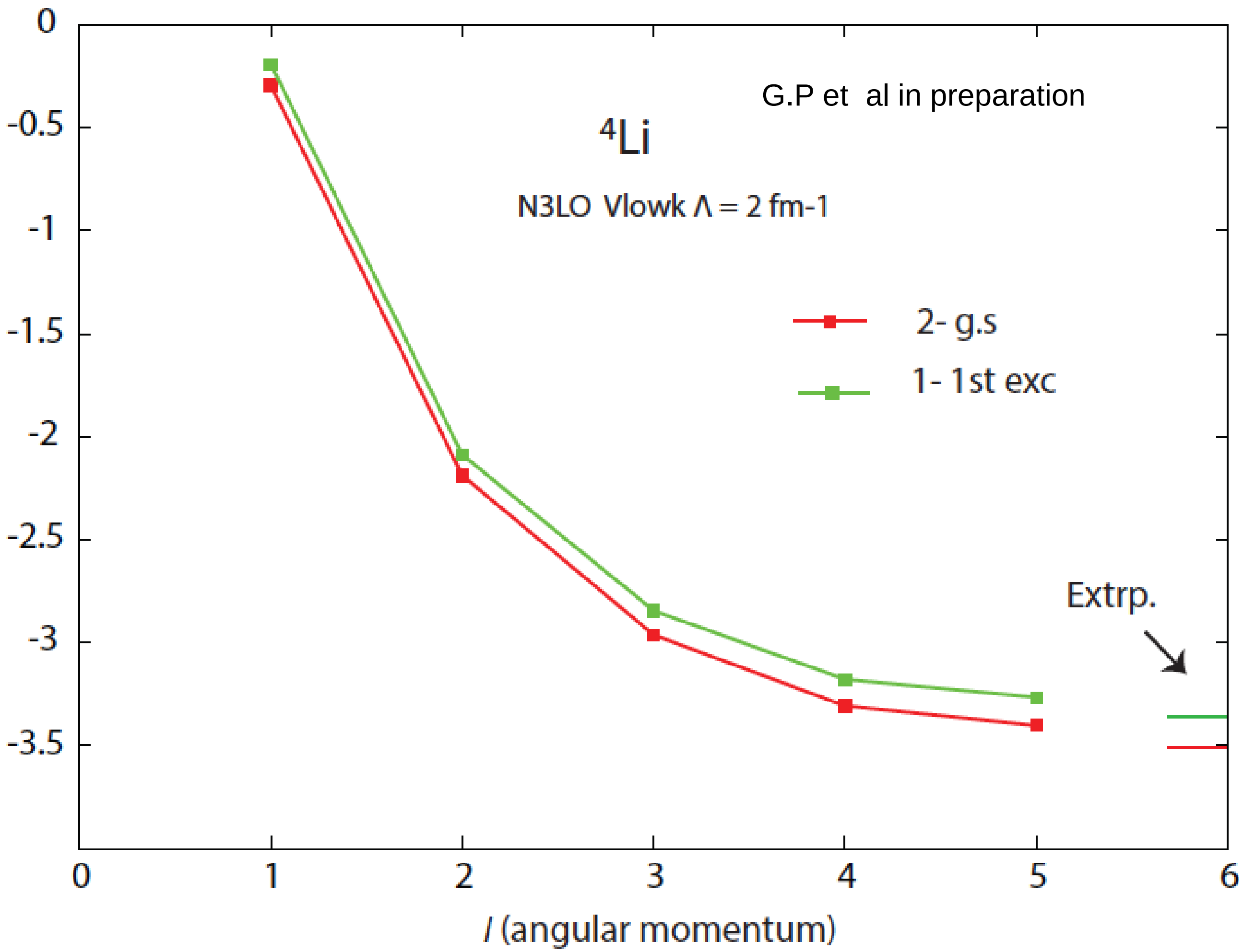
Basis:
Gamow p3/2 neutron states
(0p3/2 s.p. res) +
20 scattering continua.
Rest up to h-waves are H.O states of ħω=20 MeV

type of interactions

and 3He+p PRC 84, 054010

- Extrapolated result has an uncertainty of about +-20 keV
- Sensitivity tests to be completed

Results

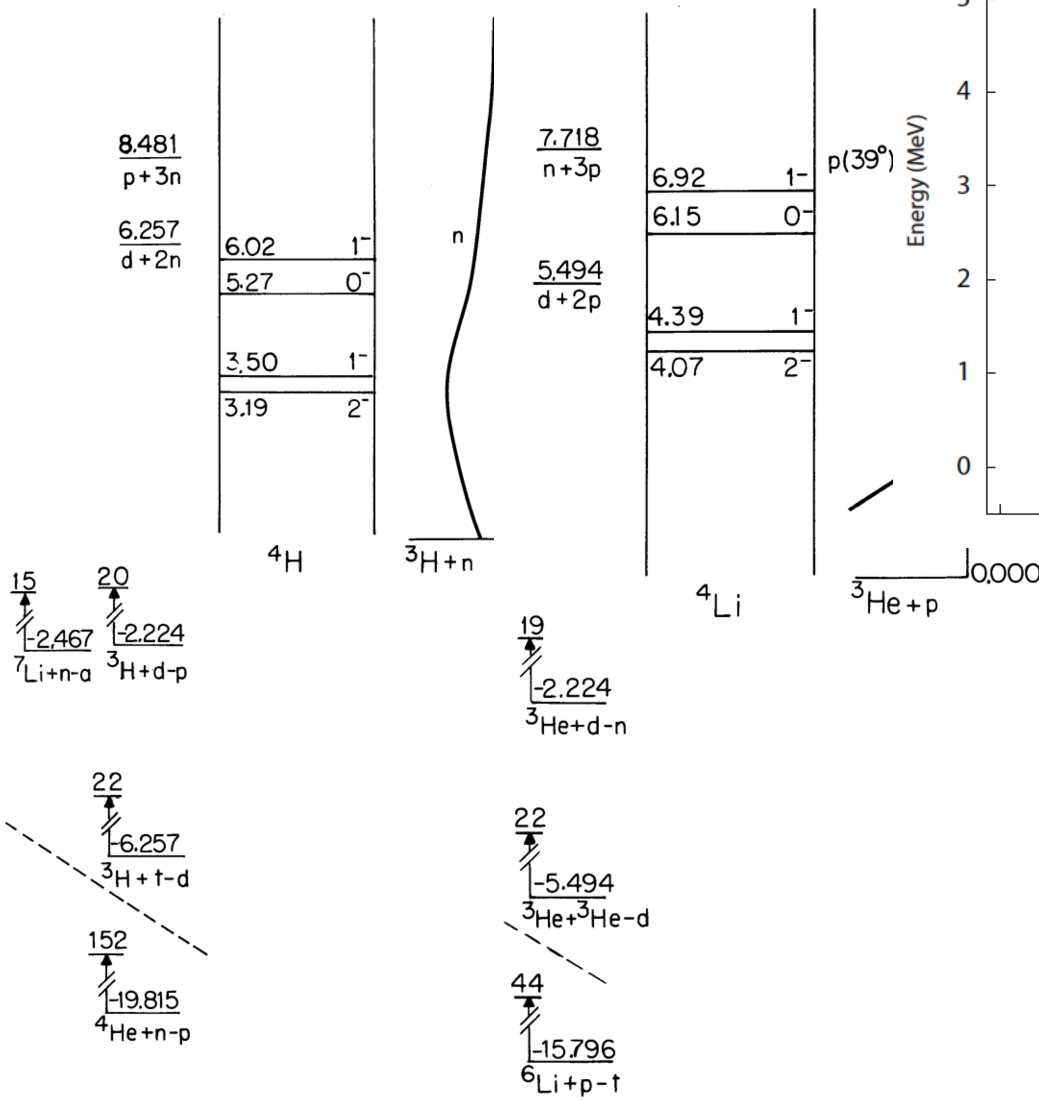


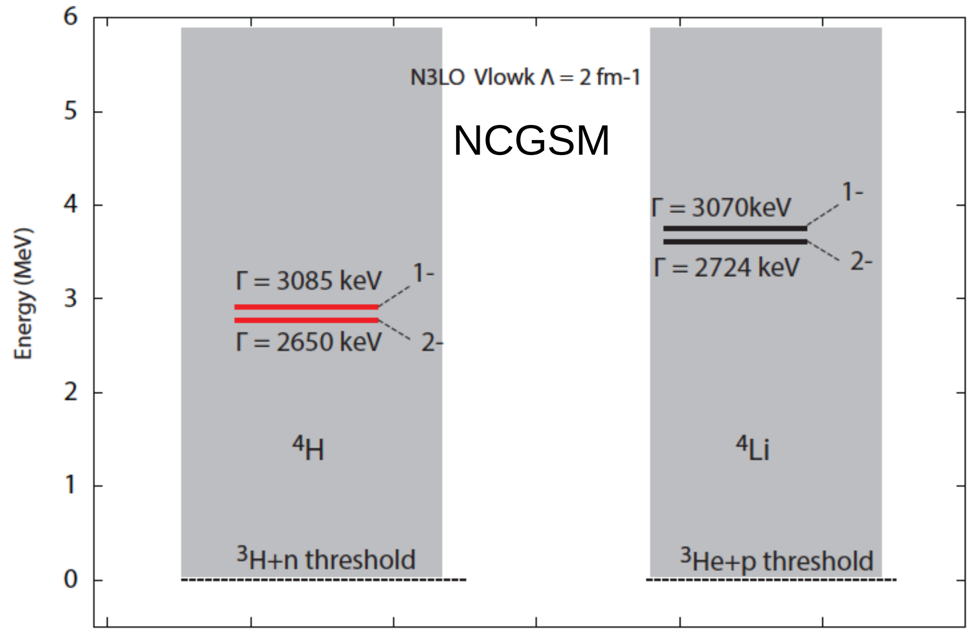
Basis:
Gamow p3/2 proton states
(0p3/2 s.p. res) +
20 scattering continua.
Rest up to h-waves are H.O
States of hw= 20 MeV

- Similar trend with ^{4}H

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

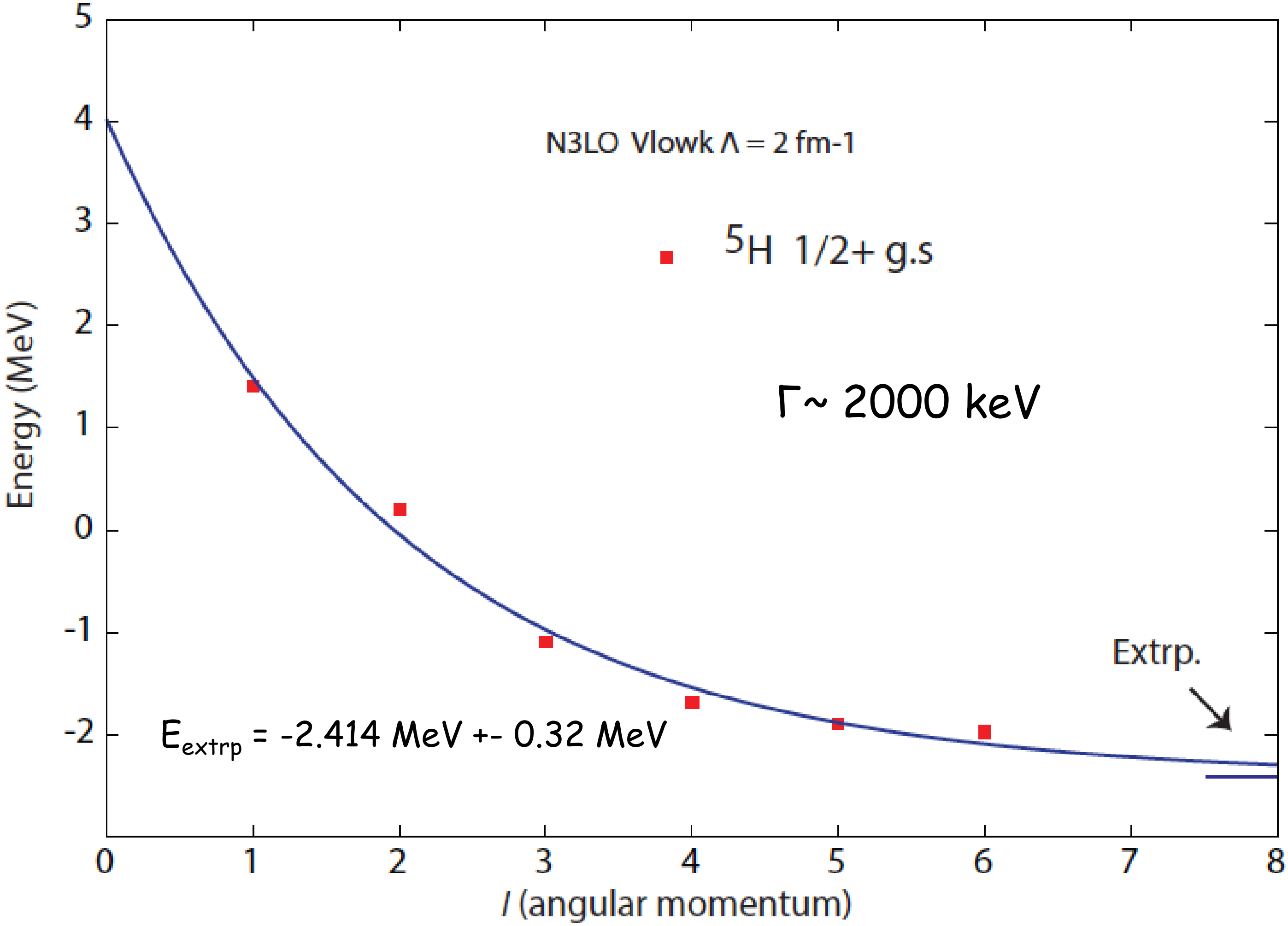
4Li:

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)

Results for ^5H



:C 62 014312)

reshold Γ ~1-4 MeV

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

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, strength functions etc
→ No boundary condition, HO basis (or other). Could take advantage of model-independent extrapolations of the HO basis (UV/IR) for resonant states.
→ Use complex scaling for few-body scattering calculations and many-body L^2 integrable basis calculations. Use together with microscopic NCSM-RGM for cluster scattering. Non-local optical potential should be OK to treat.
→ Explore other orthonormal L^2 basis beyond HO (e.g. Lagrange mesh, wavelets)

→ Back rotation was tested to calculations of observables other than densities. The back rotated state is regularized and results are in agreement with typical treatment of observables in CSM.

→ Correlation densities for ^{26}O show a hint of a possible scenario for 2n-radioactivity.
→ Provide correlations of particles data for input for experiment

→ Gamow basis has been applied successfully in an ab-initio GSM framework

Collaborators

Nicolas Michel, Marek Płoszajczak (GANIL)

Witek Nazarewicz, Yannen Jaganathen, Kevin Fossez,
Rolo Betan (MSU/NSCL)

Jimmy Rotureau (ORNL/MSU)

Andras Kruppa (Debrecen, Hungary)

James Vary and Pieter Maris (ISU)

Bruce Barrett (UA)

Heiko Hergert (MSU)
Scott Bogner (MSU)

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} …

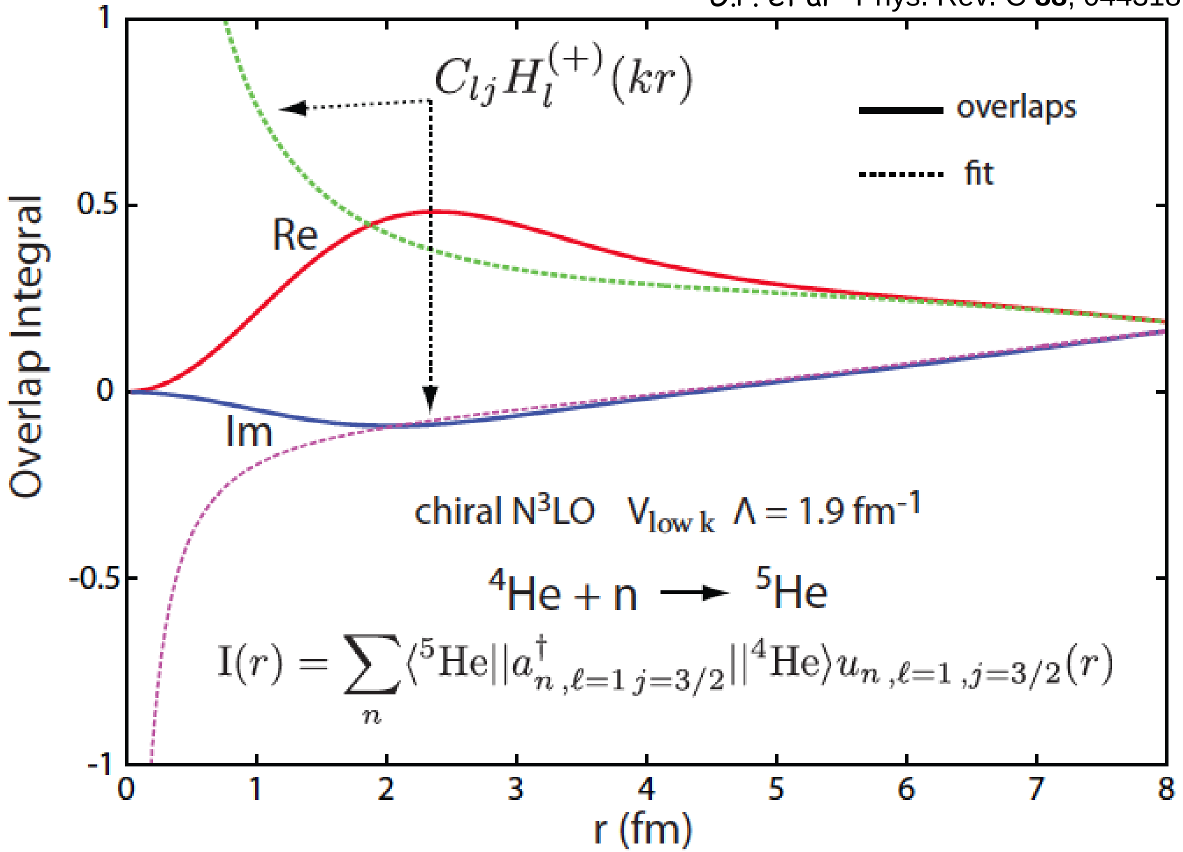
See also Okolowicz et al Phys. Rev. C85, 064320 (2012)., for properties of ANCs

Results: Ab-initio overlaps in the NC-GSM

- Basic ingredients of the theory of direct reactions

Calculations at a Vlow k Λ = 1.9 fm^{-1}

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



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

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

C = 0.197

and from (1)

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

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

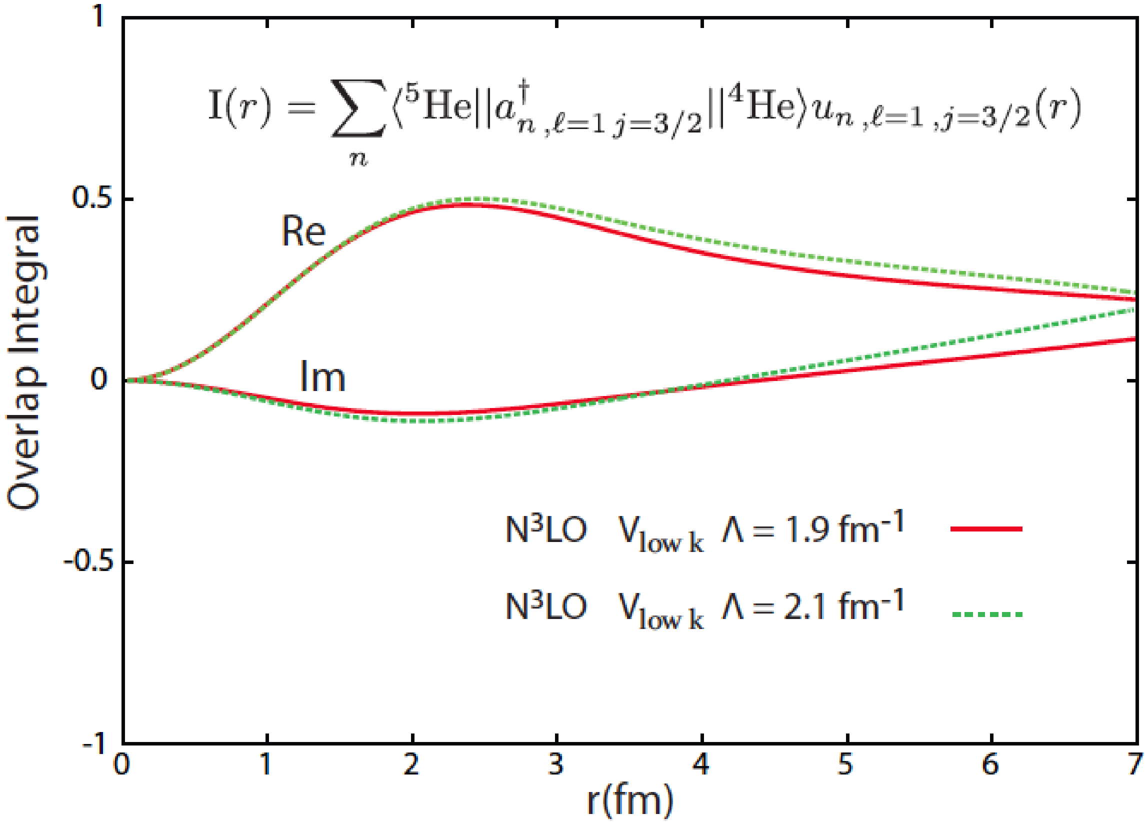
Two ways of calculating the width
a) many body diagonalization
b) from overlap function

$\longrightarrow$ Equivalent

Results: Ab-initio overlaps in the NC-GSM

Calculations at a Vlow k Λ = 1.9 fm^{-1} and 2.1 fm^{-1}

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



Overlap tail sensitive to S_{1n}

ANC (Λ = 2.1 fm^{-1}) = 0.255

S_{1n} (Λ = 2.1 fm^{-1}) = -2 MeV

$\Gamma_{diagonalization}$ = 591 keV

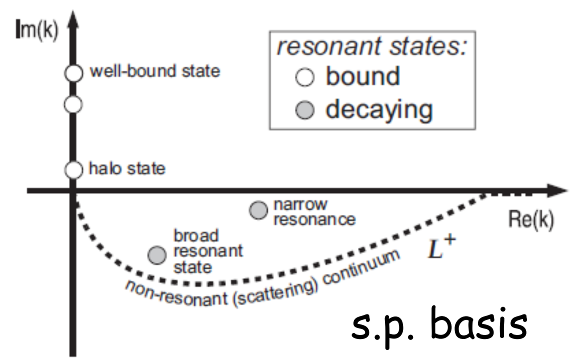
Γ_{ANC} = 570 keV

The width exhibits the correct behavior

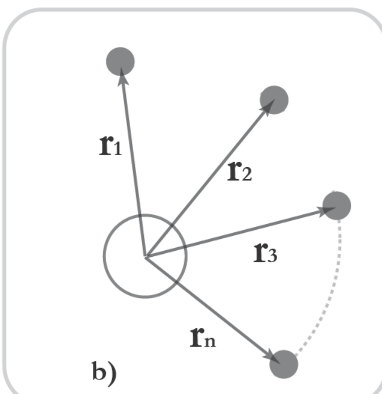
GSM HAMILTONIAN

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

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



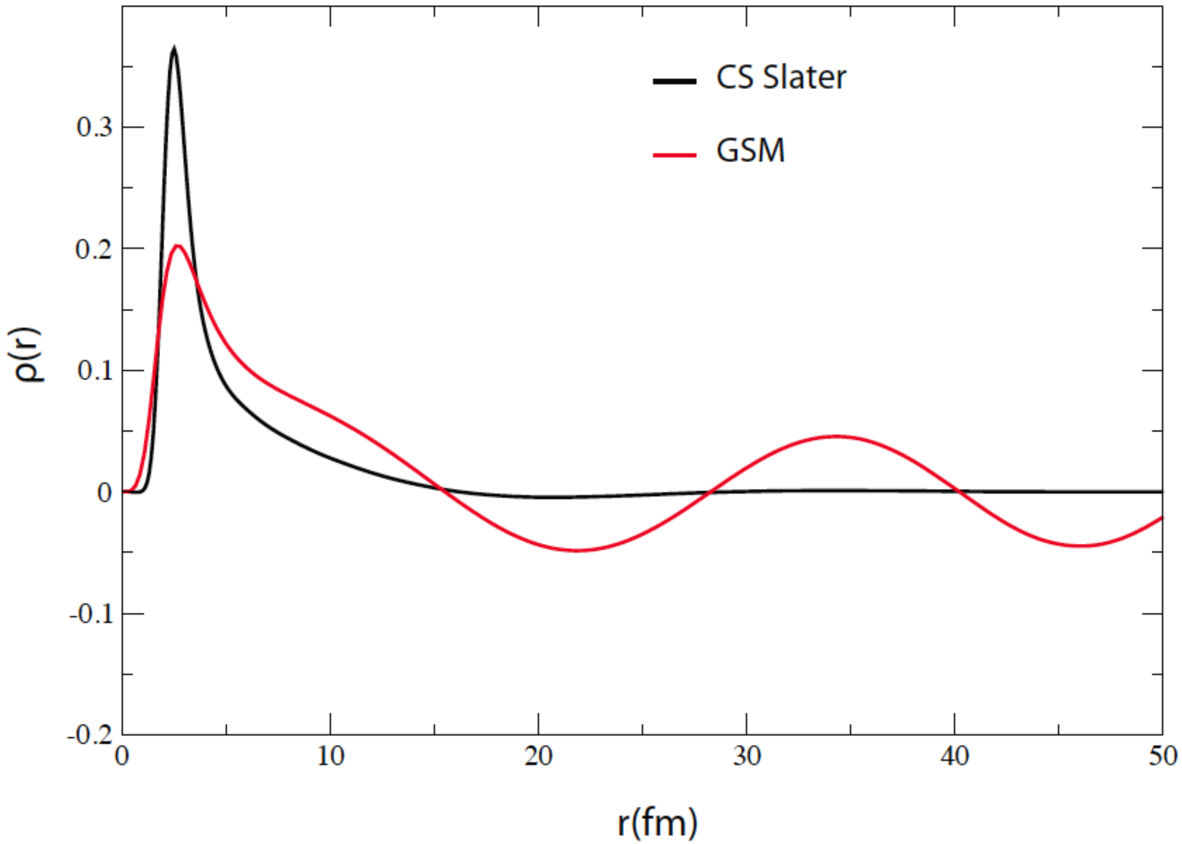
s.p. basis



V_{ij} usually a phenomelogical/schematic NN interaction, and fitted to spectra of nuclei:
Minnesota force is used, unless otherwise indicated.

Some results

2^+ first excited state in ^6He



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

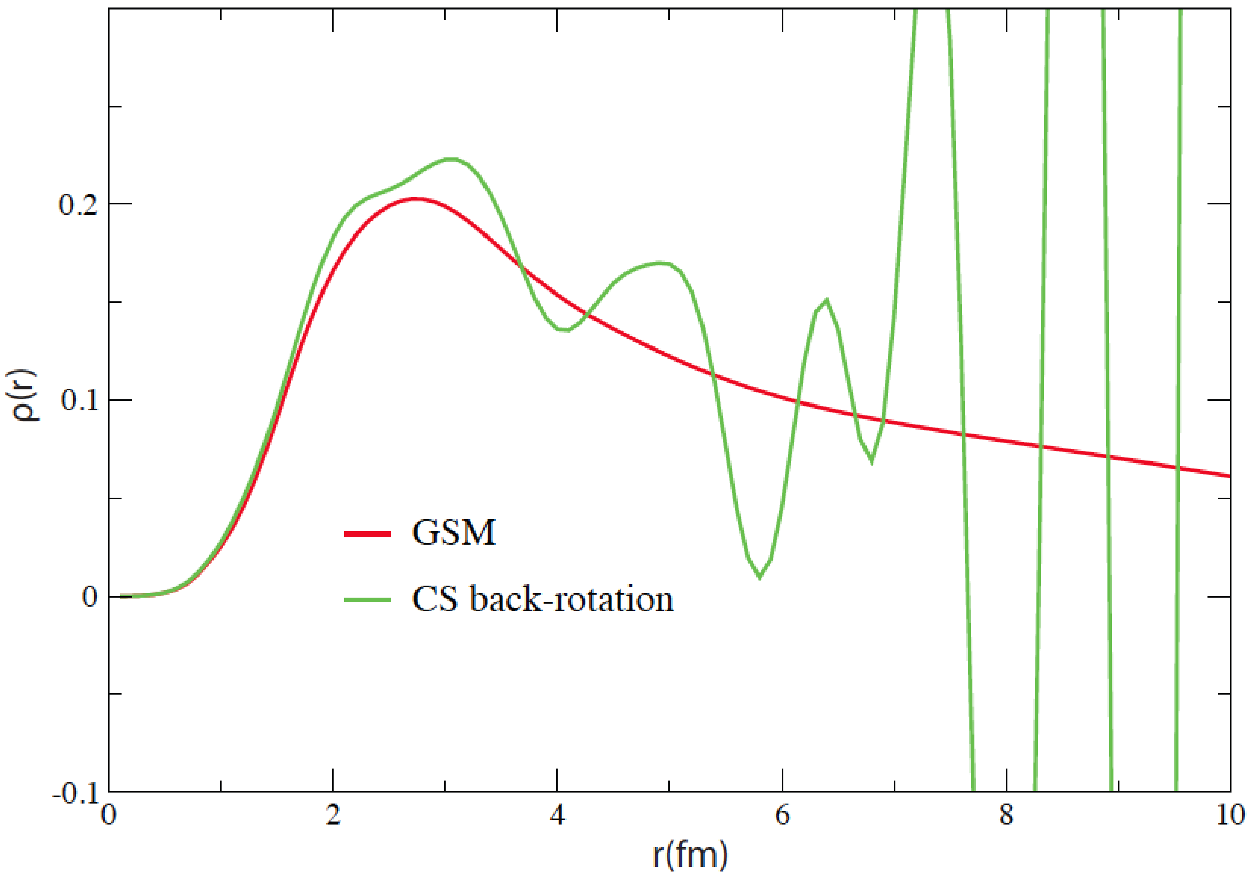
→ Perform a direct back-rotation. What is that?

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

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

In the c

$\rho(r)$ =

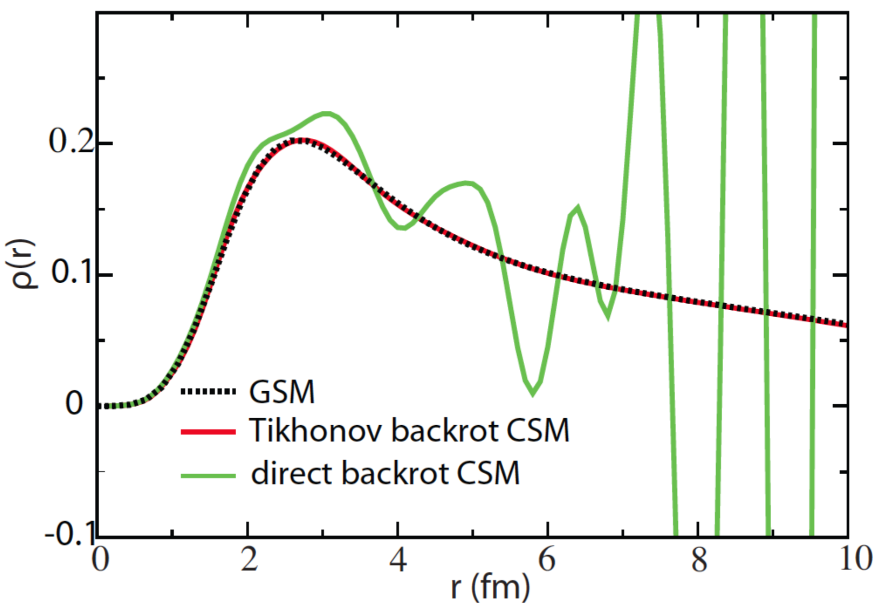


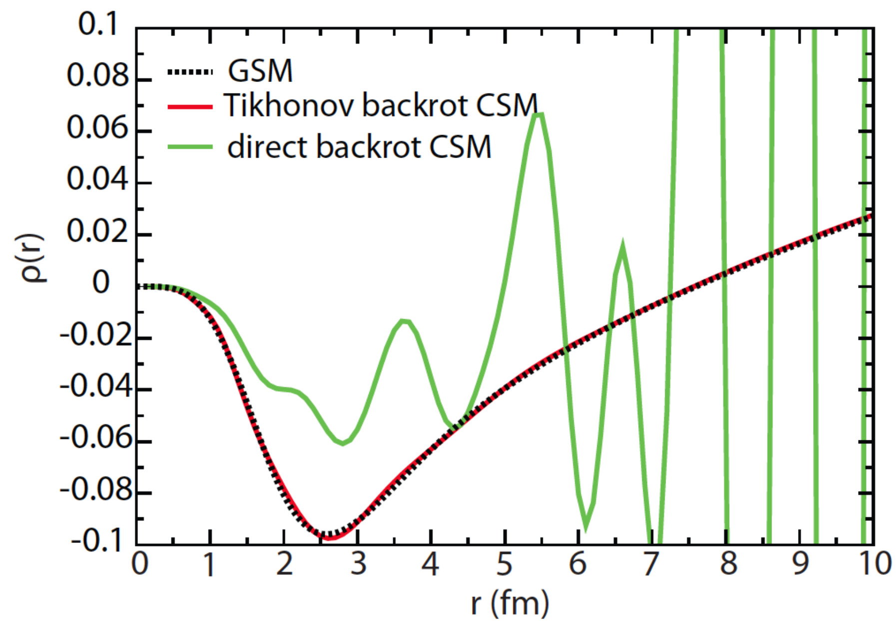
The CS density has the correct asymptotic behavior (outgoing wave)

- 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}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 (-∞,+∞)

$$f_\theta(x) = \rho_\theta(e^{-x})$$ → Now defined from (-∞,+∞)

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

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

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

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

Matrix elements of a realistic interaction in Gamow basis

$$\langle ab|V_{\mathrm{low-k}}|cd\rangle =$$

$$\langle (n_a l_a j_a t_{z_a})(n_b l_b j_b t_{z_b}) J T_z |\, V_{\mathrm{low-k}} \,| (n_c l_c j_c t_{z_c})(n_d l_d j_d t_{z_d}) J T_z \rangle$$

Latin letters denote a general Gamow (HF) basis

$$V_{\mathrm{osc}} = \sum_{\alpha \le \beta} \sum_{\gamma \le \delta} |\alpha\beta\rangle \langle \alpha\beta | V_{\mathrm{low-k}} | \gamma\delta \rangle \langle \gamma\delta |$$

Express the interaction in a HO basis (greek letters denote HO states)

$$\langle \alpha\beta | V_{\mathrm{low-k}} | \gamma\delta \rangle = \langle (n_\alpha l_\alpha j_\alpha t_{z_\alpha})(n_\beta l_\beta j_\beta t_{z_\beta}) J T_z |\, V_{\mathrm{low-k}} \,| (n_\gamma l_\gamma j_\gamma t_{z_\gamma})(n_\delta l_\delta j_\delta t_{z_\delta}) J T_z \rangle$$

Usage of Moshinksy coefficients to calculate the matrix elements

In applications we truncate the HO expansion up to Nmax oscillator quanta

PRC 73 (2006) 064307
G.Hagen et al

→ Similar treatment by Caprio, Vary, Maris in Sturmian basis

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

$$\underbrace{\langle ab|V_{\rm osc}|cd\rangle}^{\text{TBMEs in a Gamow basis}} \approx \sum_{\alpha\leq\beta}^{N}\sum_{\gamma\leq\delta}^{N}\langle ab|\alpha\beta\rangle\langle\alpha\beta|\underbrace{V_{\rm low-k}}_{\text{TBMEs in a HO basis}}|\gamma\delta\rangle\langle\gamma\delta|cd\rangle$$

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!

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

Identical particles

$$\langle ab|\alpha\beta\rangle = \langle a|\alpha\rangle\langle b|\beta\rangle$$

protons-neutrons

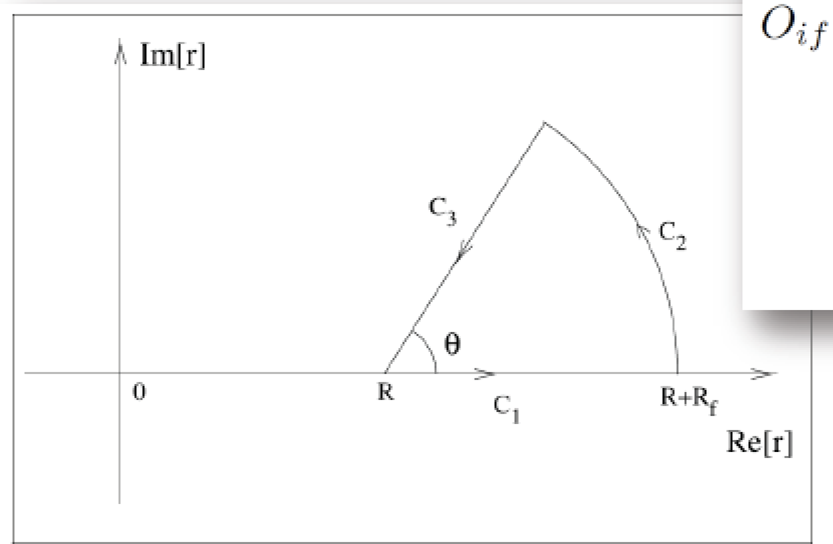
with $$\langle a|\alpha\rangle = \int d\tau\, \tau^2 \varphi_a(\tau) R_\alpha(\tau)\, \delta_{l_a l_\alpha}\delta_{j_a j_\alpha}\delta_{t_a t_\alpha}$$

Computing matrix elements with Gamow states

How can we calculate matrix elements of operators using Gamow states that are asymptotically diverging ?

$$u_n(E_n, r) \sim O_l(k_n r) \sim e^{ik_n r} \qquad k_n = \gamma_n - i\kappa_n \; (\kappa_n, \gamma_n > 0)$$

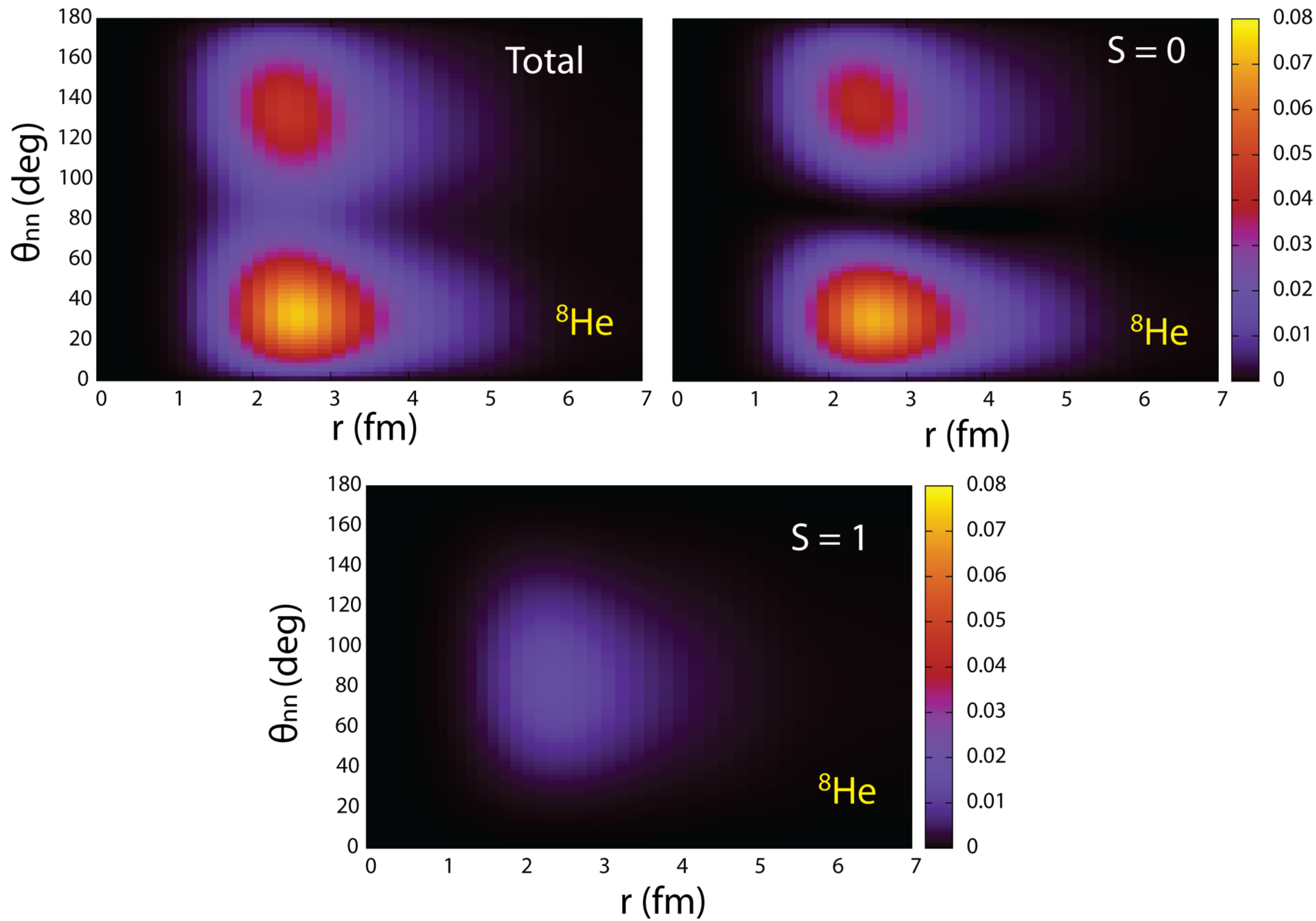
Answer: **Complex scaling!**



$$O_{if} = \int_0^R u_f(r)\, O(r)\, u_i(r)\, dr + \int_0^{+\infty} \left[u_f(R + x \cdot e^{i\theta})\, O(R + x \cdot e^{i\theta}) \times u_i(R + x \cdot e^{i\theta}) e^{i\theta}\, dx \right].$$

N. Michel Phys. Rev. C **67** 054311 (2003)

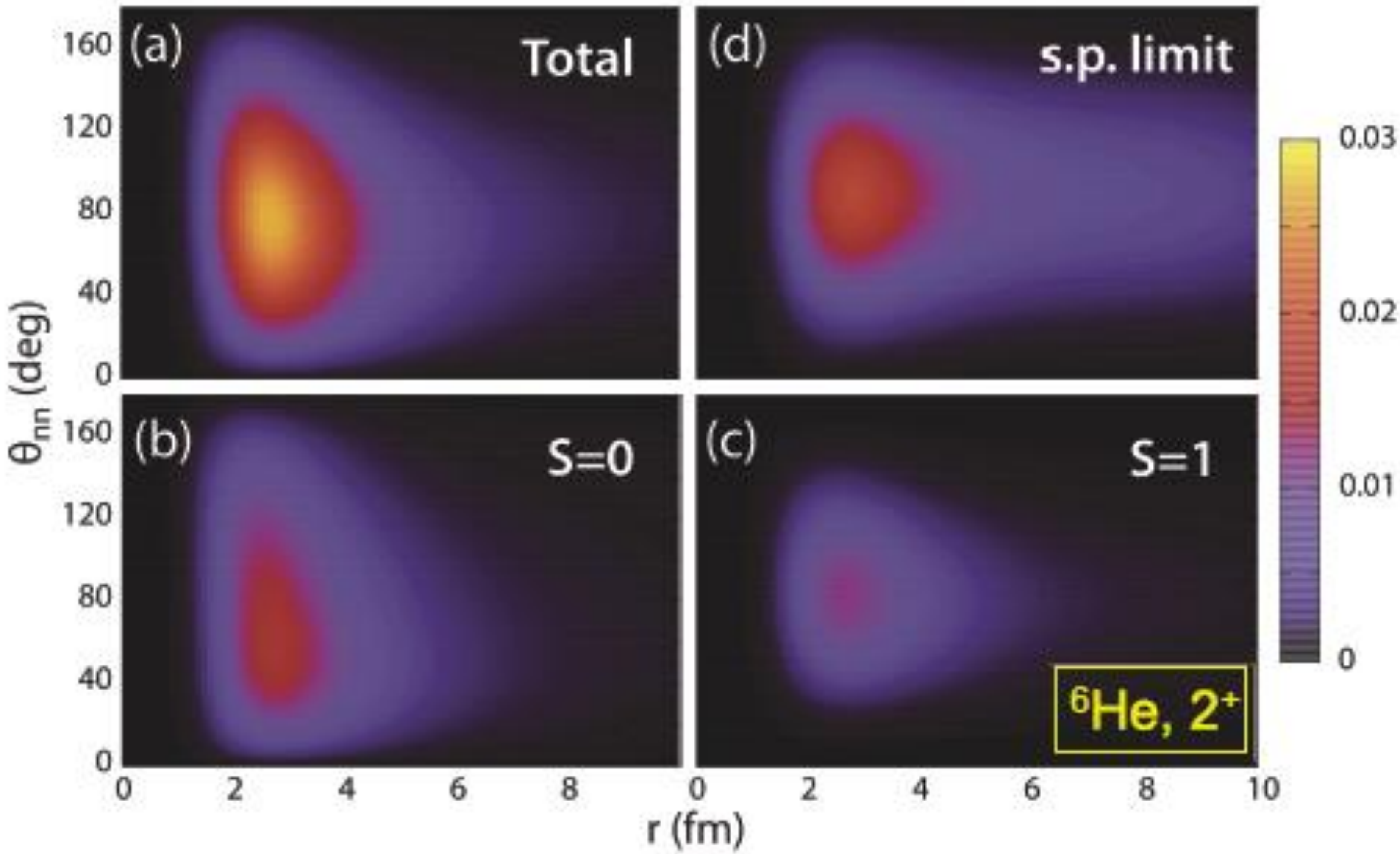
Neutron correlations in ^{8}He ground state



Neutron correlations in ^{6}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…

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

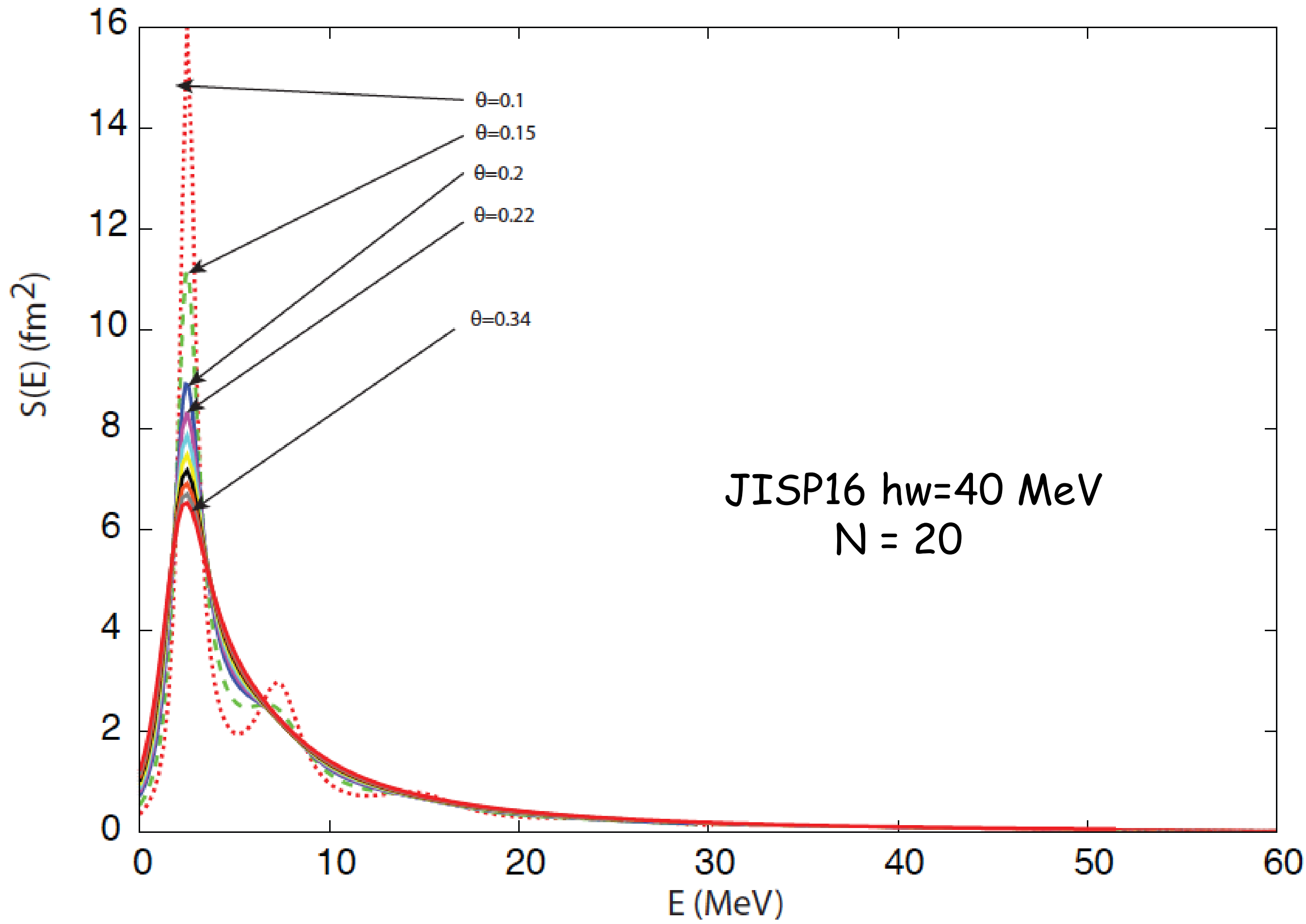
Nucleus	MFDn	NCGSM	Difference
^{2}H 1^+ ($N_{shell} = 4$)	-1.6284	-1.6284	$\leq$ 0.1 keV
^{2}H 1^+ ($N_{shell} = 8$)	-2.1419	-2.1419	$\leq$ 0.1 keV
^{3}H $1/2^+$ ($N_{shell} = 4$)	-7.6016	-7.6016	$\leq$ 0.1 keV
^{3}H $1/2^+$ ($N_{shell} = 8$)	-8.3203	-8.3203	$\leq$ 0.1 keV
^{3}He $1/2^+$ ($N_{shell} = 8$)	-7.6084	-7.6084	$\leq$ 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^2LO_{opt} ($N_{shell} = 4$)	-5.9802	-5.9806	0.4 keV
^{3}H $1/2^+$ N^2LO_{opt} ($N_{shell} = 8$)	-8.1129	-8.1132	0.3 keV
^{3}H $1/2^+$ N^2LO_{opt} ($N_{shell} = 10$)	-8.2171	-8.2174	0.3 keV

Dipole transition strength $^3S_1$-$^3D_1$ → $^3P_1$ (preliminary)



☺ Strength function is smoothing out as in the toy model potential case.
😐 Need to investigate the pattern
→ The position is not changing

More applications

→ A toy model for CS (Csoto et al PRA 41 3469, Myo et al PTP 99, 801)

- Simple Gaussian potential (attractive + repulsive)
- Supports a bound 0+ g.s
- 1- excited states resonances and continua

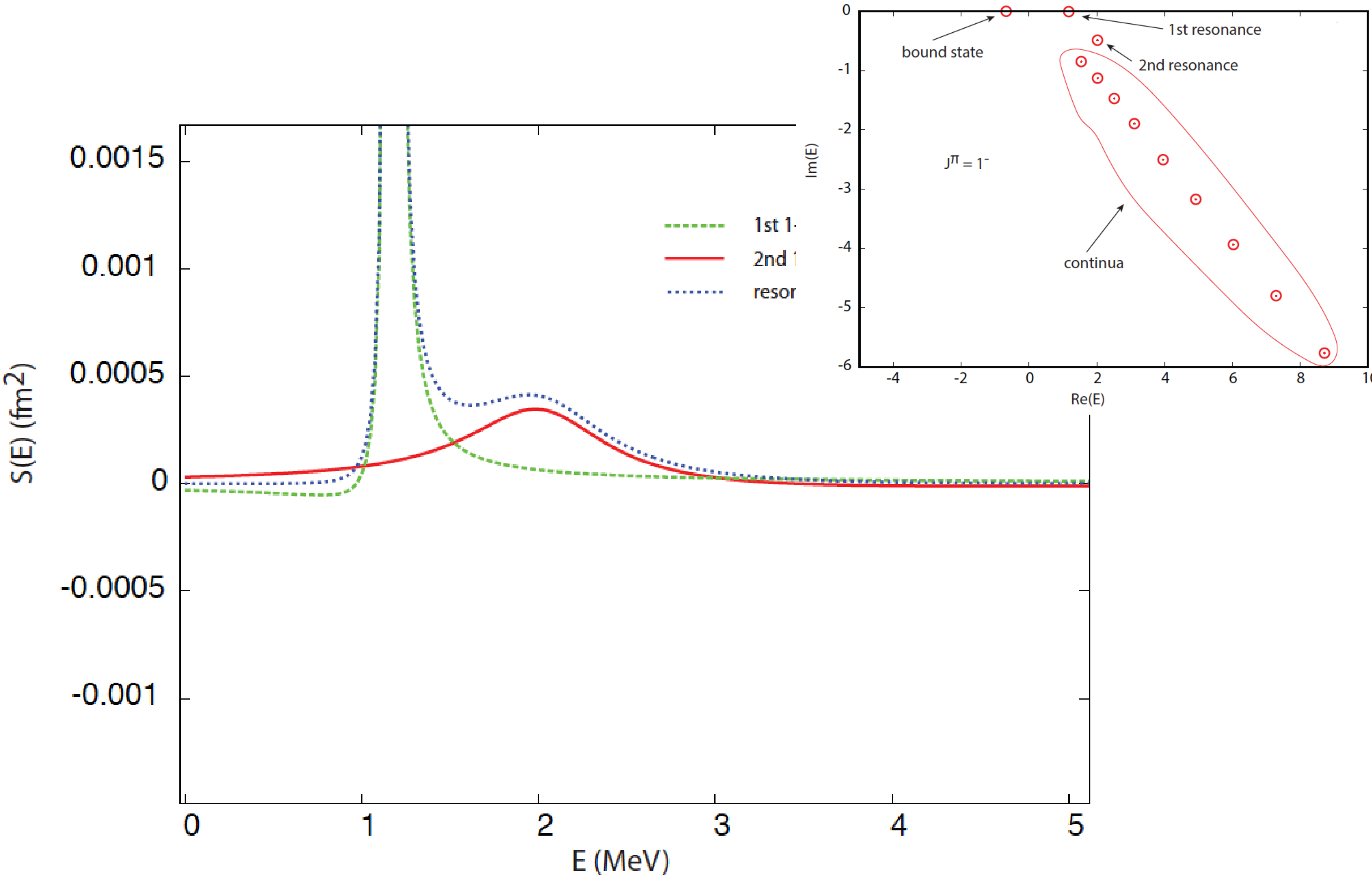
→ Study dipole transition strength from 0+ → 1- within CS

$$S_{\lambda,\nu}(E) = -\frac{1}{\pi} Im \left[\frac{\langle \tilde{\Phi}_i^\theta | O_\lambda^\theta | \Phi_\nu^\theta \rangle \langle \tilde{\Phi}_\nu^\theta | O_\lambda^\theta | \Phi_i^\theta \rangle}{E - E_\nu^\theta} \right]$$

- ✓ i is the initial state (e.g. 0+), v are the final continuum states (e.g. 1-)
- ✓ Tilde symbol is important: conjugation does not affect the radial parts (c-product)
- ✓ The decomposition is mathematically possible due to the Berggren completeness or extended completeness relation (ECR)

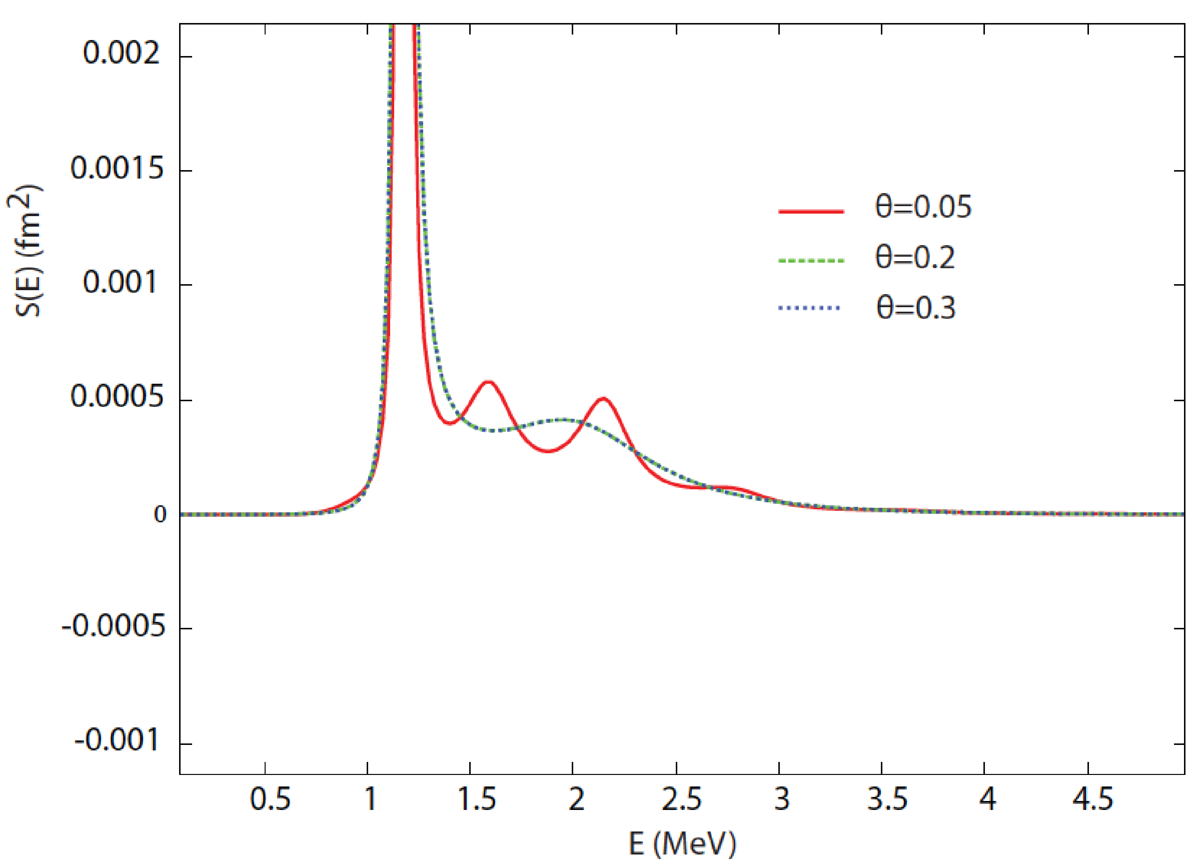
→ Decomposition of the strength function can quantify which state(s) contribute.

Decomposition of contributions to the strength function



→ Contributions from resonances and continua

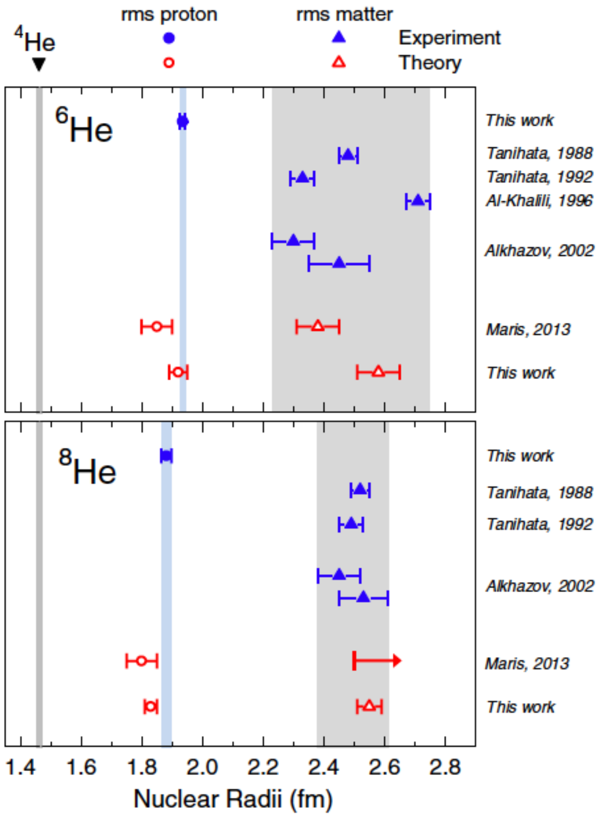
Convergence with rotation parameter θ



→ CS serves as a smoothing procedure. Need to study dependence on θ.
Already results indistinguishable for θ=0.2, 0.3

Applications → ^{6,8}He charge radii

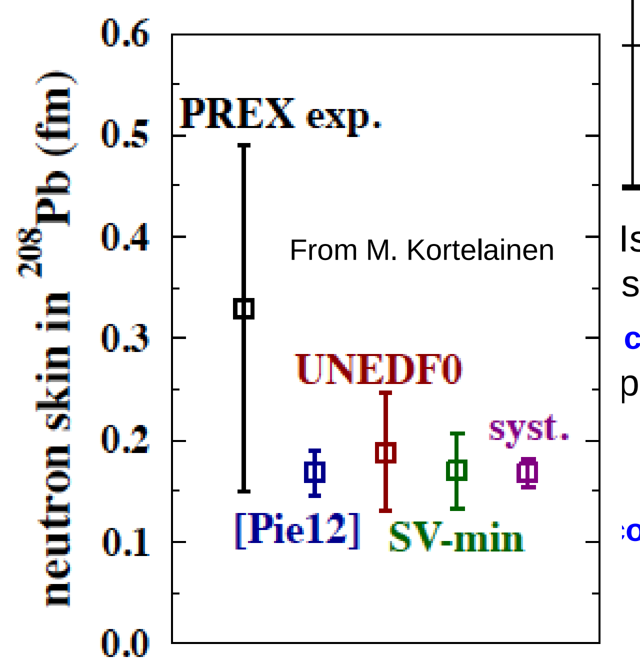
L.B.Wang *et al*, PRL **93**, 142501 (2004)
P.Mueller *et al*, PRL **99**, 252501 (2007)
M. Brodeur *et al*, PRL **108**, 052504 (2012)



Z.-T.Lu, P.Mueller, G.Drake,W.Nörtershäuser, S.C. Pieper, Z.-C.Yan
Rev.Mod.Phys. 2013, 85, (2013).
"Laser probing of neutron rich nuclei in light atoms"

RMS charge radii

	^{4}He	^{6}He	^{8}He
L.B.Wang *et al*	**1.67fm**	**2.054(18)fm**	
		2.059(7)fm	**1.959(16)fm**



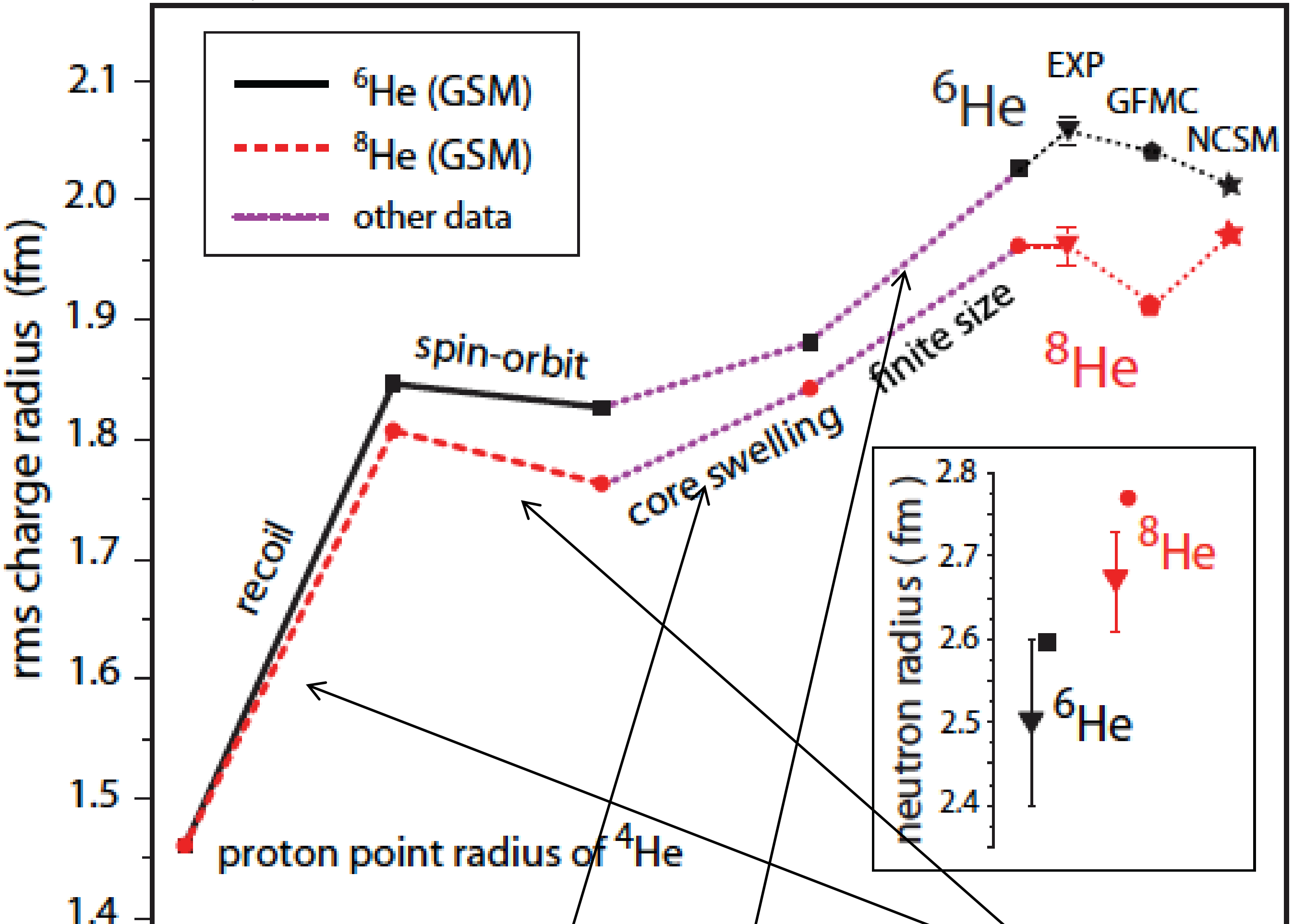
Isotopic Shifts measurements
se of this example:

cally around the

prove the nuclear Hamiltonian

:orrelations?

G. Papadimitriou et al PRC 84, 051304



^{6}He

$$\langle r^2 \rangle_{so} = -0.0718 fm^2$$

$$\langle r^2 \rangle_{so} = -0.158 fm^2$$

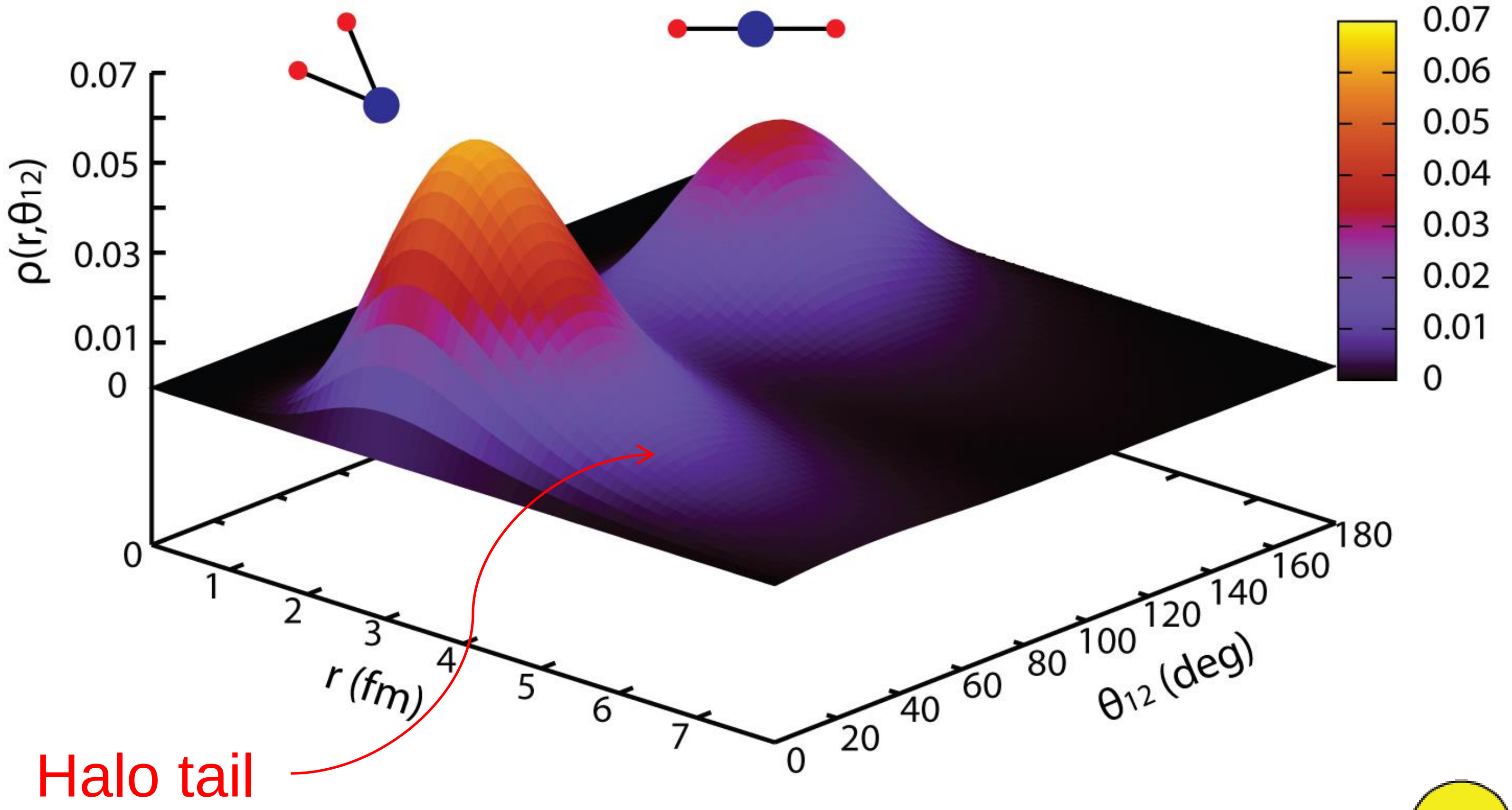
^{8}He

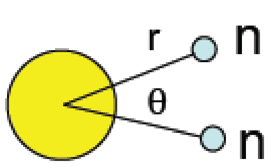
$$\left\langle r_{pp}^2\left({}^{A_C+n}X\right)\right\rangle = \boxed{\left\langle r_{pp}^2\left({}^{A_C}X\right)\right\rangle} + \boxed{\frac{1}{(A_C+n)^2}\sum_{i=1}^{n}\left\langle r_i^2\right\rangle + \frac{2}{(A_C+n)^2}\sum_{i<j}^{n}\left\langle \vec{r}_i \cdot \vec{r}_j\right\rangle}$$

$$\langle r_{ch}^2 \rangle = \langle r_{pp}^2 \rangle + \boxed{\langle R_p^2 \rangle + \frac{N}{Z}\langle R_n^2 \rangle + \frac{3}{4M_p^2}} + \boxed{\langle r^2 \rangle_{so}}$$

Neutron correlations in ^{6}He ground state

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

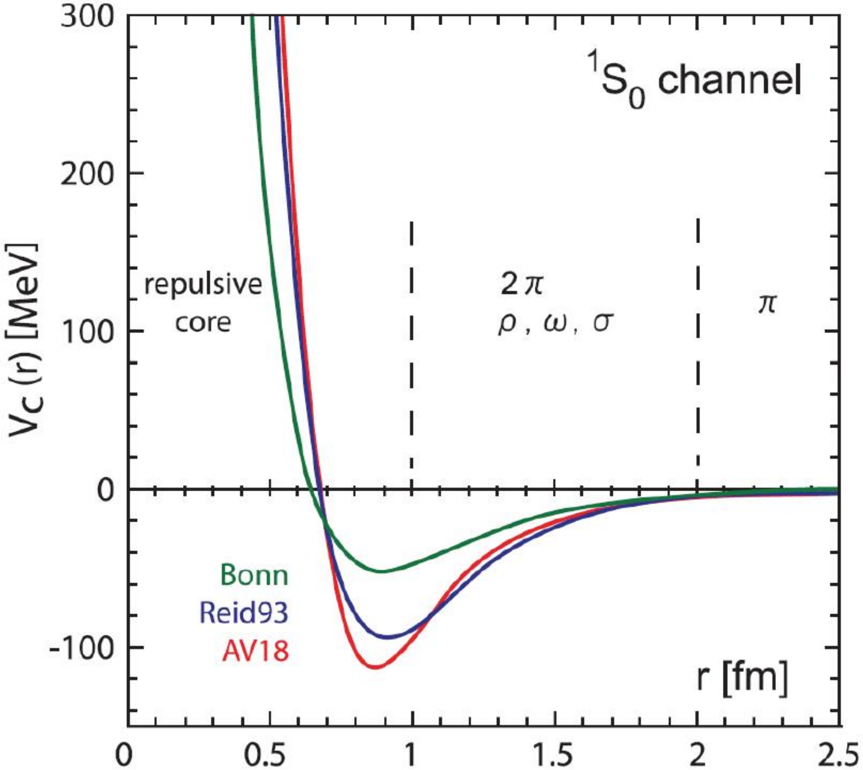




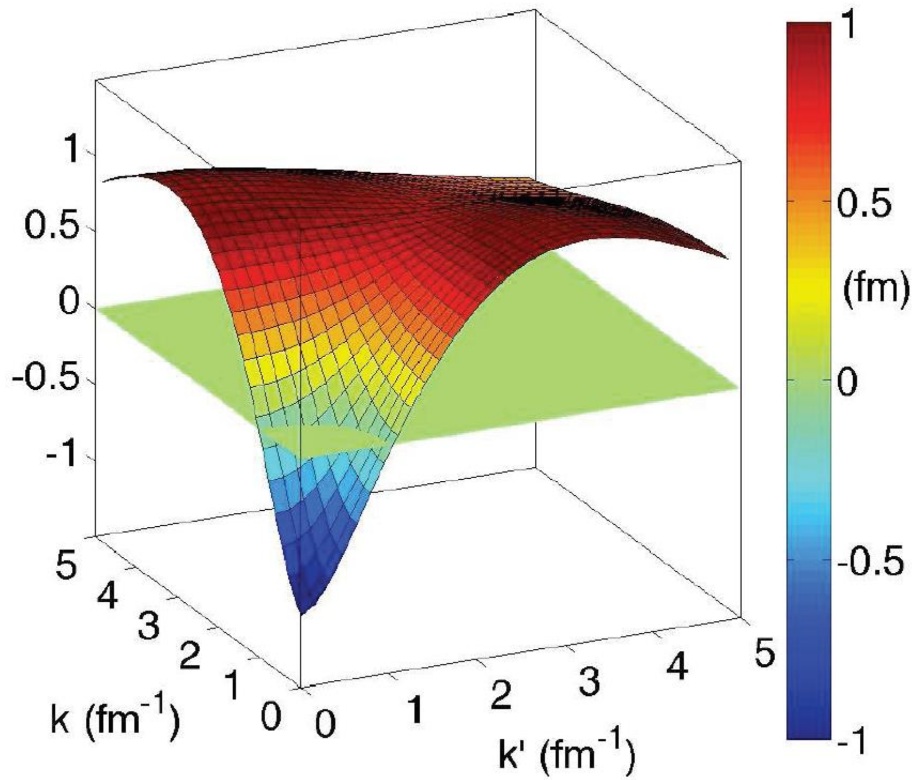
→ Probability of finding the particles at distance **r** from the core with an angle θ_{nn}

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

Realistic two-body potentials in coordinate and momentum space (Inputs)



(a)



(b)

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

Repulsive core makes calculations difficult

→ Need to decouple high/low momentum modes

✓ Achieved by V_{low-k} and/or other RG approaches (e.g. SRG, UCOM, Lee-Suzuki, G-matrix…)

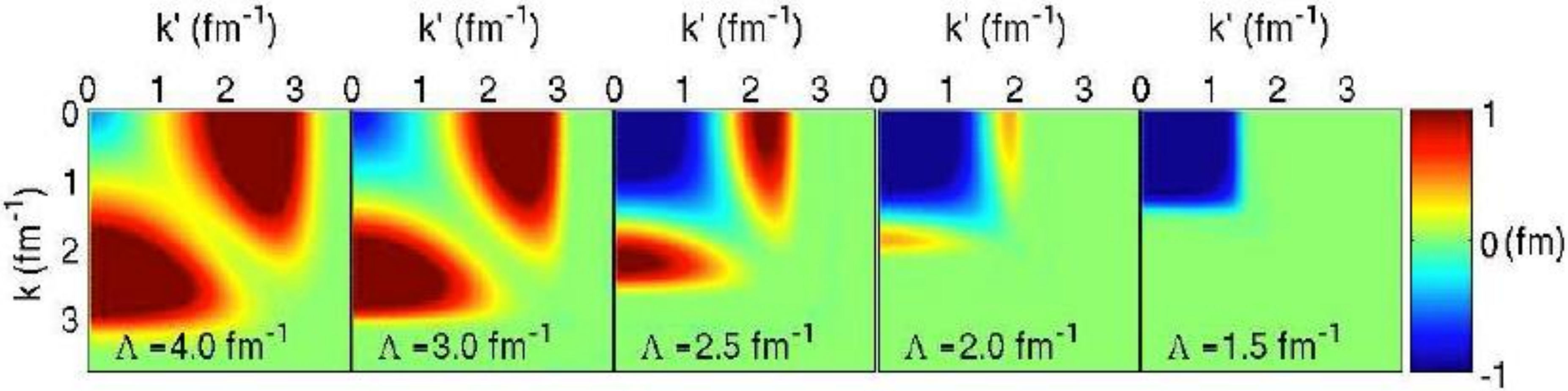
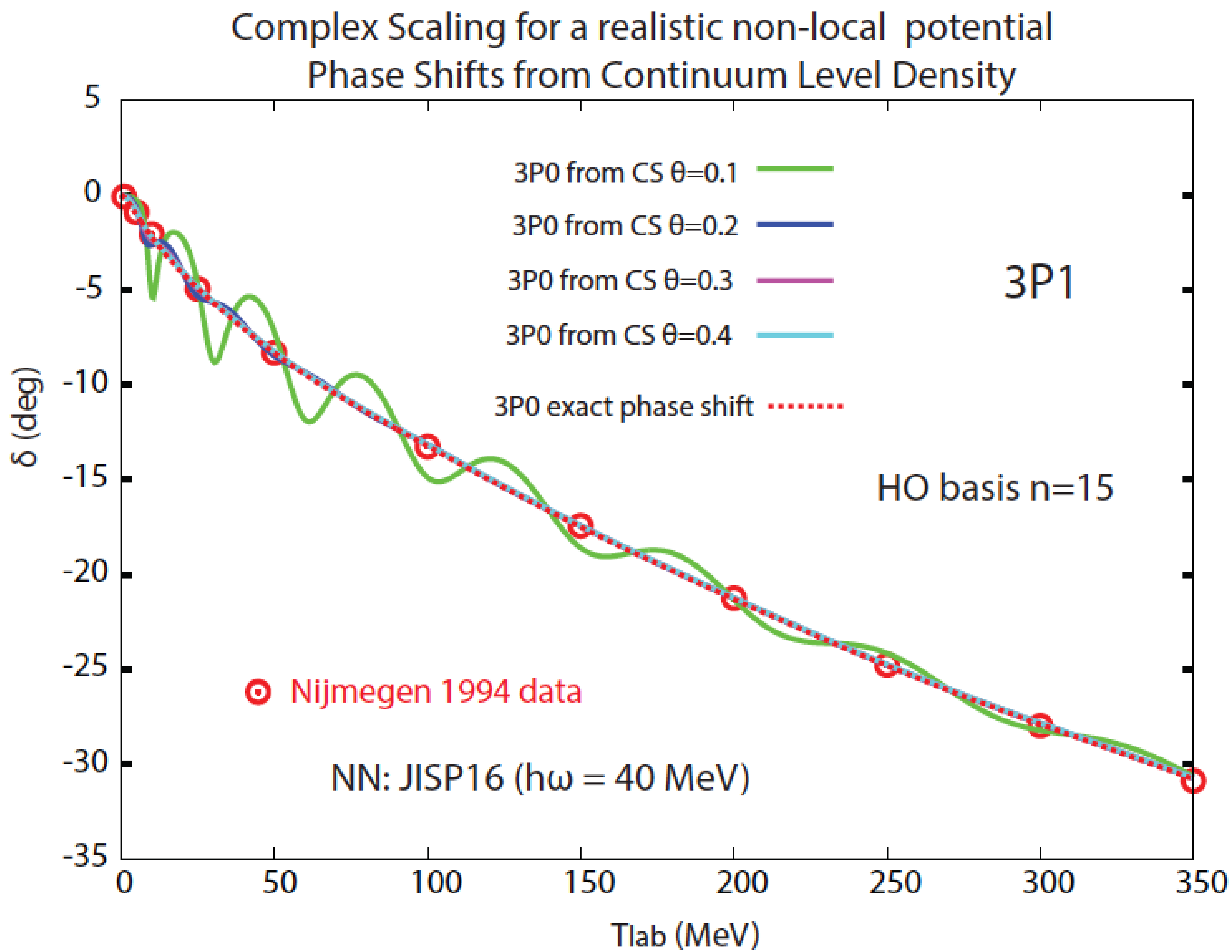


Fig. from S. Bogner et al Prog.Part.Nucl.Phys.65:94-147,2010

→ 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…

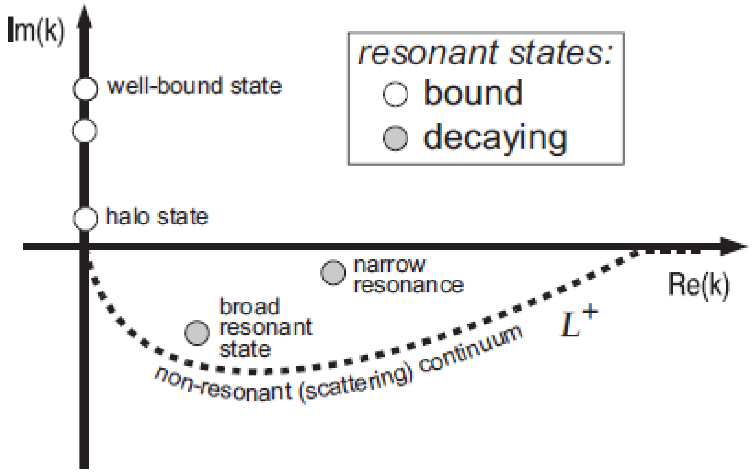


Complex Scaling for a realistic non-local potential
Phase Shifts from Continuum Level Density
3P0 from CS θ=0.1
3P0 from CS θ=0.2
3P0 from CS θ=0.3
3P0 from CS θ=0.4
3P0 exact phase shift
3P1
HO basis n=15
Nijmegen 1994 data
NN: JISP16 (hω = 40 MeV)
δ (deg)
Tlab (MeV)
5
0
-5
-10
-15
-20
-25
-30
-35
0
50
100
150
200
250
300
350

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 (bound, resonances…)

Non-resonant Continuum along the contour

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

$$\downarrow$$

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

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