Structure and Reactions of nuclei using complex energy formalisms

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Life on the edge of nuclear stability: Experimental highlights

2⁺₁ energy (keV)

• New decay modes: 2n radioactivity



A.Spyrou et al

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



- New exotic resonant states: ¹³Li, ¹⁰He,²⁶O... (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

- \rightarrow 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 Three-body models/ 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.



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, in order to 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

- \rightarrow How to obtain them?
- On the real-energy axis from the phase-shift $\delta(E)$: Position \rightarrow inflection point Width $\rightarrow 2/(d\delta/dE)|$ 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 (Hazi, Kruppa, Arai etc).
- 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

- Nuttal and Cohen PR 188, 1542 (1969)
- Lazauskas and Carbonell PRC 72 034003 (2005)
- Witala and Glöckle PRC 60 024002 (1999)
- Horiuchi, Suzuki, Arai PRC 85, 054002 (2012)
- Myo, Kikuchi, Masui, Kato Prog. Part. Nucl. Phys. 79 1 (2014)
- G.P., A.T. Kruppa et al PRC 89 014330 (2014)
- G.P., J.P. Vary PRC(R) 91, 021001 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.
- ABC theorem: Bound states and resonances invariant. Scattering and resonance states behave asymptotically as bound states.
- 2) Slater basis or Slater Type Orbitals (STOs): Basically, exponential decaying functions thresholds

 $\sum_{l_1,j_1} \sum_{l_2,j_2} \sum_{i,j=0}^{N} C_{l_1j_1l_2j_2,ij} \mathcal{A}\left(r_1^{l_1+i} r_2^{l_2+j} \exp(-ar_1 - ar_2) [\mathcal{Y}_{l_1j_1}(\hat{r}_1, s_{z_1}) \otimes \mathcal{Y}_{l_2j_2}(\hat{r}_2, s_{z_2})]^{IM}\right)$

- \rightarrow CS: Powerful method to o
- → Involves L² square integra without an implicit imposi like bound states at larhe
- \rightarrow Can (in general) be applied

Hresonant state
(hidden)in Quantum Chemistry(b)Im(E)rotated continuaIm (E)(b)Im(E)rotated continuaIrameters are obtained
Resonant states behave $H(\theta)$ resonant state
(revealed)ethods techniques
(I.e. NCSM, Faddeev, CC etc)

Some results (⁶He)

- Comparison between Complex Scaling Slater and Gamow Shell Model
- 0⁺ g.s, 2⁺ 1st excited Force Minnesota, a-n interaction KKNN

$\langle \hat{O} \rangle$	0+	GSM	$\mathrm{CS}\left(\vartheta=0\right)$	
$\langle \hat{H} \rangle$		-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	
$\left\langle \frac{\vec{p_1} \cdot \vec{p_2}}{m_3} \right\rangle$)	- 0.625	- 0.623	
\hat{O} 2 ⁺ CS ($\vartheta = \vartheta_{opt}$)			GSMI	
\hat{H}	1.	239 <i>- i</i> 0.291	1.239 - i0.292	
\hat{T}	17	.340 - i7.949	17.311 - i7.825	
V_{c-n}	-1	5.831 + i7.408	-15.805 + i7.28	
V_{nn}	-0	0.270 + i0.250	-0.267 + i0.244	

 \rightarrow Reliable calculation of widths of metastable states

Some results



Correct asymptotic behavior

More applications

 \rightarrow 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

 \rightarrow Study dipole transition strength from 0+ \rightarrow 1- within CS

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

- \checkmark 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)
- \rightarrow Decomposition of the strength function can quantify which state(s) contribute.

Decomposition of contributions to the strength function



Convergence with rotation parameter $\boldsymbol{\theta}$



 \rightarrow CS serves as a smoothing procedure

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 (351-3D1 coupled channels)
- Compute complex scaled matrix elements of the interaction
- Simple implementation: Shift CS transformation to the basis for the TBME

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

 \rightarrow Diagonalize H_{θ} with your favorite diagonalization routine



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

- \rightarrow Test is successful. Bound state position does not change after rotation.
- \rightarrow 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

 \rightarrow Connection with continuum level density (CLD)

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

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

H₀(θ) 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

Onecould check with the same Hamiltonian what each 'method' produces







Note: Similar calculation of the phase-shifts but extracted from the Busch (NPLQCD Lüscher) formula required 1800 basis states (Luu et al PRC 82 034003)

Dipole transition strength ${}^{3}S_{1} - {}^{3}D_{1} \rightarrow {}^{3}P_{1}$ (preliminary)



- © Strength function is smoothing out as in the toy model potential case.
- ☺ Need to investigate the pattern
- \rightarrow The position is not changing

Complex Scaling for structure and reactions (some comments):

- \rightarrow Doable to use realistic, non-local chiral or phenomenological potentials.
- \rightarrow **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.
- Aethod gives at the same time: widths, partial widths, position of resonances, (structure) and also reaction observables with a single diagonalization...

Another Complex Energy Method: Gamow Shell Model (see also K. Fossez talk)

Why use different basis sets for nuclei:

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

ightarrow 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 resonances as well.



Hamiltonian diagonalized

$$|\Psi\rangle = \sum_{n} c_n |SD_n\rangle$$

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



 \rightarrow 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 phenomelogical/schematic NN interaction, and fitted to spectra of nuclei:
Minnesota force is used, unless otherwise indicated.

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



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

 \rightarrow 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

Neutron correlations in ⁶He 2+ excited state



 \rightarrow 2+ neutrons almost uncorrelated...

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
 - \rightarrow All particles active (No-Core). Solve the A-body Hamiltonian.
 - → Argonne V18, (Wiringa, Stoks, Schiavilla PRC 51, 38, 1995)
 - \rightarrow N³LO (D.R.Entem and R. Machleidt PRC(R) 68, 041001, 2003)
 - → V_{lowk} technique used to decouple high/low momentum nodes. Λ_{Vlowk} = 1.9 fm⁻¹ (S. Bogner et al, Phys. Rep. 386, 1, 2003)
- Basis states

 \rightarrow s- and p- states generated by the Gamow HF or WS potential

 \rightarrow |>1 H.O states





• Diagonalization of (1) \rightarrow Applications to 4H,4Li,5H

Applications to ^{4,5}H and ⁴Li

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



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

⁴H,⁴Li:



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

Results



> Similar trend with ${}^{4}H$

Results as compared to experiment





Complex Scaling for structure and reactions (some comments):

- \rightarrow Doable to use realistic, non-local chiral or phenomenological potentials.
- \rightarrow 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.
- A 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 L² integrable functions (e.g. HO).
- \rightarrow Combine or compare with LIT for strength functions. Investigate dependence on θ vs inversion.

<u>Conclusions/Future plans</u>

- \rightarrow Complex scaling applied to non-local general realistic potentials
- → Tests on p-n system successful. Phase-shifts calculated within an L² basis.
- \rightarrow Explore CS more, strength functions etc
- → No boundary condition, HO basis (or other). 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 L² integrable basis calculations. Use together with CDCC for naturally smoothing cross-sections.
- \rightarrow Use recently developed local EFT interactions (local regulators).

Additionally calculations were shown:

- \rightarrow Gamow basis applied successfully in an ab-initio GSM framework
 - Calculations of exotic superheavy hydrogens are in the pipeline
- Calculations in Berggren basis also naturally provide widths of resonances.
- Realistic effective interactions for GSM for Oxygens → systematic improvement
- Shell Model calculations with new interactions for order-by-order assessment of error bars (NN+3N + continuum) in a CI framework

Collaborators/People affiliated with complex energy methods :

James Vary and Pieter Maris (ISU)

Nicolas Michel, Marek Płoszajczak (GANIL)

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

Andras Kruppa (Debrecen, Hungary)

Bruce Barrett (UA)

Jimmy Rotureau (ORNL/MSU)

Back up

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 (L² function)

Solution



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.



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 $(-\infty, +\infty)$

$$\begin{split} f_{\theta}(x) &= \rho_{\theta}(e^{-x}) & \rightarrow \text{Now defined from } (-\infty, +\infty) \\ f_{\theta}(\xi) &= \frac{1}{2\pi} \int_{-\infty}^{\infty} e^{-ix\xi} f_{\theta}(x) dx & \rightarrow \text{F.T} \\ f(x+iy) &= \frac{1}{2\pi} \int_{-\infty}^{\infty} e^{ix\xi} e^{-y\xi} f_{\theta}(\xi) d\xi & \rightarrow \quad \text{Value of (1) for } x+iy \\ (analytical continuation) \\ f(x+iy) &= \frac{1}{2\pi} \int_{-\infty}^{\infty} e^{ix\xi} e^{-y\xi} \frac{f_{\theta}(\xi)}{1+\alpha e^{-2y\xi}} d\xi & \rightarrow \text{Tikhonov regularization} \end{split}$$

x = -lnr , $y = \theta$

Matrix elements of a realistic interaction in Gamow basis

$$\begin{split} \langle ab|V_{\rm low-k}|cd\rangle = \\ \langle (n_a l_a j_a t_{z_a})(n_b l_b j_b t_{z_b})JT_z | V_{\rm low-k} | (n_c l_c j_c t_{z_c})(n_d l_d j_d t_{z_d})JT_z \rangle \end{split}$$

Latin letters denote a general Gamow (HF) basis

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

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

$$\langle \alpha \beta | V_{\rm low-k} | \gamma \delta \rangle = \left\langle (n_{\alpha} l_{\alpha} j_{\alpha} t_{z_{\alpha}}) (n_{\beta} l_{\beta} j_{\beta} t_{z_{\beta}}) J T_{z} \right| V_{\rm low-k} \left| (n_{\gamma} l_{\gamma} j_{\gamma} t_{z_{\gamma}}) (n_{\delta} l_{\delta} j_{\delta} t_{z_{\delta}}) J T_{z} \right\rangle$$

Usage of Moshinksy coefficients to calculate the matrix elements

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

PRC 73 (2006) 064307 G.Hagen et al

 \rightarrow 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 + 1)

$$\begin{array}{c} \text{TBMEs in a Gamow} \\ & \text{basis} \end{array} \\ & \left\langle ab \middle| V_{\text{OSC}} \middle| cd \right\rangle \approx \sum_{\alpha \leq \beta}^{N} \sum_{\gamma \leq \delta}^{N} \langle ab \middle| \alpha\beta \rangle \langle \alpha\beta \middle| V_{\text{low}-k} \middle| \gamma\delta \rangle \langle \gamma\delta \middle| cd \rangle \\ & \text{Matrix elements} \\ & \text{between Gamow States} \end{array} \\ \end{array} \\ \begin{array}{c} \text{Matrix elements} \\ \text{TBMEs in a HO} \longrightarrow \\ & \text{TBMEs in a HO} \\ & \text{basis} \end{array} \\ \end{array} \\ \begin{array}{c} \text{CD-Bonn, Av18} \\ \text{N3LO, Vlowk, SRG etc} \end{array} \\ \end{array}$$

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

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

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 ⁸He ground state



Neutron correlations in ⁶He 2+ excited state



 \rightarrow 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
$^{2}\text{H 1}^{+}$ (N _{shell} = 4)	-1.6284	-1.6284	$\leq 0.1 \text{ keV}$
$^{2}\mathrm{H}\ 1^{+}\ (\mathrm{N}_{shell}=8)$	-2.1419	-2.1419	$\leq 0.1~{\rm keV}$
${}^{3}\mathrm{H}\ 1/2^{+}\ (\mathrm{N}_{shell}=4)$	-7.6016	-7.6016	$\leq 0.1~{\rm keV}$
${}^{3}\mathrm{H}\ 1/2^{+}\ (\mathrm{N}_{shell}=8)$	-8.3203	-8.3203	$\leq 0.1~{\rm keV}$
$^{3}\text{He }1/2^{+}(N_{shell}=8)$	-7.6084	-7.6084	$\leq 0.1~{\rm keV}$
${}^{4}\text{He} \ 0^{+} \ (\text{N}_{shell} = 4)$	-27.3685	-27.3684	$0.1 \ \mathrm{keV}$
⁶ Li 1 ⁺ (N _{shell} = 4)	-24.9778	-24.9776	$0.2 \ \mathrm{keV}$
⁶ Li 3 ⁺ (N _{shell} = 4)	-22.4959	-22.4957	$0.2 { m keV}$

MFDn: Maris, Vary,... NC-GSM: Papadimitriou...

Calculations are done a pure HO basis

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







 \rightarrow 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)



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

Repulsive core makes calculations difficult

\rightarrow 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)
- \rightarrow One has to deal with "induced" many-body forces...