First results from the Gamow-NCSM

Julius Müller

Institut für Kernphysik

06.10.2022

Motivation

- Theoretical framework to describe many-body resonances
- NCSM powerful method for bound states of light nuclei
- NCSM/RGM and NCSM-C includes continuum into many-body basis
  Quaglioni et al PRL 101, 092501(2008); Baroni et al. PRL 110, 022505(2013)

- **Aim**: Include continuum in single-particle basis using Berggren basis
- **Consequence**: Complex symmetric eigenvalue problem

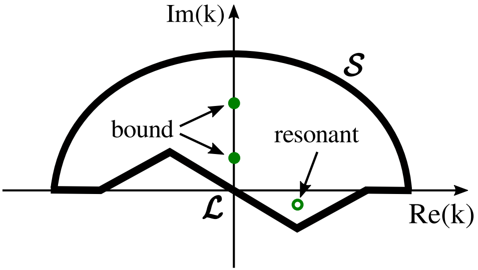
Berggren Single Particle Basis

- Find single-particle basis that includes complex continuum
- Completeness relation

$$\mathbb{1} = \sum_{\mathrm{b,r}} |u\rangle\langle\tilde{u}| + \int_{\mathcal{L}} |u(k)\rangle\langle\tilde{u}(k)|\, dk$$

- Norm in rigged Hilbert space

$$\langle\tilde{u}|u\rangle = \int u(r)^2 dr$$



Berggren Single Particle Basis

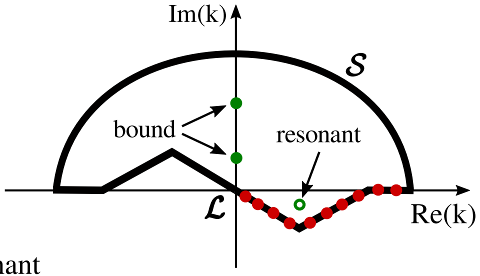
- Find single-particle basis that includes complex continuum

- Completeness relation

$$\mathbb{1} = \sum_{b,r} |u\rangle\langle\tilde{u}| + \sum_{\nu=1}^{\nu_{max}} w_\nu \, |u(k_\nu)\rangle\langle\tilde{u}(k_\nu)|$$

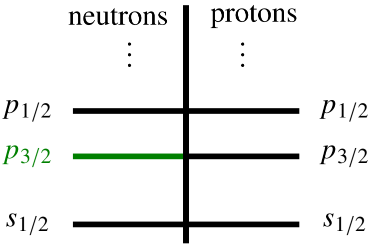
- Norm in rigged Hilbert space

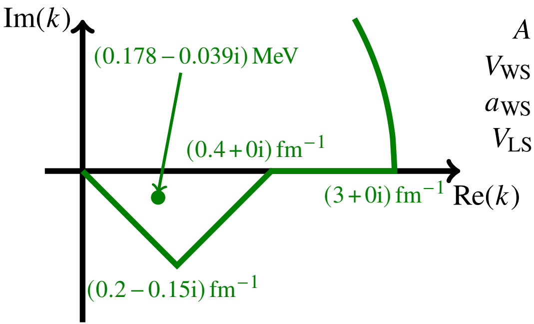
$$\langle\tilde{u}|u\rangle = \int u(r)^2 dr = \begin{cases} \delta_{\nu,\nu'}, & \text{bound/resonant} \\ w_\nu \delta_{\nu,\nu'}, & \text{scattering} \end{cases}$$



Gamow Single Particle Basis

- Setup single-particle basis for Gamow-NCSM
- Berggren basis in all partial waves creates to large model spaces
- Choose specific partial waves for Berggren basis



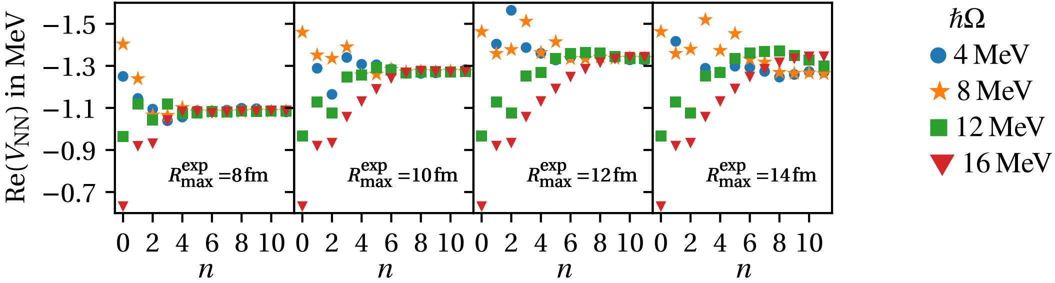


$$A = 4$$
$$V_{\mathrm{WS}} = -25\,\mathrm{MeV}$$
$$a_{\mathrm{WS}} = 0.67\,\mathrm{fm}$$
$$V_{\mathrm{LS}} = -30\,\mathrm{MeV}$$

Matrix element transformation

- Split many-body Hamiltonian in two parts $$\hat{H} = \underbrace{\hat{T}_{1b}}_{\text{exact}} + \underbrace{\hat{T}_{2b} + \hat{V}_{NN} + \cancel{\hat{V}_{3N}}}_{\text{HO approximation}}$$

- HO approximation $$\left|u_\nu^{BG}\right\rangle = \sum_{n=0}^{n_{max}} C_\nu^n \left|u_n^{HO}\right\rangle \qquad C_\nu^n = \int_0^{R_{max}^{exp}} u_\nu^{BG}(r) u_n^{HO}(r) dr$$



Gamow No Core Shell Model - Theory

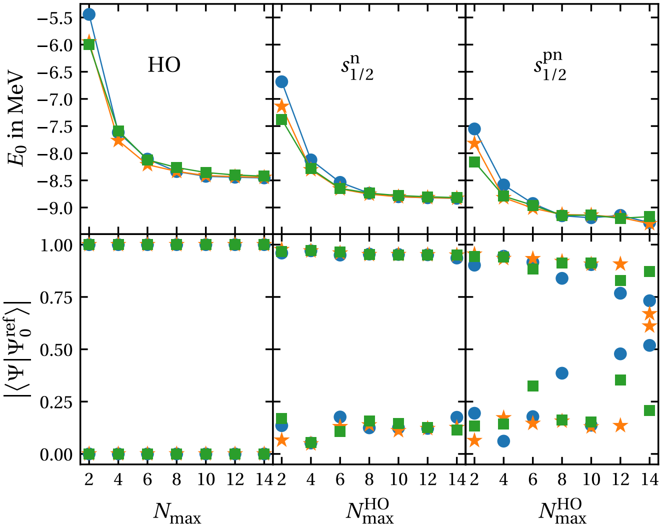
- Complex symmetric matrix eigenvalue problem

$$\sum_j \underbrace{\left\langle \phi_i \middle| \hat{H} \middle| \phi_j \right\rangle}_{\text{complex symmetric}} \left\langle \phi_j \middle| \Psi_n \right\rangle = E_n \left\langle \phi_i \middle| E_n \right\rangle$$

- Many-body truncation for HO and Berggren partial waves
  - $N_{\max}^{\text{HO}}$: maximal number of HO excitations
  - $S_{\max}$: maximal number of scattering states occupied
- Many-body resonance states indistinguishable from discretized scattering continuum
- Calculate overlap for many-body state and reference state

$$O_n = \left| \left\langle \Psi_n \middle| \Psi_0^{\text{ref}}(S_{\max} = 0) \right\rangle \right|$$

Gamow No Core Shell Model - Benchmark for ^{3}H



- Test for real scattering contour
- Instability in convergence due to degeneracy
- Different results due to non-orthonormal basis and matrix element approximation

$\hbar\Omega$

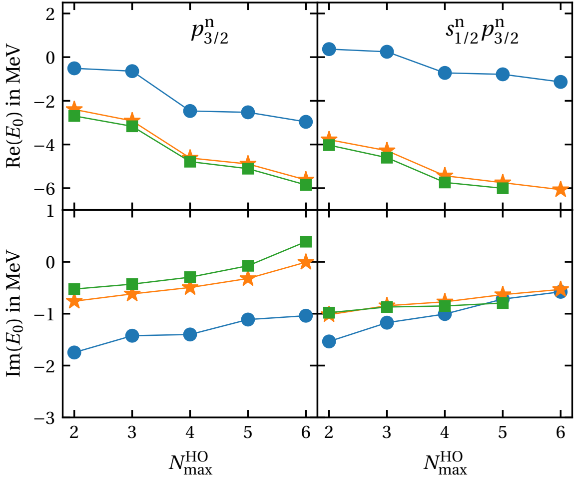
- 16 MeV
- 20 MeV
- 24 MeV

$\nu_{max} = 30$

$S_{max} = 2, 3$

NN @ N^{3}LO $\Lambda = 500$ MeV
$\alpha = 0.08\,\mathrm{fm}^4$
Entem et al. PRC 96, 024004 (2017)

Gamow No Core Shell Model - First Resonance for ^{4}H



- Include resonance and complex scattering contour
- Partial wave distribution plays a role for imaginary part

ν_{max}
- 0
- 12
- 18

$\hbar\Omega = 16\,\text{MeV}$
$S_{max} = 2$

NN @ N^{3}LO $\Lambda = 500\,\text{MeV}$
$\alpha = 0.08\,\text{fm}^4$
Entem et al. PRC 96, 024004 (2017)

Gamow No Core Shell Model 2.0 - Natural Orbitals

- Construct one-body density matrix

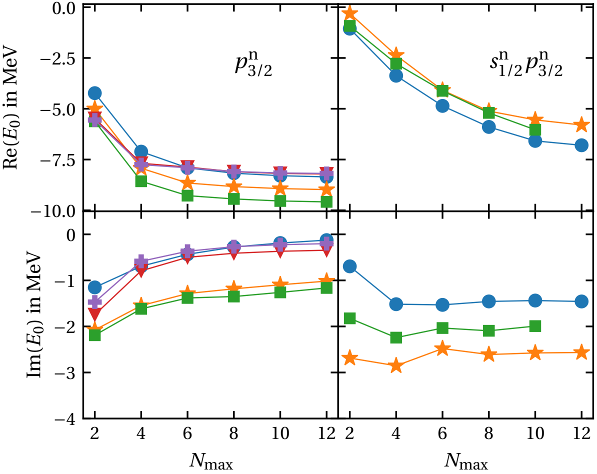
$$\rho_{ij} = \langle \Psi | \hat{a}_i^\dagger \hat{a}_j | \Psi \rangle$$

- Calculate orthonormal eigenbasis
  $\Rightarrow$ natural orbitals

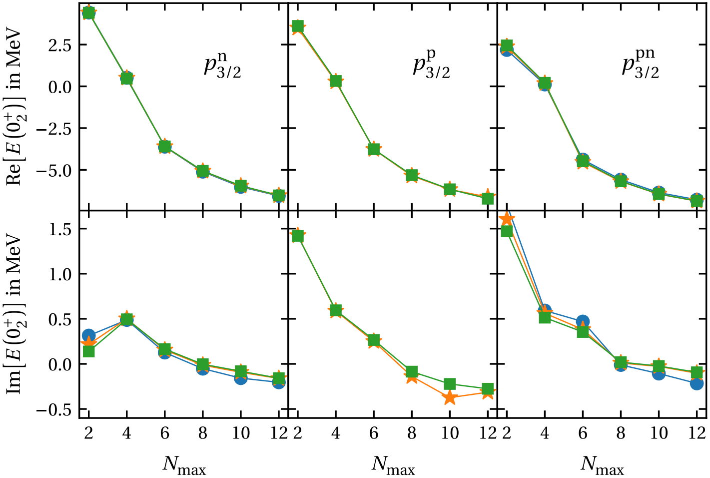
- Use only $N_{\max}$ truncation

$\hbar\Omega = 16\,\mathrm{MeV}$
$S_{\max} = 2$

$\nu_{\max}$: ● 18, ★ 21, ■ 24, ▼ 27, ✚ 30



Gamow No Core Shell Model 2.0 - ^{4}He



- Stable results for different initial Berggren partial waves

ν_{max}
- 12
- 18
- 24

$\hbar\Omega = 16\,\text{MeV}$
$S_{max} = 2, 3$

NN @ N^{3}LO $\Lambda = 500\,\text{MeV}$
$\alpha = 0.08\,\text{fm}^4$
Entem et al. PRC 96, 024004 (2017)

Summary

Setup Berggren and Gamow basis sets	⇒	- One-body potential - Partial wave distribution - Contour path
↓		
Transform nuclear matrix elements	⇒	- HO approximation - Radial cutoff
↓		
Perform Gamow-NCSM calculation	⇒	- Many-body truncations - Calculate overlap
↓		
Calculate natural orbitals	⇒	- Choose reference state
↓		
Perform NAT-Gamow-NCSM calculation	⇒	- Many-body truncation

Summary

Setup Berggren and Gamow basis sets	⇒	- One-body potential - Partial wave distribution - Contour path
↓		
Transform nuclear matrix elements	⇒	- HO approximation - Radial cutoff
↓		
Perform Gamow-NCSM calculation	⇒	- Many-body truncations - Calculate overlap
↓		
Calculate natural orbitals	⇒	- Choose reference state
↓		
Perform NAT-Gamow-NCSM calculation	⇒	- Many-body truncation

Summary

Setup Berggren and Gamow basis sets ⇒
- One-body potential
- Partial wave distribution
- Contour path

↓

Transform nuclear matrix elements ⇒
- HO approximation
- Radial cutoff

↓

Perform Gamow-NCSM calculation ⇒
- Many-body truncations
- Calculate overlap

↓

Calculate natural orbitals ⇒
- Choose reference state

↓

Perform NAT-Gamow-NCSM calculation ⇒
- Many-body truncation

Summary

Setup Berggren and Gamow basis sets	⇒	- One-body potential - Partial wave distribution - Contour path
↓		
Transform nuclear matrix elements	⇒	- HO approximation - Radial cutoff
↓		
Perform Gamow-NCSM calculation	⇒	- Many-body truncations - Calculate overlap
↓		
Calculate natural orbitals	⇒	- Choose reference state
↓		
Perform NAT-Gamow-NCSM calculation	⇒	- Many-body truncation

Summary

Setup Berggren and Gamow basis sets	⇒	- One-body potential - Partial wave distribution - Contour path
↓		
Transform nuclear matrix elements	⇒	- HO approximation - Radial cutoff
↓		
Perform Gamow-NCSM calculation	⇒	- Many-body truncations - Calculate overlap
↓		
Calculate natural orbitals	⇒	- Choose reference state
↓		
Perform NAT-Gamow-NCSM calculation	⇒	- Many-body truncation

Outlook

- Define many-body uncertainty for final results
- Analyse interaction dependence and order-by-order behavior
- Application to more interesting nuclei, e.g. ^{4}n
- Inclusion of importance-truncation scheme to optimize many-body model space

Outlook

- Define many-body uncertainty for final results
- Analyse interaction dependence and order-by-order behavior
- Application to more interesting nuclei, e.g. ^{4}n
- Inclusion of importance-truncation scheme to optimize many-body model space

Thank you for your attention!

R-Matrix Theory

- Solve single-particle Schrödinger equation for internal and external part in coordinate space

$$\hat{H}_{\text{internal}} = \hat{T} + \hat{V}_N + \hat{V}_C \qquad r < R$$
$$\hat{H}_{\text{external}} = \hat{T} + \hat{V}_C \qquad r \geq R$$

- Solve internal part on Lagrange mesh
- External part has analytical solution (Coulomb functions)
- Full wave function contained using matching conditions

Gamow No Core Shell Model - Basis dimension