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The Berggren basis for the No-Core Shell Model

by Hans Spielvogel

Outline

1. Introduction
2. Theoretical basics
3. *R*-matrix theory
4. Results
5. Summary & Outlook

Introduction

Overall goal: Describe nuclear structure, calculate observables

→ Solve Schrödinger equation

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Our goal: Enhance this model, add continuum physics explicitly to model space

Use the Berggren completeness relation

Tore Berggren, Nuc. Phys. A, 109(2), 1968

NCSM, difficulties

- Unstable or weakly bound nuclei require correct inclusion of continuum
- Properties are determined by continuum effects

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But: HO have finite range → cannot describe continuum

- Unless basis is very big
- Computational not feasible

NCSM, search for other basis

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- Basis for computation of Hamilton matrix:

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  $\rightarrow$ Need a basis with continuum included

NCSM with Berggren basis

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  $\rightarrow$ Generalization of HO-based NCSM to complex energy plane

NCSM with Berggren basis

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Berggren basis: Set of bound states, resonances and states at arbitrarily complex energy

Theoretical basics

to compute the new basis

Scattering theory and Berggren completeness relation

Scattering solutions I, Coulomb functions

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- Time-independent, two-body, radial Schrödinger equation:

$$\left(-\frac{\hbar^2}{2\mu}\frac{\mathrm{d}^2}{\mathrm{d}r^2} + \frac{\hbar^2}{2\mu}\frac{l(l+1)}{r^2} + V_N(r) + V_C(r) - E \right) u_l(r) = 0$$

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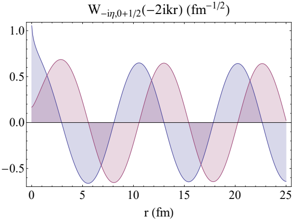
Coulomb functions:

- Special, positive energy solutions, only Coulomb potential $V_C(r)$:

$$H_l^{\pm}(kr)\propto e^{\pm i\phi_l(\eta)}W_{\mp i\eta,l+\frac{1}{2}}(\mp 2ikr)$$



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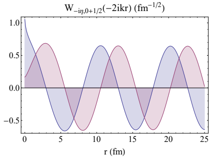

- Scattering states described by asymptotic equation ($V_N(r)=0$)

Scattering solutions II, scattering matrix

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→ General solution for scattering states:

$$u_l(k,r) \propto H_l^-(kr) - S_l(k) H_l^+(kr)$$

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  - Complex phase for positive real energies

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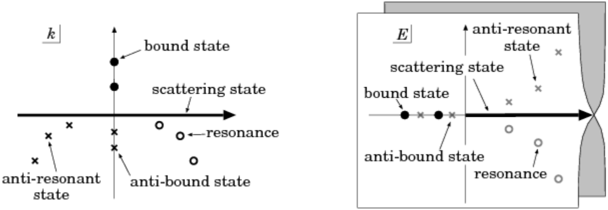

http://inspirehep.net/record/1321318/files/pole06.png

Berggren Completeness relation

- Derived from evaluating an integral in complex k plane

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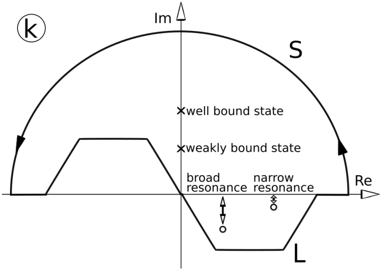

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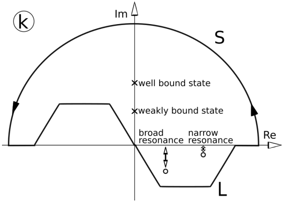

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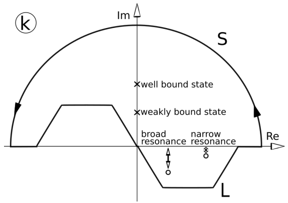

Our new basis states:

$$\hat{\mathbb{1}} = \sum_{n=b,r} |u_n\rangle \langle u_n| + \frac{1}{\pi} \int_{L^+} |u_k\rangle \langle u_k| \, dk$$

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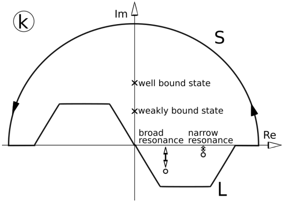

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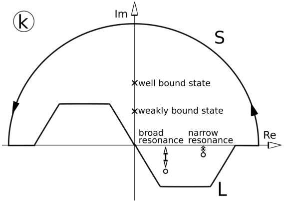

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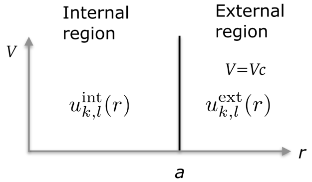
- Contour integral contains non-resonant continuum states
  - $\rightarrow$ Discretized: $\hat{\mathbb{1}} \approx \sum_{i=b,r,n} \lambda_i |u_i\rangle \langle u_i|$
  - $\rightarrow$ States need to be calculated

R-matrix theory

A technique to derive the poles and states

R-matrix theory

- Separation in internal and external region at a channel radius a



From:

Stefan Alexa,

Master's presentation

R-matrix theory

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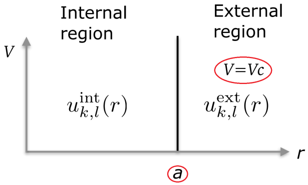

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- Wave functions:

External: General, asymptotic scattering solution with S_l:

$$u_l^{\text{ext}}(r) = \frac{i}{2} e^{-i\delta_l} [H_l^-(kr) - S_l H_l^+(kr)]$$

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  $\rightarrow$ Add Bloch operator $\mathcal{L} = \frac{\hbar^2}{2\mu}\delta(r-a)\frac{d}{dr}$

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Bloch-Schrödinger equation (B-SEQ): $(H+\mathcal{L}-E)u_l^{\text{int}} = \mathcal{L}u_l^{\text{ext}}$

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C-matrix:

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R-matrix theory III

S-matrix:

$$S_l(k) = \frac{H_l^-(ka)}{H_l^+(ka)} \frac{1 - ka \left.\frac{H_l^{-\,\prime}(kr)}{H_l^-(kr)}\right|_{r=a} R_l(k)}{1 - ka \left.\frac{H_l^{+\,\prime}(kr)}{H_l^+(kr)}\right|_{r=a} R_l(k)} = e^{2i\delta_l}$$

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Complex energies

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- States at complex energies $E = E_R - \frac{i}{2}\Gamma$ for Berggren basis
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Difficulties for wave functions:

- External wave function diverges:
- $H_l^+(kr) \propto e^{ikr}$
- $S_l(E)$ diverges at resonance
- Not a serious problem

Results

Search of poles and expansion in HO basis

Used Potential

- Woods-Saxon potential

$$V_{WS}(r) = V_0\, f(r) + \frac{1}{\hbar^2} V_{ls}\, f'(r) \frac{r_0^2}{r} \left(\hat{\vec{l}} \cdot \hat{\vec{s}}\right) + V_C(r)\, \hat{\pi}_p + \frac{\hbar^2}{2\mu} \frac{l(l+1)}{r^2}$$

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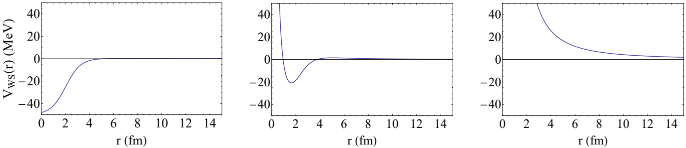
- Nucleus examined: ^{4}He



(a) $l = 0,\ j = 1/2$ (b) $l = 1,\ j = 3/2$ (c) $l = 4,\ j = 7/2$

S-matrix in complex energy plane

- Identifying resonances as S-matrix poles in complex plane

S-matrix in complex energy plane

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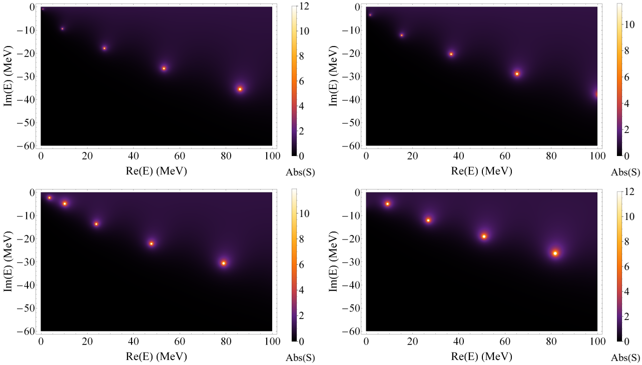
- Identifying resonances as S-matrix poles in complex plane
- Calculated on a lattice with R-matrix theory



Wave function result

- Wave functions for two resonance pole energies of $l = 0$, $j = 1/2$:

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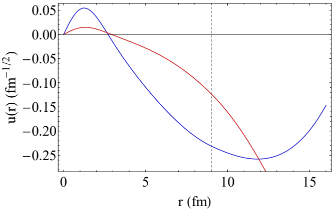
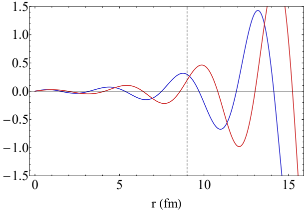


(a) $E = 0.77 - 0.95\,\mathrm{i}$ MeV



(b) $E = 53.14 - 26.62\,\mathrm{i}$ MeV

Real energy phase shifts

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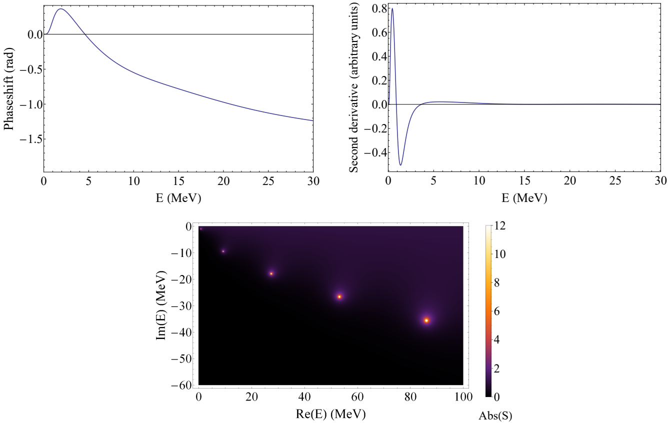
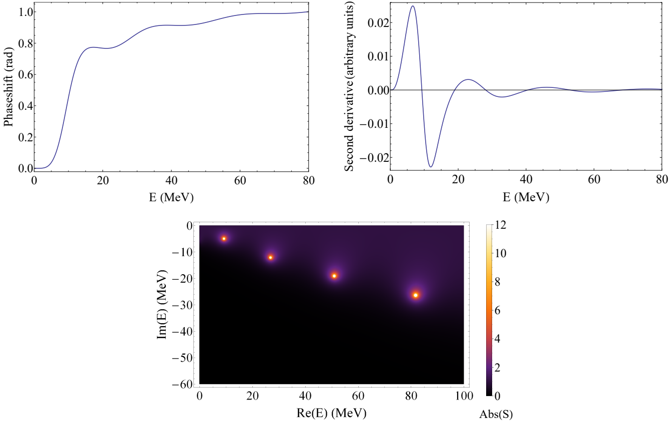
- Phase shift and second derivative for $l = 0$, $j = 1/2$



Real energy phase shifts

- Phase shift and second derivative for $l = 4$, $j = 7/2$



Real energy phase shifts

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- Phase shift and second derivative for $l = 4$, $j = 7/2$
- Unusable for precise determination of resonances

Expansion in HO functions

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- To use HO matrix elements in NCSM calculation

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Expansion integral:

$$\Phi_l^{\mathrm{BG}}(r) = \sum_{n}^{n_{\mathrm{max}}} \int_0^\infty \mathrm{d}r' \; \Phi_{l,n}^{\mathrm{HO}}(r') \Phi_l^{\mathrm{BG}}(r') \cdot \Phi_{l,n}^{\mathrm{HO}}(r)$$

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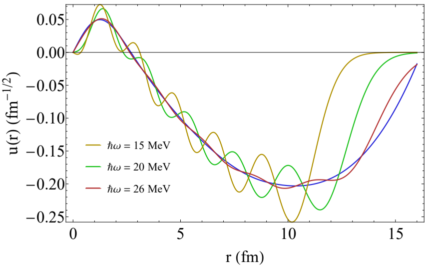

Summary and Outlook

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- R-matrix theory: Calculate the S-matrix and states at arbitrarily complex energy
- Search for resonances: S-matrix on a complex energy lattice
- Build Berggren basis out of:
  bound, resonant and non-resonant continuum states
- Use it in the NCSM to include continuum in the basis

Outlook

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- Existing implementation for NCSM usable with minor adjustments

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- Derive the Berggren basis
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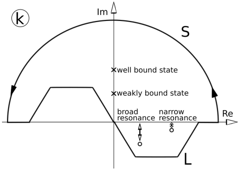
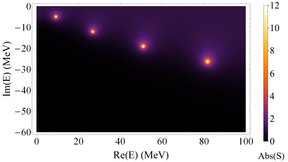
- Study truncations and convergence:
  - Different contours and number of states
  - Impact of HO expansion basis truncation





End

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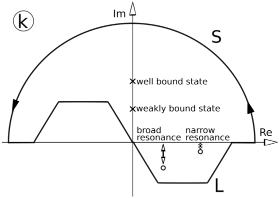
Thank you for your attention!

Appendix: Coulomb Solutions

- Differential equation:
  $$\left(\frac{d^2}{d\rho^2} - \frac{l(l+1)}{\rho^2} - \frac{2\eta}{\rho} \pm 1\right) f(\rho) = 0$$
- Scattering solutions:
  $$H_l^{\pm}(kr) = (\mp i)^l e^{\pi\eta/2 \pm i\sigma_l(\eta)} W_{\mp i\eta, l+\frac{1}{2}}(\mp 2ikr)$$
  $$F_l(kr) = \frac{1}{2i}(H_l^+(kr) - H_l^-(kr))$$
  $$G_l(kr) = \frac{1}{2}(H_l^+(kr) + H_l^-(kr))$$
  with: $\sigma_l(\eta) = \frac{1}{2i}(\ln\Gamma(1+l+i\eta) - \ln\Gamma(1+l-i\eta))$
- Bound solutions: $H_l^+(\eta, kr) = W_{-\eta, l+\frac{1}{2}}(2kr)$
  $$H_l^-(\eta, kr) = 0$$

Appendix: Completeness relation

- Unit operator: $\mathbb{1} = \sum_n |u_n\rangle \langle u_n|$
- Expand function: $|\Phi\rangle = \sum_n \langle u_n|\Phi\rangle |u_n\rangle = \sum_n c_n |u_n\rangle$
- General completeness relation:
  $\mathbb{1} = \sum_{k_n \in \mathbf{C}} |u_n\rangle \langle u_n| + \frac{1}{\pi} \int_C |v_n(k)\rangle \langle v_n(k^*)| \, dk$
- Completeness relation Berggren:
  $\mathbb{1} = \sum_{n=b,d} |u_n\rangle \langle u_n| + \frac{1}{\pi} \int_{L^+} |v_n(k)\rangle \langle v_n(k^*)| \, dk$



Appendix: Basis and C-matrix elements

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- Basis function: $\varphi_i(r) = (-1)^{N+i}\, r \sqrt{\frac{1-x_i}{a x_i}} \frac{P_N(\frac{2r}{a}-1)}{r-a x_i}$
- local potential: $\int_0^a \varphi_i(r) V_l(r) \varphi_j(r) dr = V_l(a x_i)\delta_{ij}$

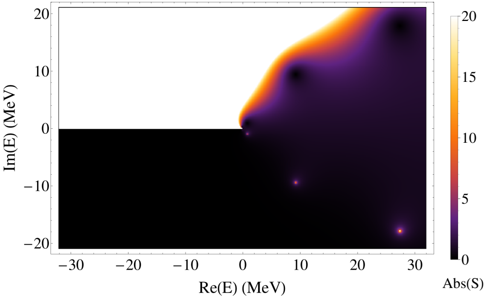
  kinetic term: $\int_0^a \varphi_i(r)(T_{l=0} + \mathcal{L}(B))\varphi_j(r) dr =$

  $i = j: \quad \frac{\hbar^2}{2\mu} \frac{1}{a^2 x_i(1-x_i)} \left(\frac{(4N^2+4N+3)x_i(1-x_i)-6x_i+1}{3x_i(1-x_i)} - B \right)$

  $i \neq j: \quad \frac{\hbar^2}{2\mu} \frac{1}{a^2\sqrt{x_i(1-x_i)x_j(1-x_j)}} \left(N^2 + N + 1 + \frac{x_i+x_j-2x_i x_j}{(x_i-x_j)^2} - \frac{1}{1-x_i} - \frac{1}{1-x_j} - B \right)$

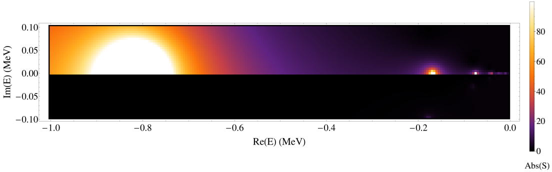
Appendix: All quadrants

Contour plot of the S-matrix for all four quadrants of the complex energy plane:



Appendix: Bound states

Contour plot of the S-matrix at the negative, real axis



Appendix: Changing potential

Contour plot of the *S*-matrix at the origin for different potential depths