Resonance properties from a calculable *R*-matrix approach

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Physics beyond the limits of stability: exploring the continuum, Villazzano, Trento, Italy, October 18th, 2016.

Introduction

Purpose

Presenting an R-matrix approach to compute resonance energies and widths

Motivation

Resonances play an important role in low-energy nuclear collisions (in scattering, capture, transfer reactions,...)

What is a resonance?

A compound nucleus characterized by some lifetime (τ) which is unstable with respect to the emission of a nucleon or a group of nucleons

Properties

- A pole of the S-matrix with complex energy

$$E = E_r - i\frac{\Gamma}{2}$$

  is associated with a resonance.

- Link between width and lifetime: $\tau \propto 1/\Gamma$

Attention!

Not all S-matrix poles correspond to resonances (bound states, virtual states, poles far from the physical axis)

Introduction

Purpose

Computing resonance energies and widths from an R-matrix approach

How?

Illustration on simple examples...

Introduction

Purpose

Computing S-matrix poles from an R-matrix approach

How?

Illustration on simple examples...

Scattering theory: single-channel case

- Radial Schrödinger equation

$$\left[-\frac{\hbar^2}{2\mu}\left(\frac{d}{dr^2}-\frac{\ell(\ell+1)}{r^2}\right)+V(r)\right]u_\ell(k,r)=Eu_\ell(k,r)=\frac{\hbar^2k^2}{2\mu}u_\ell(k,r)$$

with

$$V(r)\underset{r\to+\infty}{\longrightarrow}V_c(r)=Z_1Z_2e^2/4\pi\epsilon_0 r$$

- Boundary conditions

$$u_\ell(k,0)=0$$

$$u_\ell(k,r)\underset{r\to+\infty}{\longrightarrow}\frac{1}{v}\left[I_\ell(kr,\eta)-S_\ell(k)O_\ell(kr,\eta)\right]$$

Collision matrix

- Collision matrix computed with the R-matrix method

R-matrix

- The R-matrix approach is widely used to study scattering and reactions.

[P. Descouvemont and D. Baye, Rep. Prog. Phys. 73 (2010) 036301]
[P. G. Burke, R-Matrix Theory of Atomic Collisions, Application to Atomic, Molecular and Optical Processes, Springer Series on Atomic, Optical, and Plasma Physics, Volume 61, 2011.]

R-matrix

- The R-matrix approach is widely used to study scattering and reactions.
- This is also well suited for studying virtual and resonance states (but this is less known)

[B. I. Schneider, Phys. Rev. A 24, 1 (1981)]

R-matrix

- The R-matrix approach is widely used to study scattering and reactions.
- This is also well suited for studying virtual and resonance states (but this is less known)
- Proof in the following...

R-matrix

Internal region	External region
Expansion of u_ℓ^{int} in some basis	-Only Coulomb interaction
$\Rightarrow u_\ell^{\mathrm{int}}(k,r) = \sum_n A_{\nu n} f_n(r)$	$u_\ell^{\mathrm{ext}}(k,r) = \frac{1}{v}\left[I_\ell(kr,\eta) - S_\ell(k) O_\ell(kr,\eta)\right]$
(e.a., $[f_n(r)]$=polynomials)	

0 a r

Matching of internal and external part so that u_ℓ et $\mathrm{d}u_\ell/\mathrm{d}r$ continuous at $r = a$

S-matrix poles

$$u_\ell^{\mathrm{ext}}(k,r) = \frac{1}{v}\left[I_\ell(kr,\eta) - S_\ell(k)O_\ell(kr,\eta)\right]$$

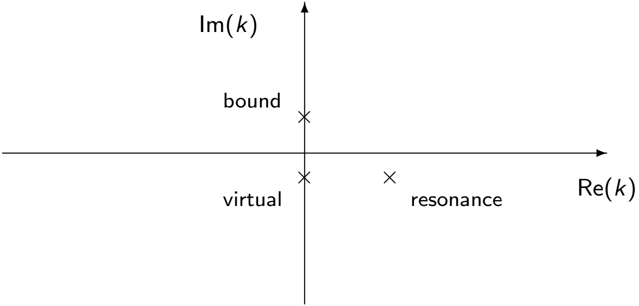
If $E = \hbar^2 k^2/2\mu$ is a pole of S_ℓ

$$\Rightarrow u_\ell^{\mathrm{ext}}(k,r) \propto O_\ell(kr,\eta) \propto e^{ikr}$$

- $k = i|k| \Rightarrow u_\ell^{\mathrm{ext}}(k,r) \propto e^{-|k|r} \Rightarrow$ bound state ($E < 0$, u_ℓ square-integrable)
- $k = -i|k| \Rightarrow u_\ell^{\mathrm{ext}}(k,r) \propto e^{|k|r} \Rightarrow$ virtual state ($E < 0$, u_ℓ diverges exponentially)
- $k = |k_R| - i|k_I| \Rightarrow u_\ell^{\mathrm{ext}}(k,r) \propto e^{i|k_R|r}e^{|k_I|r} \Rightarrow$ resonance state ($Re(E) > 0$, u_ℓ diverges exponentially, $|k_I| \ll |k_R|$)

S-matrix poles

S-matrix poles correspond to bound, virtual, and resonance states



R-matrix in equations

Radial Schrödinger equation

$$H_\ell u_\ell(r) = E u_\ell(r)$$

replaced by

$$(H_\ell + \mathcal{L}(B)) u_\ell^{int}(r) = E u_\ell^{int}(r) + \mathcal{L}(B) u_\ell^{ext}(r)$$

on the internal region

Bloch operator

=surface operator

$$\mathcal{L}(B) = \frac{\hbar^2}{2\mu} \delta(r-a) \left(\frac{d}{dr} - \frac{B}{r} \right)$$

- makes $H_\ell + \mathcal{L}(B)$ Hermitian over the internal region
- enforces the continuity $\mathrm{d}u_\ell/\mathrm{d}r$ at $r = a$

Choice of B

$$B = ka \frac{\mathrm{d}O_\ell(ka,\eta)/\mathrm{d}a}{O_\ell(ka,\eta)} \Rightarrow \mathcal{L}(B) u_\ell^{ext}(r) = 0$$

R-matrix in equations

Bloch-Schrödinger equation

$$(H_\ell + \mathcal{L}(B))u_\ell^{\mathrm{int}}(r) = E u_\ell^{int}(r)$$

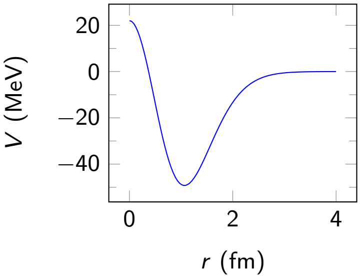
- Expansion of $u_\ell^{\mathrm{int}}(r)$ into some discrete basis
- $\Rightarrow$ Eigenvalue problem to solve

Comments

- The complex component in $H_\ell + \mathcal{L}(B)$ comes only from B
- B is energy-dependent $\Rightarrow$ iterations needed (typically, $\approx$10-100))
- The eigenvalue is real or complex and is a pole of the S-matrix
- $\Rightarrow$ the method provides as well bound-, virtual-, or resonance-state energies

Bound state

Minnesota potential $J^{\pi}ST = 1^{+}10$



Deuteron energy (MeV)

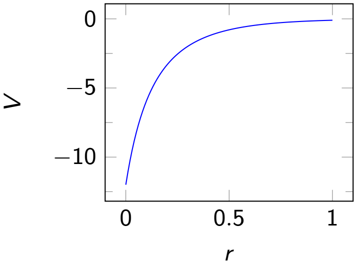
a=channel radius

N=number of basis functions

$N\backslash a$ (fm)	8	10
10	-2.4	-2.0
20	-2.20173	-2.202
30	-2.201763435	-2.20176342
40	-2.201763433	-2.201763433

Virtual state

Bargmann potential



$$V(r) = -\frac{16}{3}\frac{e^{-4r}}{(1+e^{-4r}/3)^2}$$

Virtual energy

a=5 ;N=20

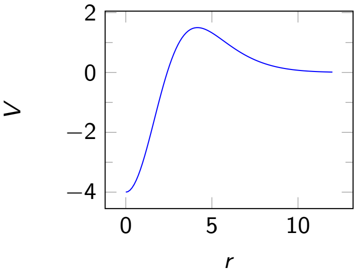
exact	approx.
-0.5	-0.50008

Comment

Iterative process less stable than for bound-state research!

Resonance state

Double Gausian potential



$$V(r) = -8e^{-0.16r^2} + 4e^{-0.04r^2}$$

CSM results from [D. Baye, Phys. Rep. 565 (2015) 1]

	Re(E)	Im(E)
this work	1.1710425	-4.864$\times 10^{-3}$
CSM	1.171041	-4.864$\times 10^{-3}$
this work	2.0175	-0.4864
CSM	2.017498	-0.486300

Outlook

- An *ab initio* approach: the no-core shell model with continuum
- $\alpha + {}^{3}\mathrm{He}$
- ${}^{8}\mathrm{Be} + n$

Starting point

Microscopic Schrödinger equation

$$\Big(\sum_{i=1}^{A} \frac{p_i^2}{2m_N} + \sum_{i>j=1}^{A} v_{ij} + \sum_{i>j>k=1}^{A} v_{ijk} - T_{\mathrm{c.m.}}\Big)|\Psi_A^{J^\pi T}\rangle = E|\Psi_A^{J^\pi T}\rangle$$

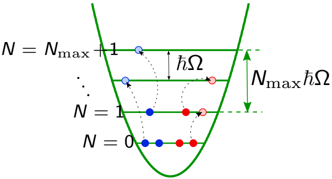
kinetic energy of nucleon i

chiral NN (+3N) interactions typically softened by the similarity renormalization group method to facilitate convergence

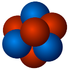
No-core shell model with continuum w.f.

D. R. Entem and R. Machleidt, Phys. Rev. C 68, 041001 (2003)
P. Navrátil, Few-Body Syst. 41, 117 (2007)

S. K. Bogner, R. J. Furnstahl, and R. J. Perry, Phys. Rev. C 75, 061001 (2007)



No-core shell model (NCSM)

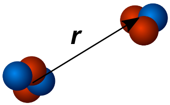


- Slater determinants of harmonic oscillator functions
- Exact c.m. factorization
- Short- and medium-range correlations
- Bound-state method

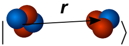
$$|\Psi_A^{J^\pi T}\rangle = \sum_\lambda c_\lambda^{J\pi T} \underbrace{|\;\rangle}_{NCSM}$$

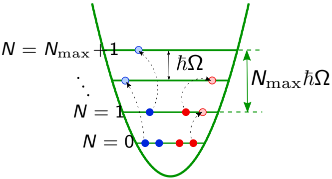
+NCSM/resonating group method (RGM)

- NCSM cluster wave functions
- Long-range correlations
- Bound and scattering states; reactions



$$|\Psi_A^{J^\pi T}\rangle = \sum_\nu \int dr\; r^2\, \frac{\gamma_\nu^{J\pi T}(r)}{r}\, \mathcal{A}_\nu \underbrace{|\qquad\qquad\rangle}_{NCSM/RGM}$$





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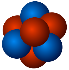

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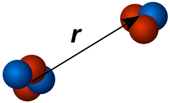
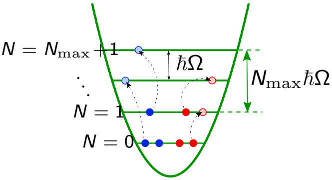


= No-core shell model with continuum (NCSMC)

[S. Baroni, P. Navratil, and S. Quaglioni, PRL 110, 022505 (2013); PRC 87, 034326 (2013).]

$$|\Psi_A^{J^\pi T}\rangle = \sum_\lambda c_\lambda^{J\pi T} \underbrace{|\quad\rangle}_{NCSM} + \sum_\nu \int dr\; r^2 \frac{\gamma_\nu^{J\pi T}(r)}{r} \mathcal{A}_\nu \underbrace{|\quad \overset{\boldsymbol{r}}{\longrightarrow} \quad\rangle}_{NCSM/RGM}$$



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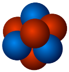

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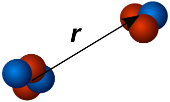

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unknowns

NCSMC equations

$$|\Psi_A^{J^\pi T}\rangle = \sum_\lambda \underbrace{c_\lambda^{J\pi T}}_{unknown} |\ \rangle + \sum_\nu \int dr\ r^2 \underbrace{\frac{\gamma_\nu^{J\pi T}(r)}{r}}_{unknown} \mathcal{A}_\nu | \xrightarrow{r} \rangle$$

- Variational amplitudes ($c_\lambda^{J\pi T}$ and $\gamma_\nu^{J\pi T}$) obtained by solving the NCSMC equations

$$\begin{pmatrix} E_\lambda \delta_{\lambda\lambda'} & \langle\ |H\mathcal{A}_\nu| \xrightarrow{r} \rangle \\ \langle \xrightarrow{r} |\mathcal{A}_{\nu'} H|\ \rangle & \langle \xrightarrow{r} |\mathcal{A}_{\nu'} H \mathcal{A}_\nu| \xrightarrow{r} \rangle \end{pmatrix} \begin{pmatrix} c \\ \gamma \end{pmatrix} = E \begin{pmatrix} \delta_{\lambda\lambda'} & \langle\ |\mathcal{A}_\nu| \xrightarrow{r} \rangle \\ \langle \xrightarrow{r} |\mathcal{A}_{\nu'}|\ \rangle & \langle \xrightarrow{r} |\mathcal{A}_{\nu'} \mathcal{A}_\nu| \xrightarrow{r} \rangle \end{pmatrix} \begin{pmatrix} c \\ \gamma \end{pmatrix}$$

- Most challenging: calculation of kernels (mostly due to $\mathcal{A}_\nu$)
- NCSMC equations solved with the microscopic R-matrix method (MRM) on a Lagrange mesh

[M. Hesse, J.-M. Sparenberg, F. Van Raemdonck, and D. Baye, Nucl. Phys. A 640, 37 (1998)]

MRM on a Lagrange mesh

Internal region

Microscopic description

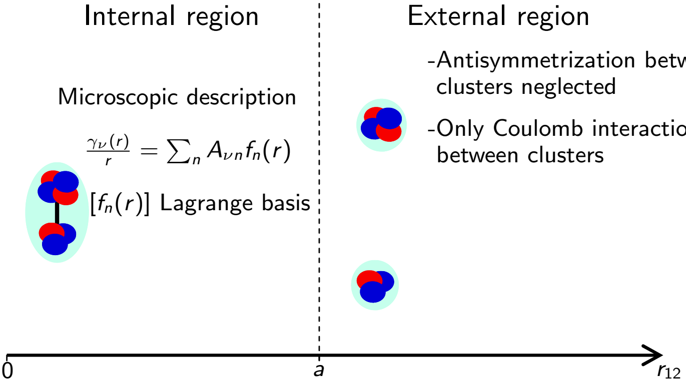
$\frac{\gamma_\nu(r)}{r} = \sum_n A_{\nu n} f_n(r)$

$[f_n(r)]$ Lagrange basis

External region

-Antisymmetrization between clusters neglected

-Only Coulomb interaction between clusters



[D. Baye, P.-H. Heenen, and M. Libert-Heinemann, Nucl. Phys. A 291 (1977) 230]

[M. Hesse, J.-M. Sparenberg, F. Van Raemdonck, and D. Baye, Nucl. Phys. A 640, 37 (1998)]

[P. Descouvemont and D. Baye, Rep. Prog. Phys. 73 (2010) 036301]

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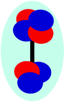


$[f_n(r)]$ Lagrange basis

External region

-Antisymmetrization between clusters neglected

-Only Coulomb interaction between clusters

$\Rightarrow \gamma_\nu(r) \propto C_\nu W(k_\nu r)$ (closed channels)

$\propto O_\nu(k_\nu r)$ (open channels)

0 $\qquad a \qquad r_{12}$

[D. Baye, P.-H. Heenen, and M. Libert-Heinemann, Nucl. Phys. A 291 (1977) 230]

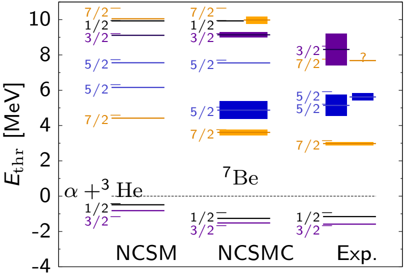
[M. Hesse, J.-M. Sparenberg, F. Van Raemdonck, and D. Baye, Nucl. Phys. A 640, 37 (1998)]

[P. Descouvemont and D. Baye, Rep. Prog. Phys. 73 (2010) 036301]

Applications

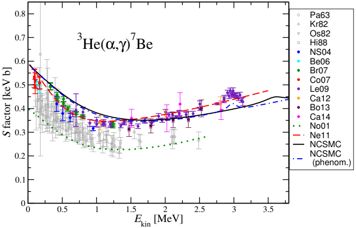
- $\alpha + N$
- $\alpha + {}^3\mathrm{He}/{}^3\mathrm{H}$
- ${}^{10}\mathrm{Be} + n$
- ${}^{8}\mathrm{Be} + n$
- $\ldots$

$\alpha + {}^3\mathrm{He}$



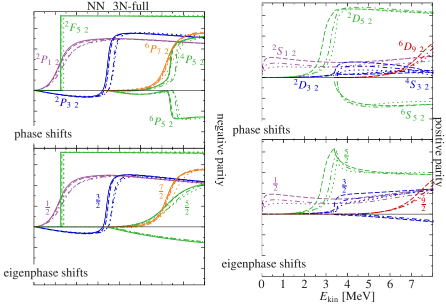
Impact of the 7/2− resonance on the astrophysical

S factor



[JDE *et al.*, Phys. Lett. B 757 (2016) 430]

^{8}Be + n: New analysis in progress



[J. Langhammer *et al*,, Phys. Rev. C 91, 021301(R)]

Previous resonance analysis from the phase-shift inflexion point

^{9}Be states	NCSMC E_R [MeV]	NCSMC Γ [MeV]	experiment E_R [MeV]	experiment Γ [MeV]
$\frac{1}{2}^+$	0.012	0.09	0.019	0.22
$\frac{5}{2}^+$	2.85	0.41	1.38	0.28
$\frac{3}{2}^+$	3.39	0.17	3.03	0.74
$\frac{9}{2}^+$	7.48	2.25	5.09	1.33
$\frac{3}{2}^-$	-1.367	-	-1.66	-
$\frac{1}{2}^-$	1.15	0.95	1.11	1.08
$\frac{5}{2}^-$	1.25	0.02 keV	0.76	0.78 keV
$\frac{3}{2}^-$	3.4	0.26	3.92	1.33
$\frac{5}{2}^-$	6.21	2.22	6.27	1.0
$\frac{7}{2}^-$	6.21	0.84	4.71	1.21

Conclusions

- The R-matrix approach is a powerful method to compute the poles of the S-matrix close to the physical axis
- For broad resonances, more justified and reliable than an extraction from the phase shifts.
- For narrow resonances, more efficient than an extraction from the phase shifts.
- The R-matrix approach allows a correct interpretation/analysis of the neutral s-wave "resonances"

Conclusions

The R-matrix approach is a unified approach to describe bound, scattering, resonance, and virtual states!

Collaborators

In alphabetic order

- A. Calci (TRIUMF)
- W. Horiuchi (Hokkaido U.)
- G. Hupin (CEA)
- P. Navrátil (TRIUMF)
- S. Quaglioni (LLNL)
- F. Raimondi (U. Surrey)
- R. Roth (TUD)