R-Matrix Theory for the NCSM/RGM

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Outline

1. Motivation
2. Scattering
3. NCSM/RGM
4. R-Matrix Theory
5. Lagrange Mesh
6. Benchmarks
7. Summary

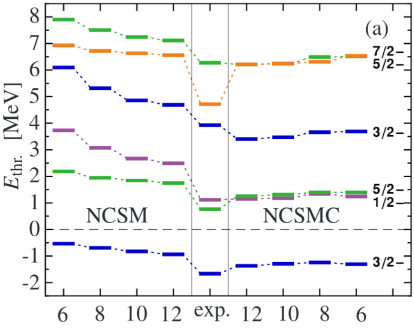
Motivation

Inclusion of continuum into *ab-inito* nuclear structure unavoidable

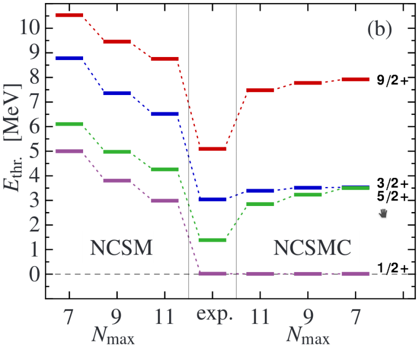
- Experimental data obtained from scattering
- Nuclear reactions
- Inclusion of resonances
- Unified framework for bound states and scattering effects
- Discrepancies in experiment and theory

Motivation
^{9}Be

- ^{9}Be as system of ^{8}Be+n
- ^{8}Be+n Threshold at 1.665 MeV



Langhammer et al, PRC 91, 021301(R) (2015)



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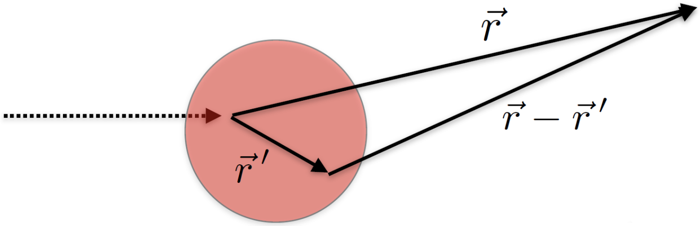
Scattering

- Lippmann-Schwinger equation

$$|\psi\rangle = |\psi_0\rangle + (E - H_0)^{-1} V |\psi\rangle$$

- Lippmann-Schwinger in coordinate space

$$\psi(\vec{r}) \sim \mathrm{e}^{i\vec{k}\vec{r}} + \int_{\vec{r}\,'} \int_{\vec{r}\,''} \frac{\mathrm{e}^{ik|\vec{r}-\vec{r}\,'|}}{|\vec{r}-\vec{r}\,'|} T(\vec{r}\,', \vec{r}\,'') \mathrm{e}^{i\vec{k}\vec{r}\,''}$$

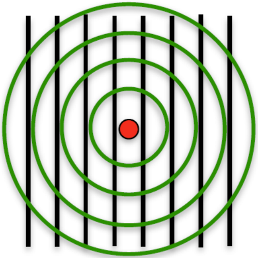


Scattering

- Plane and spherical wave for large r

$$\psi(\vec{r}) = \mathrm{e}^{i\vec{k}\vec{r}} + f_{\vec{k}}(\theta, \phi)\,\frac{\mathrm{e}^{ikr}}{r}$$

- Scattering information in scattering amplitude $f_{\vec{k}}(\theta, \phi)$



Scattering

- Partial wave decomposition for large r

$$\psi(\vec{r}) \to \sum_{l=0}^{\infty}(2l+1)\frac{P_l(\cos\theta)}{2ik}\left[(-1)^{l+1}\frac{\mathrm{e}^{-ikr}}{r} + S_l(k)\frac{\mathrm{e}^{ikr}}{r}\right]$$

- Scattering matrix S_l

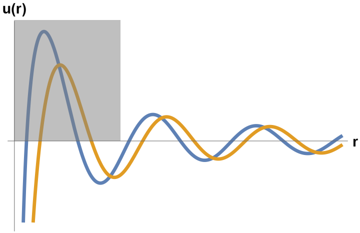
$$S_l(k) = 1 + 2ikf_l(k)$$

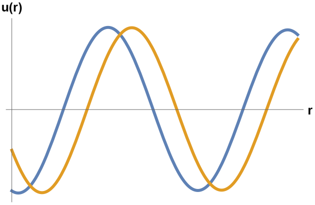
- Unitarity of S_l

$$S_l(k) = \mathrm{e}^{2i\delta_l(k)}$$

Scattering

- Phaseshift interpretation





- Radial Schrödinger equation

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

- Long range behaviour

$$u_l(r) = \cos(\delta_l)F_l(\eta, kr) + \sin(\delta_l)G_l(\eta, kr)$$

$$u_l(r) = C_l\left(H_l^-(\eta, kr) - S_l H_l^+(\eta, kr)\right)$$

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NCSM/RGM

- See lecture by Petr Navrátil
- Partial wave binary cluster basis

$$|\Psi^{J\pi T}\rangle = \sum_{\nu} \int \mathrm{d}r\, r^2\, \frac{u_\nu(r)}{r} \mathcal{A}_\nu \, |\Phi^{J\pi T}_{\nu r}\rangle$$

- Generalized eigenvalue problem

$$\sum_{\nu} \int \mathrm{d}r\, r^2 \left(\mathcal{H}_{\nu',\nu}(r',r) - E\mathcal{N}_{\nu',\nu}(r',r)\right) \frac{u_\nu(r)}{r} = 0$$

- Non-local potential

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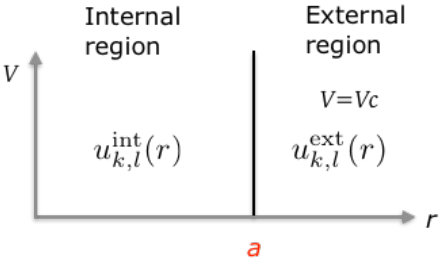
R-Matrix Theory

- Define channel radius a



- Continuity condition of logarithmic derivative

$$\frac{u_l^{\mathrm{int}\prime}(a)}{u_l^{\mathrm{int}}(a)} = \frac{u_l^{\mathrm{ext}\prime}(a)}{u_l^{\mathrm{ext}}(a)}$$

R-Matrix Theory

- Definition of R-matrix

$$u_l(a) = R_l(E)\Big(a u_l'(a) - B u_l(a)\Big)$$

- Hamiltonian not Hermitian

$$\int_0^a \mathrm{d}r\, r^2 \Big(\psi_1^*(r)\big(\mathcal{H}_l\psi_2(r)\big) - \big(\mathcal{H}_l\psi_1(r)\big)^*\psi_2(r)\Big) \neq 0$$

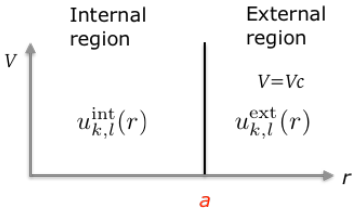
- Introduce Bloch-Operator into Hamiltonian

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

R-Matrix Theory

- Bloch-Schrödinger equation

$$(\mathcal{H}_l + \mathcal{L}(B) - E)u_l^{\text{int}}(r) = \mathcal{L}(B)u_l^{\text{int}}(r) = \mathcal{L}(B)u_l^{\text{ext}}(r)$$



- Expand interior solution

$$u_l^{\text{int}}(r) = \sum_{j=1}^{N} c_j \varphi_j(r)$$

R-Matrix Theory

- Project onto expansion basis

$$\sum_j \underbrace{\int_0^a \mathrm{d}r\, \varphi_i(r)\big(\mathcal{H}_l + \mathcal{L}(B) - E\big)\varphi_j(r)}_{C_{ij}}\, c_j = \int_0^a \mathrm{d}r\, \varphi_i(r)\mathcal{L}(B)u_l^{\mathrm{ext}}(r)$$

- Solve for $u_l(a)$

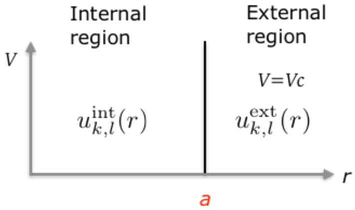
$$u_l(a) = \sum_i \varphi_i(a)c_i = \frac{\hbar^2}{2\mu a}\sum_{i,j}\varphi_i(a)(C^{-1})_{ij}\,\varphi_j(a)\Big(au_l'(a) - Bu_l(a)\Big)$$

- Compare to R-matrix definition

$$R_l(E) = \frac{\hbar^2}{2\mu a}\sum_{i,j}\varphi_i(a)(C^{-1})_{ij}\,\varphi_j(a)$$

R-Matrix Theory

- Reminder of ansatz



$$\frac{u_l^{\mathrm{int}\prime}(a)}{u_l^{\mathrm{int}}(a)} = \frac{u_l^{\mathrm{ext}\prime}(a)}{u_l^{\mathrm{ext}}(a)} = \frac{\cos(\delta_l)\,k\,F_l'(\eta,ka) + \sin(\delta_l)\,k\,G_l'(\eta,ka)}{\cos(\delta_l)F_l(\eta,ka) + \sin(\delta_l)G_l(\eta,ka)}$$

- Solve for phaseshift

$$\tan(\delta_l) = -\frac{F_l(\eta,ka) + ka\,R_l(E)F_l'(\eta,ka)}{G_l(\eta,ka) + ka\,R_l(E)G_l'(\eta,ka)}$$

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Lagrange Mesh

- Free choice of basis functions: Lagrange functions

$$\varphi_i(r) = (-1)^{N+i} \frac{r}{ax_i} \sqrt{ax_i(1-x_i)} \frac{P_N(2r/a-1)}{r-ax_i}$$

- Mesh points

$$P_N(2x_i - 1) = 0$$

- Simple integration with Gauss quadrature

$$\int_0^a \mathrm{d}r \int_0^\infty \mathrm{d}r' r'^2 \varphi_i(r) W(r,r') \varphi_j(r) \stackrel{\text{Gauss}}{=} a\sqrt{\lambda_i \lambda_j} W(ax_i, ax_j)$$

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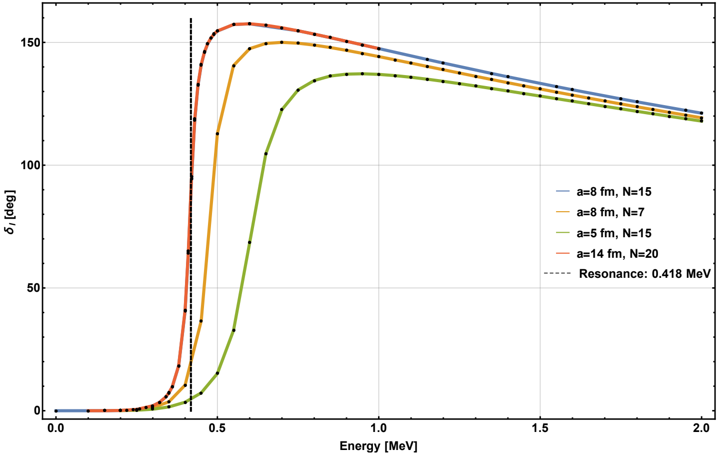
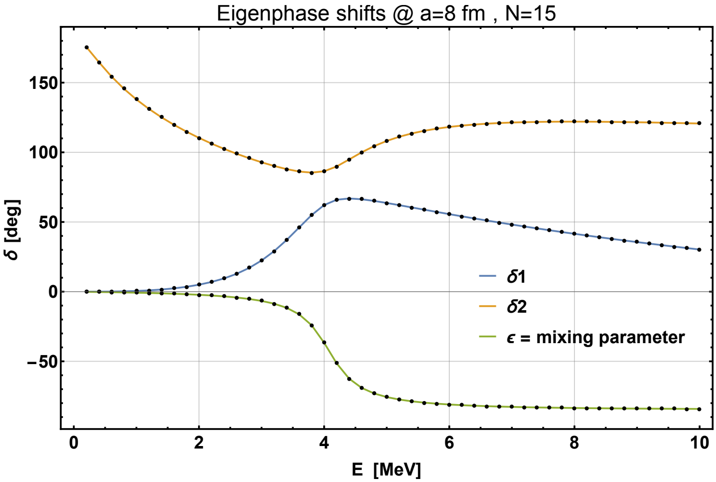
Benchmarks

- ^{12}C+p scattering, effective potential
- $l = 0$ single channel



Benchmarks

- α+d scattering
- ^{6}Li effective potential
- $l = 0$ and $l = 2$ channel



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Summary

- Necessity for continuum in nuclear structure
- Basics of scattering physics
- Relative motion wave function in NCSM/RGM

R-matrix Theory on Lagrange Mesh

- Use of asymptotic solution
- Reformulation to matrix inversion
- Simple integral evaluation
- Non-local potential treatment

Epilog

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- **Thank you for your attention!**

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