Calculable *R*-matrix method on a Lagrange mesh for the Schrödinger and Dirac equations

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Calculable *R*-matrix method on a Lagrange mesh for the Schrödinger and Dirac equations

- Introduction
- Principle of *R*-matrix methods
- *R*-matrix method for Schrödinger equation
- Lagrange-mesh simplification
- Applications
- *R*-matrix method for Dirac equation
- Examples
- [*R*-matrix method for Dirac bound states]
- Conclusion

Principle of *R*-matrix methods

Phenomenological
R-matrix

↓

Nuclear physics:
Resonances
Fit of cross sections

Calculable
R-matrix

↓

Atomic physics

Nuclear physics

Many misconceptions !

Short history of *R*-matrix methods

Phenomenological *R* matrix

- Fit of resonances (Wigner and Eisenbud 1947)
- Fit of low-energy cross sections
- Mostly used in nuclear physics (Lane and Thomas 1958)

Calculable *R* matrix

- Numerical solution of Schrödinger equation
- Convergence problems → Buttle correction (1967)
- Use of Bloch operator (Bloch 1957)
- Mostly used in atomic physics

- Convergence problems due to use of a common boundary condition for all basis states → solved by bases without that constraint (also valid for Dirac equation)

Review: P. Descouvemont, D.B., Rep. Prog. Phys. 73 (2010) 036301

Some key steps

1938: original but not practical idea by Kapur and Peierls
1947: (Phenomenological) *R* matrix (PRM) introduced by Wigner and Eisenbud
1957: Bloch operator
1958: Rev. Mod. Phys. paper on PRM by Lane and Thomas
1965: idea of Calculable *R* matrix (CRM) by Haglund and Robson
1967: first application of CRM by Buttle
1973: introduction of CRM in atomic physics by Burke
1974: microscopic *R* matrix (D.B. and Heenen)
1976: propagation (Light and Walker)
1994: CRM on a Lagrange mesh (Malegat)

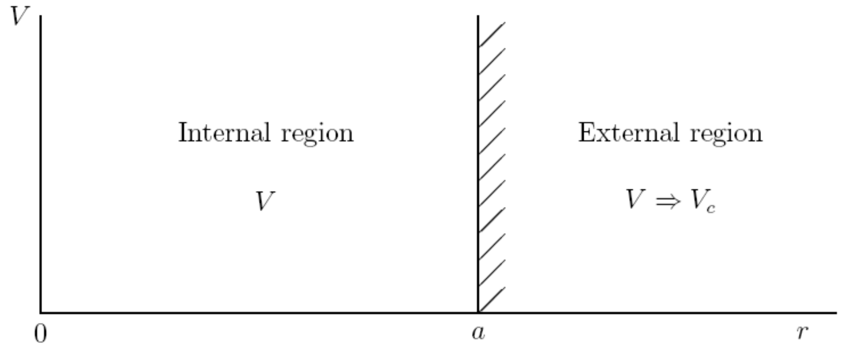
But many misunderstandings till now

- Choice of channel radius (PRM versus CRM)
- Choice of boundary condition parameter
- Choice of basis in CRM
- Utility of Bloch operator (underestimated)

Calculable *R* matrix

Principle for Schrödinger equation:

Division of the configuration space into two regions at channel radius *a*



- internal region: $r < a$
  expansion of solution of Schrödinger equation on [0, *a*] interval with *N* (not necessarily orthogonal) basis functions

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

- external region: $r > a$
  exact asymptotic expression for Coulomb potential V_c

$$u_l^{\text{ext}}(r) = \cos\delta_l\, F_l(kr) + \sin\delta_l\, G_l(kr)$$

Schrödinger equation for lth partial wave

$$(H_l - E)u_l = 0 \qquad H_l = T_l + V(r) \qquad T_l = -\frac{\hbar^2}{2\mu}\left(\frac{d^2}{dr^2} - \frac{l(l+1)}{r^2}\right)$$

Bloch operator

→ H_l not Hermitian over finite interval

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

→ $H_l + \mathcal{L}$ Hermitian over $(0,a)$

→ and more…

Bloch-Schrödinger equation

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

Continuity $\quad u_l^{\text{int}}(a) = u_l^{\text{ext}}(a)$

Important role of Bloch operator $\quad u_l^{\text{int}\prime}(a) = u_l^{\text{ext}\prime}(a)$

Calculation of *R* matrix

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

$$(H_l + \mathcal{L}(B) - E) \sum_{j=1}^{N} c_j \varphi_j(r) = \mathcal{L}(B) u_l^{\text{ext}}(r)$$

Matrix elements (integral from 0 to *a*)

$$C_{ij}(E,B) = \langle \varphi_i | T_l + \mathcal{L}(B) + V - E | \varphi_j \rangle$$

Internal solution

$$\sum_{i=1}^{N} C_{ij}(E,B) c_j = \frac{\hbar^2}{2\mu a} \varphi_i(a) \left[a u_l^{\text{ext}\prime}(a) - B u_l^{\text{ext}}(a) \right]$$

$$c_j = \frac{\hbar^2}{2\mu a} \left[a u_l^{\text{ext}\prime}(a) - B u_l^{\text{ext}}(a) \right] \sum_{i=1}^{N} (\boldsymbol{C}^{-1})_{ij} \varphi_i(a)$$

Continuity

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

***R* matrix**

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

$$u_l^{\text{ext}}(a) = R_l(E,B) \left[a u_l^{\text{ext}\prime}(a) - B u_l^{\text{ext}}(a) \right]$$

Interpretation of *R* matrix

$$\frac{a u_l^{\text{ext}\prime}(a)}{u_l^{\text{ext}}(a)} = \frac{1}{R_l(E,B)} + B = \frac{1}{R_l(E,0)}$$

→ inverse of logarithmic derivative at channel radius
→ calculated in the internal region
→ used in the external region to determine the phase shift
→ depends on channel radius

Phase shift $u_l^{\text{ext}}(r) = \cos\delta_l\, F_l(kr) + \sin\delta_l\, G_l(kr)$

$$\tan\delta_l = -\frac{F_l(ka) - kaR_l(E,0)F_l'(ka)}{G_l(ka) - kaR_l(E,0)G_l'(ka)}$$

→ independent of *B* !
→ weakly dependent on *a* (if *a* large enough)

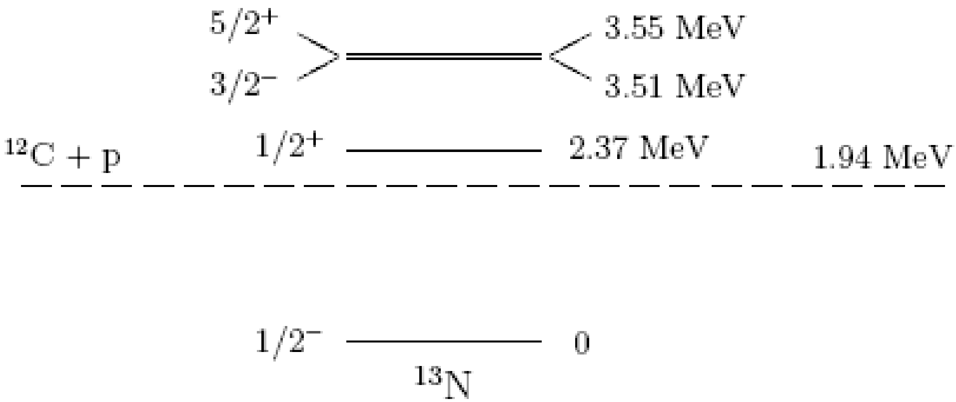
Calculable / phenomenological *R* matrix

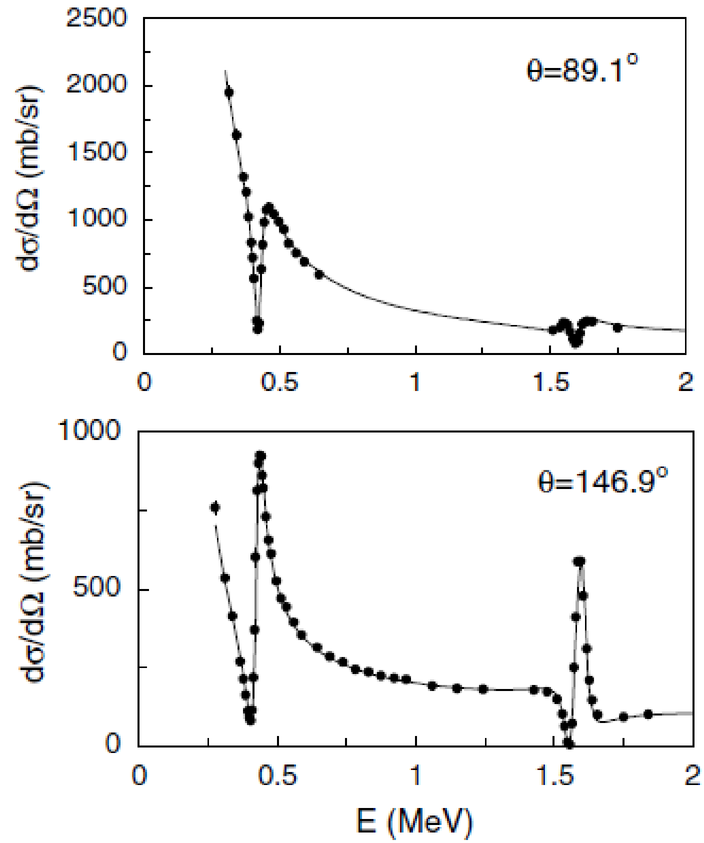
$$R_l(E,B) = \frac{\hbar^2}{2\mu a}\sum_{i,j=1}^{N}\varphi_i(a)(C^{-1})_{ij}\varphi_j(a) = \sum_{n=1}^{N}\frac{\gamma_{nl}^2}{E_{nl}-E}$$

CRM $N \geq 10$

PRM $N \leq 3$

PRM example:
^{12}C + p below 2 MeV





2 parameters per resonance

a = 4 – 6 fm

Cross section fitted between resonances!

Various misconceptions about CRM

- Depends on the channel radius!

The independence on the channel radius is a test of accuracy

- Choice of basis functions → basis states must satisfy: $\dfrac{a\varphi_j'(a)}{\varphi_j(a)} = B$

  (see Wigner and Eisenbud)

Wrong !: $\lim_{r \to a^-} u_l^{\mathrm{int}\,\prime}(r) = u_l^{\mathrm{ext}\,\prime}(a) \neq u_l^{\mathrm{int}\,\prime}(a)$

On the contrary, basis functions must provide a variety of values $\dfrac{a\varphi_j'(a)}{\varphi_j(a)}$

- Bloch operator is not really necessary!

- restores Hermiticity
- imposes the continuity of the logarithmic derivative
  (Wigner-Eisenbud condition unnecessary)

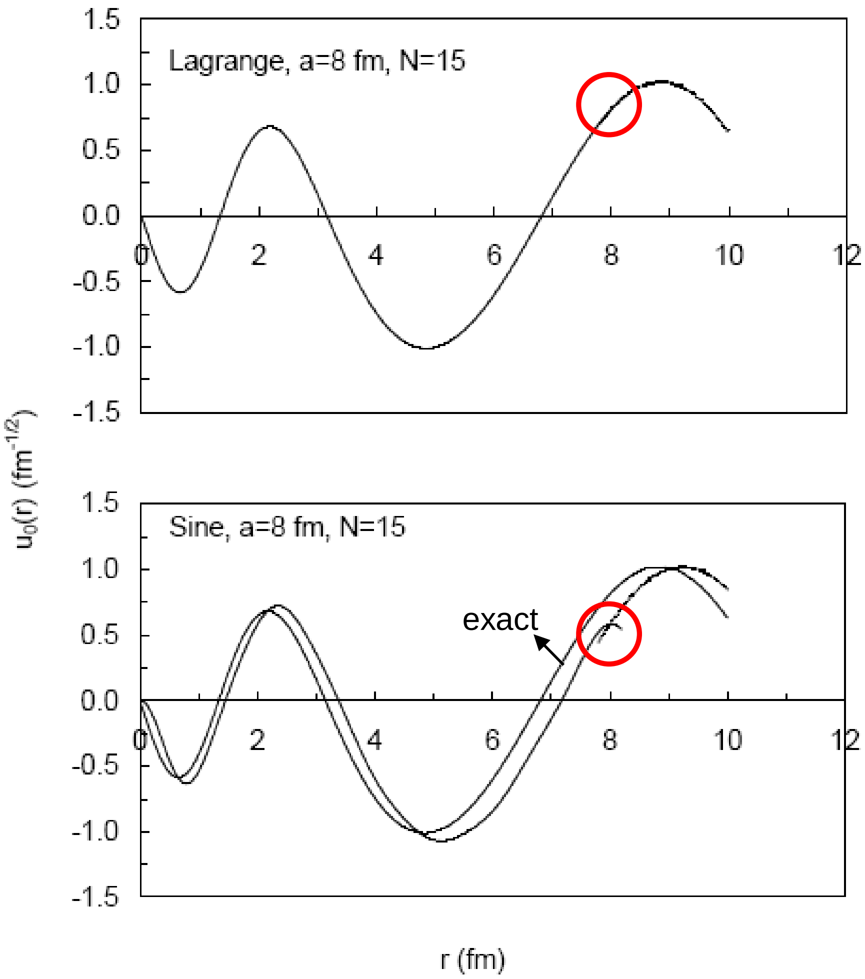
- Optimization of boundary parameter *B*

Useless ! The results *do not* depend on *B*: $\dfrac{1}{R_l(E,0)} = \dfrac{1}{R_l(E,B)} + B$

Matching at the boundary: Lagrange and sine bases

α + ^{3}He potential, *s* wave, E = 8 MeV

a = 8, N = 15



Various $\frac{a\varphi_j'(a)}{\varphi_j(a)}$

→ indistinguishable from exact solution

$$\varphi_j(r) = \sin[(j - \tfrac{1}{2})\pi r/a]$$

$$\frac{a\varphi_j'(a)}{\varphi_j(a)} = 0$$

→ bad matching,

→ poor phase shift

Lagrange-mesh simplification

Lagrange mesh and Lagrange basis

N mesh points x_i associated with Gauss quadrature

$$\int_a^b g(x)\,dx \approx \sum_{k=1}^{N} \lambda_k g(x_k)$$

N functions $f_j(x)$ satisfying Lagrange conditions

$$f_j(x_i) = \lambda_i^{-1/2} \delta_{ij}$$

Lagrange functions orthonormal at the Gauss approximation

$$\int_a^b f_i(x) f_j(x) dx \approx \sum_{k=1}^{N} \lambda_k f_i(x_k) f_j(x_k) = \delta_{ij}$$

Potential matrix elements diagonal at the Gauss approximation

$$\langle f_i | V | f_j \rangle \approx \sum_k \lambda_k f_i(x_k) V(x_k) f_j(x_k) = V(x_i)\delta_{ij}$$

D. B., P.-H. Heenen, J. Phys. A 19 (1986) 2041

D. B., Phys. Reports 565 (2015) 1

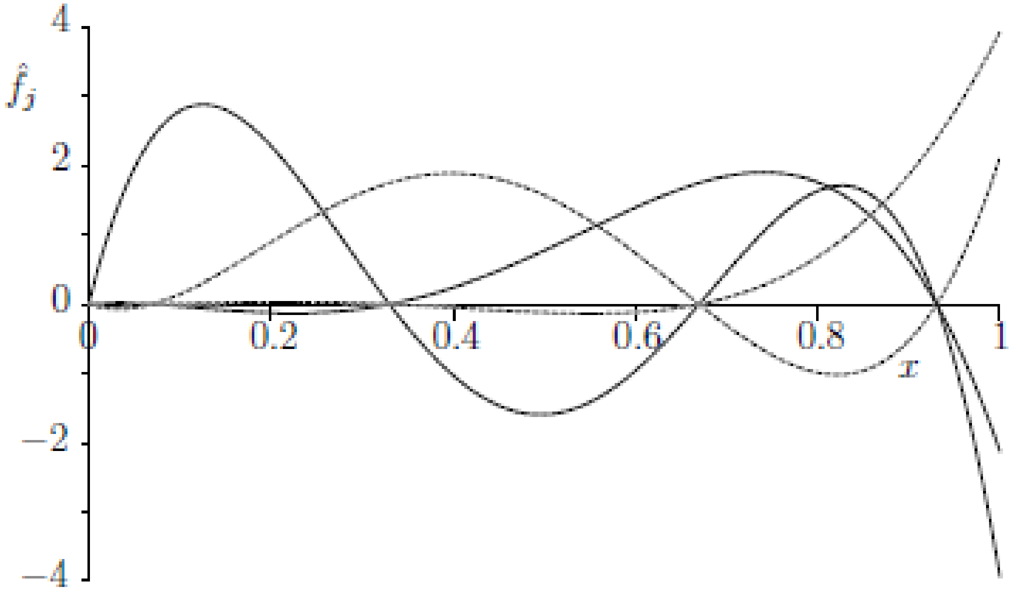
Shifted Legendre mesh

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

Regularized Lagrange-Legendre functions over [0,1]

$$f_j(x) = (-1)^{N-j} \left(\frac{1 - x_j}{x_j} \right)^{1/2} \frac{x P_N(2x - 1)}{x - x_j}$$

Non-orthogonal but orthonormal at the Gauss approximation



$$f_j(0) = 0$$

$$f_j(x_i) = \lambda_i^{-1/2} \delta_{ij}$$

D.B., Phys. Reports 565 (2015) 1

Internal wave function $u_l^{\text{int}}(r) = \sum_{i=1}^{N} c_i f_i(r)$

Shifted Lagrange-Legendre mesh on [0,1]: $P_N(2x_i - 1) = 0$

Regularized Lagrange basis (treated as orthonormal)

$$f_i(r) = (-1)^{N-i} \left(\frac{1-x_i}{ax_i}\right)^{1/2} \frac{rP_N(2r/a-1)}{r-ax_i}$$

Matrix elements of $H_l + \mathcal{L}$

$$C_{ij} = -\frac{\hbar^2}{2\mu a^2}\left(T_{ij} + \frac{l(l+1)}{x_i^2}\delta_{ij}\right) + V(ax_i)\delta_{ij}$$

Matrix elements $T_{ij} = \langle f_i | T + \mathcal{L} | f_j \rangle$ are simple functions of x_i and x_j

Properties:

- no calculations of integrals
- no loss of accuracy due to Gauss quadrature

L.Malegat, J. Phys. B 27 (1994) L691
M. Hesse, J.-M. Sparenberg, F. Van Raemdonck, D. B., Nucl. Phys. A 640 (1998) 37

Recent improvement for high *l* values: Lagrange-Jacobi mesh

Applications

- Resonating-group method (RGM)
- Continuum-discretized coupled-channel method (CDCC)
- Three-body scattering

Resonating-group method

- antisymmetrized wave functions
- non-local RGM equation (with forbidden states)

$$\left[-\frac{\hbar^2}{2\mu}\left(\frac{d^2}{dr^2}-\frac{l(l+1)}{r^2}\right)+V(r)\right]u_l(r)+\int_0^\infty W_l(r,r')u_l(r')dr' = Eu_l(r)$$

- equivalent to microscopic cluster model (MCM)

+ microscopic *R*-matrix method (MRM)

D.B., P.-H. Heenen, Nucl. Phys. A233 (1974) 304

α + p scattering (*s* wave)

E (MeV)	CRM + Lagrange a	N	δ_0	MCM + MRM N	δ_0
1	8	10	−15.466	9	−15.482
	10	20	−15.482 6	10	−15.481
100	8	15	21.142	9	21.089
	10	25	21.133 9	10	21.134

M. Hesse, J. Roland, D.B., Nucl. Phys. A709 (2002) 184

Continuum-discretized coupled-channel method (CDCC)

$$H = H_0 + T_R + V_{Tc}\left(\boldsymbol{R} + \frac{A_f}{A_p}\boldsymbol{r}\right) + V_{Tf}\left(\boldsymbol{R} - \frac{A_c}{A_p}\boldsymbol{r}\right) \qquad H_0 = T_r + V_{cf}(r)$$

Continuum represented by square-integrable functions
(pseudostates or bins = averages of continuum states)
CDCC expansion

$$\Psi^{JM\pi}(\boldsymbol{R},\boldsymbol{r}) = \frac{1}{rR}\sum_{lLi}\left[Y_l(\Omega_r)\otimes Y_L(\Omega_R)\right]^{JM} u^{J\pi}_{lLi}(R)\,\hat{\phi}_{li}(r)$$

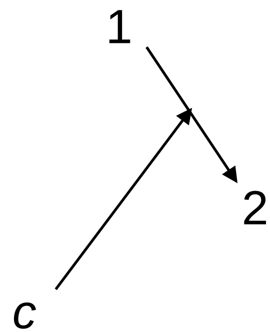
→ standard coupled-channels system of equations

$$\left[-\frac{\hbar^2}{2\mu}\left(\frac{d^2}{dR^2} - \frac{L(L+1)}{R^2}\right) + E_{li} - E\right]u^{J\pi}_{\gamma i}(R) + \sum_{\gamma' i'} V^{J\pi}_{\gamma i,\gamma' i'}(R)u^{J\pi}_{\gamma' i'}(R) = 0$$

Double use of Lagrange-mesh *R*-matrix method
- Construction of bins
- Resolution of coupled system of equations

Need for propagation (several intervals, easy with Lagrange mesh)
Application to elastic scattering and breakup
T. Druet, D.B., P. Descouvemont, J.-M. Sparenberg, Nucl. Phys. A 845 (2010) 88

c + n + n three-body scattering



Hyperspherical coordinates

$$\boldsymbol{x} = \frac{1}{\sqrt{2}}\boldsymbol{r}_{21} \qquad \boldsymbol{y} = \sqrt{\frac{4}{3}}\boldsymbol{r}_{\alpha(12)}$$

$$\rho = \sqrt{x^2 + y^2} \qquad \alpha = \arctan\frac{y}{x}$$

$$\Omega_5 = (\Omega_x, \Omega_y, \alpha)$$

Expansion in hyperspherical harmonics $\gamma = (l_x, l_y, L, S)$

$$\Psi^{JM\pi}(\rho, \Omega_5) = \rho^{-5/2}\sum_{\gamma K}\chi^{J\pi}_{\gamma K}(\rho)\ \mathcal{Y}^{JM}_{\gamma K}(\Omega_5)$$

Infinite system of coupled equations (truncated at K_{max})

$$\left[-\frac{\hbar^2}{2m_N}\left(\frac{d^2}{d\rho^2} - \frac{(K+3/2)(K+5/2)}{\rho^2}\right) - E\right]\chi^{J\pi}_{\gamma K}(\rho) + \sum_{K'\gamma'} V^{J\pi}_{K\gamma,K'\gamma'}(\rho)\,\chi^{J\pi}_{\gamma' K'}(\rho) = 0$$

Lagrange-mesh *R*-matrix $$\chi^{J\pi}_{\gamma K,\,\mathrm{int}}(\rho) = \sum_{i=1}^{N} c^{J\pi}_{\gamma K i} f_i(\rho)$$

$$\chi^{J\pi}_{\gamma K,\,\mathrm{ext}}(\rho) = H^{-}_{K+2}(k\rho)\delta_{\gamma\gamma_\omega}\delta_{KK_\omega} - U^{J\pi}_{\gamma K,\gamma_\omega K_\omega} H^{+}_{K+2}(k\rho)$$

$$H^{\pm}_{K}(x) = \pm i(\pi x/2)^{1/2}\left[J_K(x) \pm iY_K(x)\right]$$

Difficulties

- Collision matrix infinite in principle → many channels after truncation
- Asymptotic at very large distances *a* (250 – 300 fm)

  → propagation:

  - internal region from 0 to a_0 = 25 - 30 fm
  - propagation from a_0 to *a*
  - external region beyond *a*

Advantages

- Simplicity and accuracy of Lagrange mesh

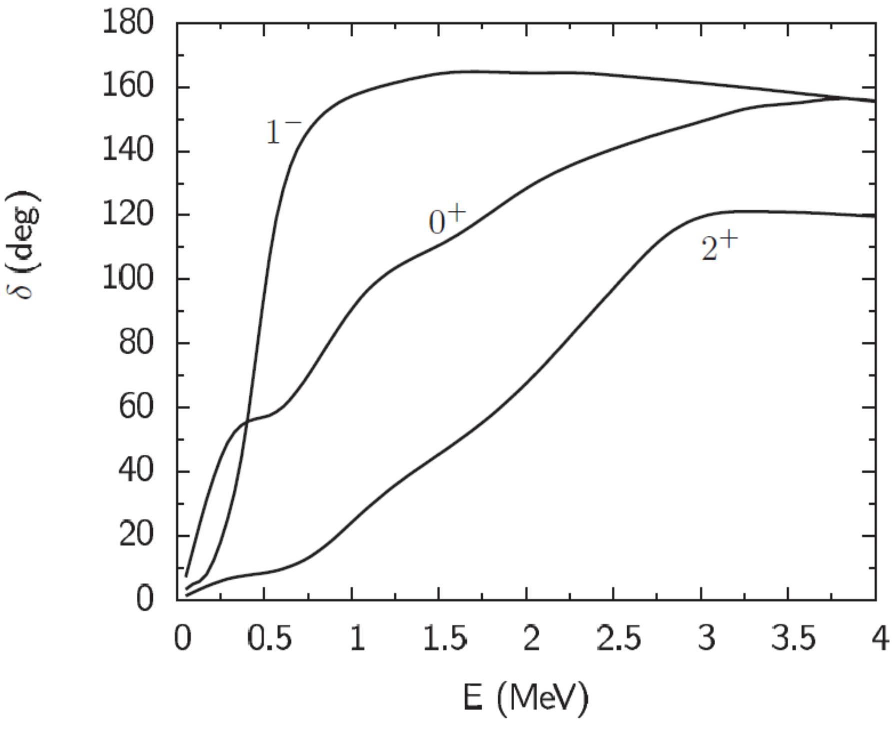
  No integration over the hyperradius
- Small hyperradial basis (*N* = 30)
- Analytical wave functions available for applications (breakup)

^{9}Li + n + n eigenphases

(^{11}Li continuum)

$J = 0 \;\; K_{max} = 32 \;\; N_c = 66$
$J = 1 \;\; K_{max} = 25 \;\; N_c = 155$
$J = 2 \;\; K_{max} = 22 \;\; N_c = 133$

a = 400. N =30



E.C. Pinilla, P. Descouvemont, D.B., Phys. Rev. C 85 (2012) 054610

R matrix for Dirac equation

A controversy existed about the accuracy of the *R*-matrix method for the Dirac equation. The origin of the problem was the same as for the Schrödinger equation.

Accurate calculable *R*-matrix method for the Dirac equation
- Relativistic matrix Bloch operator (3 parameters)
- Use of bases without constraint at boundary
- No restriction on parameters of Bloch operator (contrary to literature)

Facultative simplification:
- Lagrange-mesh technique
- Very simple: no analytical calculation of matrix elements
- Very accurate

Applied to:
- Determination of phase shifts and scattering wave functions
- Determination of bound-state energies and wave functions

D.B., Phys. Rev. A 92 (2015) 042112

Dirac equation

$$[c\boldsymbol{\alpha}\cdot\boldsymbol{p}+\beta mc^2+V(r)]\Psi_{\kappa m}(\boldsymbol{r})=(E+mc^2)\Psi_{\kappa m}(\boldsymbol{r})$$

Dirac spinor

$$\Psi_{\kappa m}(\boldsymbol{r})=\frac{1}{r}\begin{pmatrix} P_\kappa(r)\chi_{\kappa m} \\ iQ_\kappa(r)\chi_{-\kappa m}\end{pmatrix}$$

Quantum numbers

$$j=|\kappa|+\tfrac{1}{2},\quad l=j+\tfrac{1}{2}\operatorname{sgn}\kappa$$

Coupled radial equations

$$H_\kappa\begin{pmatrix} P_\kappa(r) \\ Q_\kappa(r)\end{pmatrix}=E\begin{pmatrix} P_\kappa(r) \\ Q_\kappa(r)\end{pmatrix}$$

2 x 2 matrix radial Hamiltonian

$$H_\kappa=\begin{pmatrix} V(r) & \hbar c\left(-\frac{d}{dr}+\frac{\kappa}{r}\right) \\ \hbar c\left(\frac{d}{dr}+\frac{\kappa}{r}\right) & V(r)-2mc^2\end{pmatrix}$$

Bloch – Dirac equations

2 x 2 Bloch operator (no derivative!)

$$\mathcal{L} = \tfrac{1}{2}\hbar c\,(\boldsymbol{J} + \boldsymbol{B})\,\delta(r-a) \qquad \boldsymbol{J} = \begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix} \qquad \boldsymbol{B} = \begin{pmatrix} b_{11} & b_{12} \\ b_{12} & b_{22} \end{pmatrix}$$

Internal Bloch - Dirac equation

$$(H_\kappa + \mathcal{L} - E)\begin{pmatrix} P_\kappa^{\mathrm{int}}(r) \\ Q_\kappa^{\mathrm{int}}(r) \end{pmatrix} = \mathcal{L}\begin{pmatrix} P_\kappa^{\mathrm{ext}}(r) \\ Q_\kappa^{\mathrm{ext}}(r) \end{pmatrix}$$

External Bloch - Dirac equation

$$(H_\kappa - \mathcal{L} - E)\begin{pmatrix} P_\kappa^{\mathrm{ext}}(r) \\ Q_\kappa^{\mathrm{ext}}(r) \end{pmatrix} = -\mathcal{L}\begin{pmatrix} P_\kappa^{\mathrm{int}}(r) \\ Q_\kappa^{\mathrm{int}}(r) \end{pmatrix}$$

Hermiticity over finite intervals

$$\int_0^a \Phi_{\kappa,1}^T (H_\kappa + \mathcal{L})\Phi_{\kappa,2}\,dr = \int_0^a [(H_\kappa + \mathcal{L})\Phi_{\kappa,1}]^T \Phi_{\kappa,2}\,dr$$

$$\int_a^\infty \Phi_{\kappa,1}^T (H_\kappa - \mathcal{L})\Phi_{\kappa,2}\,dr = \int_a^\infty [(H_\kappa - \mathcal{L})\Phi_{\kappa,1}]^T \Phi_{\kappa,2}\,dr$$

$$\Phi_{\kappa,i}(r) = (P_{\kappa,i}(r), Q_{\kappa,i}(r))^T$$

Continuum with *R*-matrix method:
Short-range potential

Solution in the external region: vanishing potential

$$P_\kappa^{\rm ext}(r) = Ckr[j_l(kr)\cos\delta_\kappa + n_l(kr)\sin\delta_\kappa]$$

$$Q_\kappa^{\rm ext}(r) = {\rm sgn}\,\kappa\sqrt{\frac{E}{E+2mc^2}}Ckr[j_{\bar{l}}(kr)\cos\delta_\kappa + n_{\bar{l}}(kr)\sin\delta_\kappa]$$

$$k = \sqrt{E(E+2mc^2)}/\hbar c \qquad \bar{l} = l - {\rm sgn}\,\kappa$$

Solution in the internal region: expansion over an orthonormal basis

$$\varphi_j(r) \quad (j = 1,\ldots,N) \qquad \varphi_j(0) = 0$$

$$P_\kappa^{\rm int}(r) = \sum_{j=1}^N p_{\kappa j}^{\rm int}\varphi_j(r) \qquad Q_\kappa^{\rm int}(r) = \sum_{j=1}^N q_{\kappa j}^{\rm int}\varphi_j(r)$$

$$\boldsymbol{p}_\kappa = (p_{\kappa 1}, p_{\kappa 2}, \ldots, p_{\kappa N})^T, \; \boldsymbol{q}_\kappa = (q_{\kappa 1}, q_{\kappa 2}, \ldots, q_{\kappa N})^T$$

No constraint imposed at $r = a$!

Internal Bloch-Dirac equation

$$(H_\kappa + \mathcal{L} - E)\begin{pmatrix} P_\kappa^{\text{int}}(r) \\ Q_\kappa^{\text{int}}(r) \end{pmatrix} = \mathcal{L}\begin{pmatrix} P_\kappa^{\text{ext}}(r) \\ Q_\kappa^{\text{ext}}(r) \end{pmatrix}$$

Expansion on an orthonormal basis ($\boldsymbol{B} = 0$)

$$(\boldsymbol{M}_\kappa^{\text{int}} - E\boldsymbol{I})\begin{pmatrix} \boldsymbol{p}_\kappa^{\text{int}} \\ \boldsymbol{q}_\kappa^{\text{int}} \end{pmatrix} = \tfrac{1}{2}\hbar c\boldsymbol{F}\begin{pmatrix} Q_\kappa^{\text{ext}}(a) \\ -P_\kappa^{\text{ext}}(a) \end{pmatrix}$$

Matrix elements

$$\boldsymbol{M}_\kappa^{\text{int}} = \begin{pmatrix} \boldsymbol{M}_\kappa^{\text{int}(1,1)} & \boldsymbol{M}_\kappa^{\text{int}(1,2)} \\ \boldsymbol{M}_\kappa^{\text{int}(2,1)} & \boldsymbol{M}_\kappa^{\text{int}(2,2)} \end{pmatrix}$$

$$M_{\kappa ij}^{\text{int}(1,1)} = \langle\varphi_i|V(r)|\varphi_j\rangle \qquad M_{\kappa ij}^{\text{int}(2,2)} = \langle\varphi_i|V(r) - 2mc^2|\varphi_j\rangle$$

$$M_{\kappa ij}^{\text{int}(1,2)} = \hbar c\langle\varphi_i| - d/dr + \kappa/r + \tfrac{1}{2}\delta(r-a)|\varphi_j\rangle$$

$$M_{\kappa ij}^{\text{int}(2,1)} = M_{\kappa ji}^{\text{int}(1,2)}$$

$$F_{i,1} = F_{N+i,2} = \varphi_i(a), \quad F_{i,2} = F_{N+i,1} = 0, \quad i = 1, \ldots, N$$

R matrix and phase shifts for ***B*** = 0

$$\begin{pmatrix} \boldsymbol{p}_\kappa^{\rm int} \\ \boldsymbol{q}_\kappa^{\rm int} \end{pmatrix} = \tfrac{1}{2}\hbar c(\boldsymbol{M}_\kappa^{\rm int} - E\boldsymbol{I})^{-1}\boldsymbol{F}\begin{pmatrix} Q_\kappa^{\rm ext}(a) \\ -P_\kappa^{\rm ext}(a) \end{pmatrix}$$

Continuity

$$P_\kappa^{\rm int}(a) = P_\kappa^{\rm ext}(a), \quad Q_\kappa^{\rm int}(a) = Q_\kappa^{\rm ext}(a)$$

Generalized *R* matrix

$$\begin{pmatrix} P_\kappa^{\rm ext}(a) \\ Q_\kappa^{\rm ext}(a) \end{pmatrix} = \boldsymbol{\mathcal{R}}_0\begin{pmatrix} Q_\kappa^{\rm ext}(a) \\ -P_\kappa^{\rm ext}(a) \end{pmatrix}$$

$$\boldsymbol{\mathcal{R}}_0 = \tfrac{1}{2}\hbar c\boldsymbol{F}^T(\boldsymbol{M}_\kappa^{\rm int} - E\boldsymbol{I})^{-1}\boldsymbol{F}$$

Compatibility

$$\det \boldsymbol{\mathcal{R}}_0 = -1$$

R matrix

$$P_\kappa^{\rm ext}(a) = R_\kappa Q_\kappa^{\rm ext}(a)$$

$$R_\kappa = \frac{\mathcal{R}_{0,11}}{\mathcal{R}_{0,12}+1} = \frac{\mathcal{R}_{0,12}-1}{\mathcal{R}_{0,22}}$$

Phase shift (should be essentially independent of *a*)

$$\tan\delta_\kappa = -\frac{j_l(ka) - \lambda R_\kappa j_{\bar{l}}(ka)}{n_l(ka) - \lambda R_\kappa n_{\bar{l}}(ka)} \qquad \lambda = \operatorname{sgn}\kappa\sqrt{\frac{E}{E+2mc^2}}$$

R matrix for arbitrary *B*

Bloch operator

$$\mathcal{L} = \frac{1}{2}\hbar c \left[\begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix} + \begin{pmatrix} b_{11} & b_{12} \\ b_{12} & b_{22} \end{pmatrix} \right] \delta(r-a)$$

Generalized *R* matrix

$$\boldsymbol{\mathcal{R}}^{-1} = \boldsymbol{\mathcal{R}}_0^{-1} + \boldsymbol{B}$$

Continuity

$$\begin{pmatrix} P_\kappa^{\rm ext}(a) \\ Q_\kappa^{\rm ext}(a) \end{pmatrix} = \boldsymbol{\mathcal{R}}(\boldsymbol{J} + \boldsymbol{B}) \begin{pmatrix} P_\kappa^{\rm ext}(a) \\ Q_\kappa^{\rm ext}(a) \end{pmatrix}$$

Compatibility

$$(\det \boldsymbol{B} + 1) \det \boldsymbol{\mathcal{R}} - \mathrm{Tr}\, \boldsymbol{B}\boldsymbol{\mathcal{R}} = -1$$

General forms of *R* matrix

$$R_\kappa = \frac{(1+b_{12})\mathcal{R}_{11} + b_{22}\mathcal{R}_{12}}{1 - b_{11}\mathcal{R}_{11} + (1-b_{12})\mathcal{R}_{12}} = \frac{1 - (1+b_{12})\mathcal{R}_{12} - b_{22}\mathcal{R}_{22}}{b_{11}\mathcal{R}_{12} - (1-b_{12})\mathcal{R}_{22}}$$

- converges for any ***B***
- speed of convergence depends on choice of ***B***

Lagrange-Legendre basis in internal region: $\varphi_j(r) = a^{-1/2}\hat{f}_j(r/a)$

$$\hat{f}_j(x) = (-1)^{N-j}\sqrt{\frac{1-\hat{x}_j}{\hat{x}_j}}\frac{xP_N(2x-1)}{x-\hat{x}_j} \qquad P_N(2\hat{x}_i - 1) = 0$$

Gauss approximation for potential

$$\int_0^1 \hat{f}_i(x)V(x)\hat{f}_j(x)dx \approx \sum_{k=1}^{N} \hat{\lambda}_k \hat{f}_i(\hat{x}_k)V(\hat{x}_k)\hat{f}_j(\hat{x}_k) = V(\hat{x}_i)\delta_{ij}$$

Lagrange-mesh 'Hamiltonian + Bloch operator' matrix

$$M^{\mathrm{int}(1,1)}_{\kappa ij} = V(ax_i)\delta_{ij} \qquad M^{\mathrm{int}(2,2)}_{\kappa ij} = [V(ax_i) - 2mc^2]\delta_{ij}$$

$$M^{\mathrm{int}(2,1)}_{\kappa ij} = M^{\mathrm{int}(1,2)}_{\kappa ji} = \frac{\hbar c}{a}\left(\langle \hat{f}_i|\frac{d}{dx} - \frac{1}{2}\delta(x-1)|\hat{f}_j\rangle + \frac{\kappa}{x_i}\delta_{ij}\right)$$

$$\langle \hat{f}_i|\frac{d}{dx} - \frac{1}{2}\delta(x-1)|\hat{f}_j\rangle = (-1)^{i-j}\frac{\hat{x}_i + \hat{x}_j - 2\hat{x}_i\hat{x}_j}{2\sqrt{\hat{x}_i(1-\hat{x}_i)\hat{x}_j(1-\hat{x}_j)}\,(\hat{x}_i - \hat{x}_j)} \qquad i \neq j$$

$$\langle \hat{f}_i|\frac{d}{dx} - \frac{1}{2}\delta(x-1)|\hat{f}_i\rangle = 0$$

- No calculation of integrals → potential values at mesh points

Examples of phase-shift calculations

Square well

$$V(r) = -V_0, \quad r < a; \quad V(r) = 0, \quad r > a$$

Exact *R* matrix

$$R_\kappa = \operatorname{sgn}\kappa\,(2mc^2 + V_0 + E)\,\frac{j_l(pa)}{\hbar c p\, j_{\bar{l}}(pa)}$$

$$p = \sqrt{(V_0 + E)(2mc^2 + V_0 + E)}/\hbar c$$

Woods-Saxon potential

$$V(r) = -\frac{V_0}{1 + \exp[(r - R)/a_0]}$$

Square well (a = 1, V_0 = 4): Examples of choice of B

$$\hbar = c = 1$$

E = 1 with N = 12

b_{11}	b_{12}	b_{22}	condition	δ_{-1} (first)	δ_{-1} (second)
0	0	0	−0.9999995012	64.714757	64.7147757
0	1	0	−1.0000011585	64.714777718163	
0	−1	0	−0.9999998874		64.714777718165
1	0	1	−0.9999999055	64.714780	64.7147766
1	1	1	−0.9999998703	64.7147798	64.71470
	exact		−1	64.714777718179	64.714777718179

Simplest cases

$$\boldsymbol{B} = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \qquad R_\kappa = 2\mathcal{R}_{11}$$

$$\boldsymbol{B} = \begin{pmatrix} 0 & -1 \\ -1 & 0 \end{pmatrix} \qquad R_\kappa = -\frac{1}{2\mathcal{R}_{22}}$$

Square well: Examples of convergence

κ = -1 (s1/2)

E	N	$(b_{11}, b_{12}, b_{22}) = (0, 0, 0)$	$(b_{11}, b_{12}, b_{22}) = (0, -1, 0)$
1	6	64.93	64.67
	8	64.707	64.71471
	10	64.71492	64.71477767
	12	64.714775720	64.714777718165
	15	64.7147777185	64.714777718179
exact		64.71477771818	64.714777718179
100	60	49.02	49.01
	65	49.1689	49.1683
	70	49.168654	49.16866386
	75	49.16866389	49.168664041763
exact		49.168664041791	49.168664041791

$$\hbar = c = 1$$

Woods-Saxon potential

Potential from Halderson 1988
E = 49.3 MeV

a	$N=10$	$N=20$	$N=30$	$N=40$
		$\kappa=-1$		
5	1.346494	1.346637	1.346637	1.346637
6	1.346965	1.348382	1.348382	1.348382
7	1.330724	1.349453	1.349454	1.349454
8		1.349513	1.349499	1.349499
9		1.349468	1.349527	1.349527

- Stable results
- Fast convergence with respect to N
- Slower convergence with respect to a

Bound states with *R*-matrix method

N_i basis functions in the internal region: $\varphi_j(r)$

N_e basis functions in the external region: $\chi_j(r)$

$$P_\kappa^{\text{ext}}(r) = \sum_{j=1}^{N_e} p_{\kappa j}^{\text{ext}} \chi_j(r) \qquad Q_\kappa^{\text{ext}}(r) = \sum_{j=1}^{N_e} q_{\kappa j}^{\text{ext}} \chi_j(r)$$

Internal matrix equations

$$(\boldsymbol{\mathcal{M}}_\kappa^{\text{int}} - E\boldsymbol{I}) \begin{pmatrix} \boldsymbol{p}_\kappa^{\text{int}} \\ \boldsymbol{q}_\kappa^{\text{int}} \end{pmatrix} = \boldsymbol{L} \begin{pmatrix} \boldsymbol{p}_\kappa^{\text{ext}} \\ \boldsymbol{q}_\kappa^{\text{ext}} \end{pmatrix}$$

External matrix equations

$$(\boldsymbol{\mathcal{M}}_\kappa^{\text{ext}} - E\boldsymbol{I}) \begin{pmatrix} \boldsymbol{p}_\kappa^{\text{ext}} \\ \boldsymbol{q}_\kappa^{\text{ext}} \end{pmatrix} = \boldsymbol{L}^T \begin{pmatrix} \boldsymbol{p}_\kappa^{\text{int}} \\ \boldsymbol{q}_\kappa^{\text{int}} \end{pmatrix}$$

$$\boldsymbol{L} = \tfrac{1}{2}\hbar c \boldsymbol{F}^{\text{int}} (\boldsymbol{J} + \boldsymbol{B})(\boldsymbol{F}^{\text{ext}})^T$$

External non-linear equations

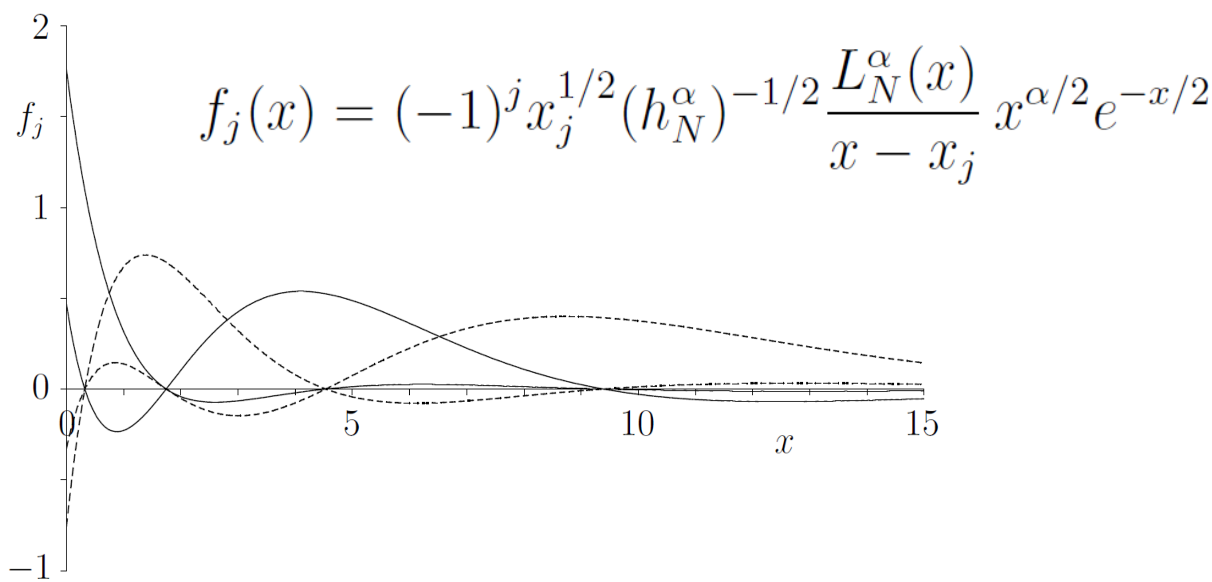
$$\left[\boldsymbol{\mathcal{M}}_\kappa^{\text{ext}} - \boldsymbol{L}^T \left(\boldsymbol{\mathcal{M}}_\kappa^{\text{int}} - E\boldsymbol{I}\right)^{-1} \boldsymbol{L}\right] \begin{pmatrix} \boldsymbol{p}_\kappa^{\text{ext}} \\ \boldsymbol{q}_\kappa^{\text{ext}} \end{pmatrix} = E \begin{pmatrix} \boldsymbol{p}_\kappa^{\text{ext}} \\ \boldsymbol{q}_\kappa^{\text{ext}} \end{pmatrix}$$

Internal non-linear equations

$$\left[\boldsymbol{\mathcal{M}}_\kappa^{\text{int}} - \boldsymbol{L} \left(\boldsymbol{\mathcal{M}}_\kappa^{\text{ext}} - E\boldsymbol{I}\right)^{-1} \boldsymbol{L}^T\right] \begin{pmatrix} \boldsymbol{p}_\kappa^{\text{int}} \\ \boldsymbol{q}_\kappa^{\text{int}} \end{pmatrix} = E \begin{pmatrix} \boldsymbol{p}_\kappa^{\text{int}} \\ \boldsymbol{q}_\kappa^{\text{int}} \end{pmatrix}$$

Resolution by iteration

Regularized Lagrange-Legendre functions in the internal region
Shifted Lagrange-Laguerre functions in the external region



Example: Ground-state of Coulomb potential for $Z = 1$

Lagrange-Legendre functions in internal region
Lagrange-Laguerre functions in external region

- No need for analytical expression
- No need for evaluation of matrix elements

N_i	N_e	a	$E_{0,-1}$	a	$E_{0,-1}$
10	10	3	-0.50000665659458	5	-0.50000665658562
10	20		-0.50000665659451		-0.50000665658534
10	30		-0.50000665659447		-0.50000665658520
20	10		-0.50000665659639		-0.50000665659619
20	20		-0.50000665659638		-0.50000665659616
20	30		-0.50000665659637		-0.50000665659616
30	10		-0.50000665659646		-0.50000665659645
30	20		-0.50000665659649		-0.50000665659645
30	30		-0.50000665659648		-0.50000665659645
exact			-0.50000665659655		-0.50000665659655

Fast convergence with respect to N_i and N_e for both a values

Example: potential – erf(r) / r

N_i	N_e	h	$a = 3$	$a = 5$	N	h	Laguerre mesh
$n = 0$							
10	10	0.4	−0.3311413562	−0.3311398	60	0.4	−0.331141353619722
10	20		−0.3311413562	−0.3311398		0.5	−0.331141353619743
20	10		−0.3311413536179	−0.33114135361966	70	0.4	−0.331141353619718
20	20		−0.331141353619727	−0.331141353619735		0.5	−0.331141353619716
$n = 1$							
10	10	0.8	−0.1014472097	−0.1014468	60	0.5	−0.101447208869135
20	20		−0.1014472088686	−0.101447208869143	70	0.5	−0.101447208869125
30	30		−0.101447208869150	−0.101447208869172			
$n = 2$							
10	10	1.1	−0.04827838	−0.04827825	60	0.5	−0.048278412436445
20	20		−0.048278412440	−0.048278412436461	70	0.5	−0.048278412436438
30	30		−0.048278412436378	−0.048278412436470			

Comparison with Lagrange-Laguerre calculation on (0,∞)

Conclusion

R-matrix description of Schrödinger or Dirac continuum

- Accurate phase shifts (no condition at boundary)
- Lagrange-mesh simplification
- Wave functions available
- Fast convergence

P. Descouvemont, D. B., Rep. Prog. Phys. 73 (2010) 036301

R-matrix description of Dirac bound-states

- New approach with internal and external *R*-matrices
- Iteration
- Accurate bound-state energies
- Wave functions available

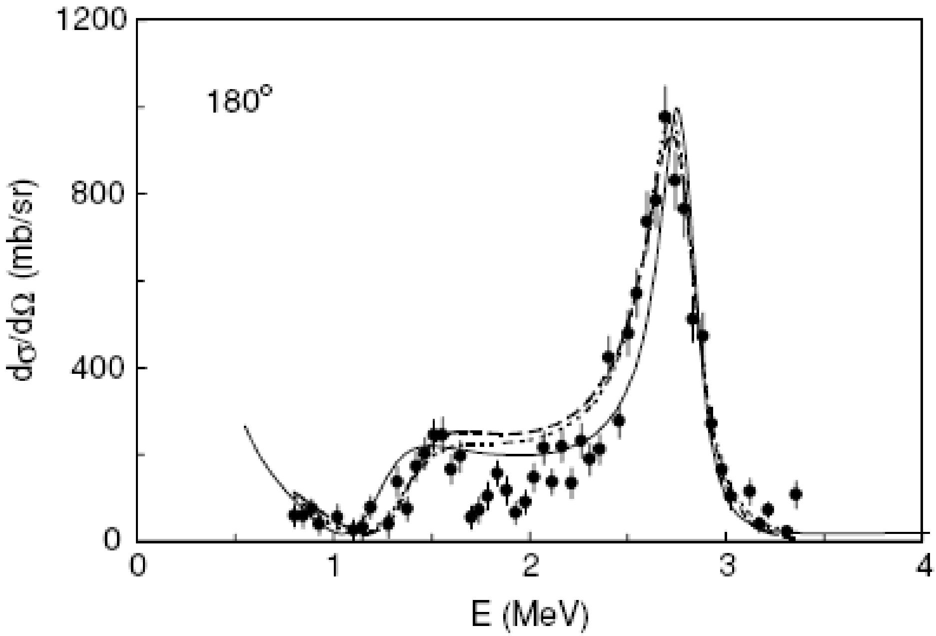
D. B., Phys. Rev. A 92 (2015) 042112

Comparison of PRM and CRM

Phenomenological:
single pole
(dotted: a = 4 fm,
dashed: a = 5 fm)

Calculable:
microscopic cluster model
(RGM, full line)
$a > 8$ fm

$^{14}O + p$



D.B., P. Descouvemont, F. Leo, Phys. Rev. C 72 (2005) 024309

Exp: V.Z. Goldberg et al, Phys. Rev. C 69 (2004) 031302