Continuum of Dirac equation with *R*-matrix method

CANHP, Kyoto, 28 October 2015

Daniel Baye
Université Libre de Bruxelles (ULB)
Brussels,Belgium

Continuum of Dirac equation with *R*-matrix method

- Introduction
- Principle of *R*-matrix methods
- Bloch-Dirac equations
- *R*-matrix method for Dirac scattering
- Lagrange-mesh simplification
- Examples
- [*R*-matrix method for Dirac bound states]
- [Examples]
- Conclusion

Introduction

- Numerical solutions of Dirac equation for bound states:
- Stability of variational techniques?
- Role of negative-energy continuum?

- Very accurate energies and wave functions with simple Lagrange-mesh calculations:
- Accurate energies, wave functions and matrix elements for singular and non-singular potentials

- Very accurate results for the continuum?
- *R*-matrix method

Pedagogical example:
Dirac-Coulomb problem

The Lagrange-Laguerre mesh provides the exact energies and wave functions of the Dirac equation for a Coulomb potential with small numbers N of mesh points for any Z.

- Exact ground-state energy, wave function, mean radius for any Z with only two mesh points ($N = 2$).

- Accurate dipole polarizability of ground state (13+ digits): $N = 6$ for $Z = 1$ to $N = 100$ for $Z = 100$.

- Two-photon transition probabilities.

D. B., L. Filippin, M. Godefroid, Phys. Rev. E 89 (2014) 043305
L. Filippin, M. Godefroid, D. B., Phys. Rev. A 90 (2014) 052520
D. B., Phys. Reports 565 (2015) 1

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)
- Relativistic extension (Goertzel 1948)

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

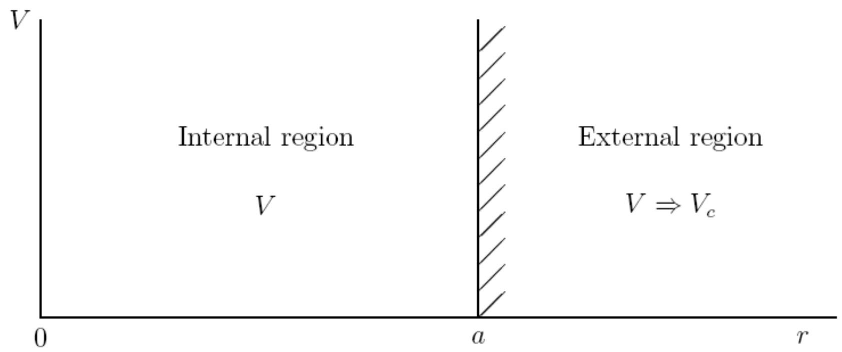
- Relativistic extension (Chang 1975, Halderson 1988)
- Convergence problems

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

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

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

$$(H_l - E)u_l = 0 \qquad H_l = T_l + V(r)$$

Bloch operator

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

$$\int_0^a f(H_l + \mathcal{L})g\,dr = \int_0^a g(H_l + \mathcal{L})f\,dr$$

Bloch-Schrödinger equation

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

R matrix

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

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

Phase shift (independent of *B* !, weakly dependent on *a* if *a* large enough)

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

Contrary to some claims, the *R*-matrix method can provide a simple and accurate description of the continuum of the Schrödinger equation.

A controversy still exist about its accuracy for the Dirac equation

Present goal:
Derive an accurate calculable *R*-matrix method for the Dirac equation

To this end:
- 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

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

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

Quantum numbers

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

Coupled radial equations

$$H_\kappa \left(\begin{array}{c} P_\kappa(r) \\ Q_\kappa(r) \end{array}\right) = E \left(\begin{array}{c} P_\kappa(r) \\ Q_\kappa(r) \end{array}\right)$$

2 x 2 matrix radial Hamiltonian

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

Bloch – Dirac equations

2 x 2 Bloch operator (no derivative!)

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

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

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

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

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

Solution in the internal region: expansion over an orthonormal basis

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

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

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

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 $\boldsymbol{B} = 0$

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

Continuity

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

Auxiliary R matrix

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

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

Compatibility

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

R matrix

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

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

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 $\boldsymbol{B}$

Bloch operator

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

Auxiliary R matrix

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

Continuity

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

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

General form of R matrix

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

Utility?

Lagrange-mesh simplification

N Lagrange functions $f_i(x)$ infinitely differentiable over (*a*,*b*) associated with *N* mesh points x_i, verifying two conditions.

(i) Lagrange condition:
→ Lagrange functions vanish at all mesh points but one

$$f_i(x_j) = \lambda_i^{-1/2} \delta_{ij}$$

(ii) Gauss condition:
→ Gauss quadrature approximation is exact for products of Lagrange functions

Corollary: Lagrange functions are orthonormal

$$\langle f_i | f_j \rangle = \int_a^b f_i(x) f_j(x) dx = \langle f_i | f_j \rangle_G = \sum_{k=1}^{N} \lambda_k f_i(x_k) f_j(x_k)$$

$$\langle f_i | f_j \rangle_G = \sum_{k=1} \lambda_k \lambda_i^{-1/2} \delta_{ik} \lambda_j^{-1/2} \delta_{jk} = \delta_{ij} \quad \Rightarrow \quad \langle f_i | f_j \rangle = \int_a^b f_i(x) f_j(x) dx = \delta_{ij}$$

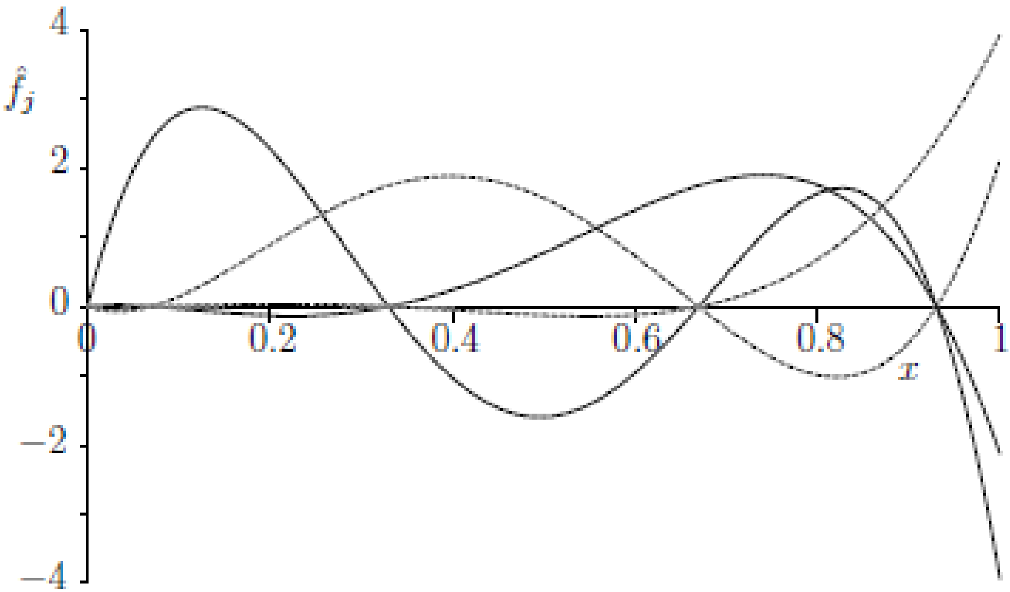
D. B., P.-H. Heenen, J. Phys. A 19 (1986) 2041
D. B, Phys. Reports 565 (2015) 1

Regularized Lagrange-Legendre functions over [0,1]

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

$$\hat{f}_j(x) = (-1)^{N-i}\sqrt{\frac{1-x_j}{x_j}}\,\frac{xP_N(2x-1)}{x-x_j}$$

$$\hat{f}_j(0) = 0 \qquad \hat{f}_j(\hat{x}_i) = \hat{\lambda}_i^{-1/2}\delta_{ij}$$



T. Druet, D.B., P. Descouvemont, J.-M. Sparenberg, Nucl. Phys. A 845 (2010) 88
D.B., Phys. Reports 565 (2015) 1

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

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

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

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

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

- 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

$$\hbar = c = 1$$

Simplest cases

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

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

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

$E = 1$ with $N = 12$

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		64.7147771818	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

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

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

Matrix elements

$$F^{\mathrm{int}}_{i,1} = F^{\mathrm{int}}_{N+i,2} = \varphi_i(a), \quad F^{\mathrm{int}}_{i,2} = F^{\mathrm{int}}_{N+i,1} = 0, \quad i = 1, \ldots, N$$

$$\boldsymbol{\mathcal{M}}^{\mathrm{int}}_{\kappa} = \boldsymbol{M}^{\mathrm{int}}_{\kappa} + \tfrac{1}{2}\hbar c \boldsymbol{F}^{\mathrm{int}} \boldsymbol{B} (\boldsymbol{F}^{\mathrm{int}})^T$$

$$F^{\mathrm{ext}}_{i,1} = F^{\mathrm{ext}}_{N+i,2} = \chi_i(a), \quad F^{\mathrm{ext}}_{i,2} = F^{\mathrm{ext}}_{N+i,1} = 0, \quad i = 1, \ldots, N$$

$$\boldsymbol{\mathcal{M}}^{\mathrm{ext}}_{\kappa} = \boldsymbol{M}^{\mathrm{ext}}_{\kappa} + \tfrac{1}{2}\hbar c \boldsymbol{F}^{\mathrm{ext}} \boldsymbol{B} (\boldsymbol{F}^{\mathrm{ext}})^T$$

$$M^{\mathrm{ext}(1,1)}_{\kappa ij} = \langle \chi_i | V(r) | \chi_j \rangle \qquad M^{\mathrm{ext}(2,2)}_{\kappa ij} = \langle \chi_i | V(r) - 2mc^2 | \chi_j \rangle$$

$$M^{\mathrm{ext}(2,1)}_{\kappa ij} = \quad M^{\mathrm{ext}(1,2)}_{\kappa ij} = \hbar c \langle \chi_i | - d/dr + \kappa/r - \tfrac{1}{2}\delta(r-a) | \chi_j \rangle$$

External non-linear equations

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

$$\left[\boldsymbol{\mathcal{M}}_\kappa^{\rm ext} - \tfrac{1}{2}\hbar c\boldsymbol{F}^{\rm ext}(-\boldsymbol{J}+\boldsymbol{B})\boldsymbol{\mathcal{R}}^{\rm int}(\boldsymbol{J}+\boldsymbol{B})(\boldsymbol{F}^{\rm ext})^T\right]\left(\begin{array}{c}\boldsymbol{p}_\kappa^{\rm ext}\\ \boldsymbol{q}_\kappa^{\rm ext}\end{array}\right) = E\left(\begin{array}{c}\boldsymbol{p}_\kappa^{\rm ext}\\ \boldsymbol{q}_\kappa^{\rm ext}\end{array}\right)$$

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

Internal non-linear equations

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

$$\left[\boldsymbol{\mathcal{M}}_\kappa^{\rm int} - \tfrac{1}{2}\hbar c\boldsymbol{F}^{\rm int}(\boldsymbol{J}+\boldsymbol{B})\boldsymbol{\mathcal{R}}^{\rm ext}(-\boldsymbol{J}+\boldsymbol{B})(\boldsymbol{F}^{\rm int})^T\right]\left(\begin{array}{c}\boldsymbol{p}_\kappa^{\rm int}\\ \boldsymbol{q}_\kappa^{\rm int}\end{array}\right) = E\left(\begin{array}{c}\boldsymbol{p}_\kappa^{\rm int}\\ \boldsymbol{q}_\kappa^{\rm int}\end{array}\right)$$

External auxiliary *R* matrix

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

Resolution by iteration

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 Dirac continuum

- Fast convergence
- Accurate phase shifts
- Wave functions available
- Extension to the Coulomb case possible but more complicated asymptotic expressions

R-matrix description of Dirac bound-states

- New approach with internal and external *R*-matrices
- Iteration
- Accurate bound-state energies
- Wave functions available
- No restriction on potential

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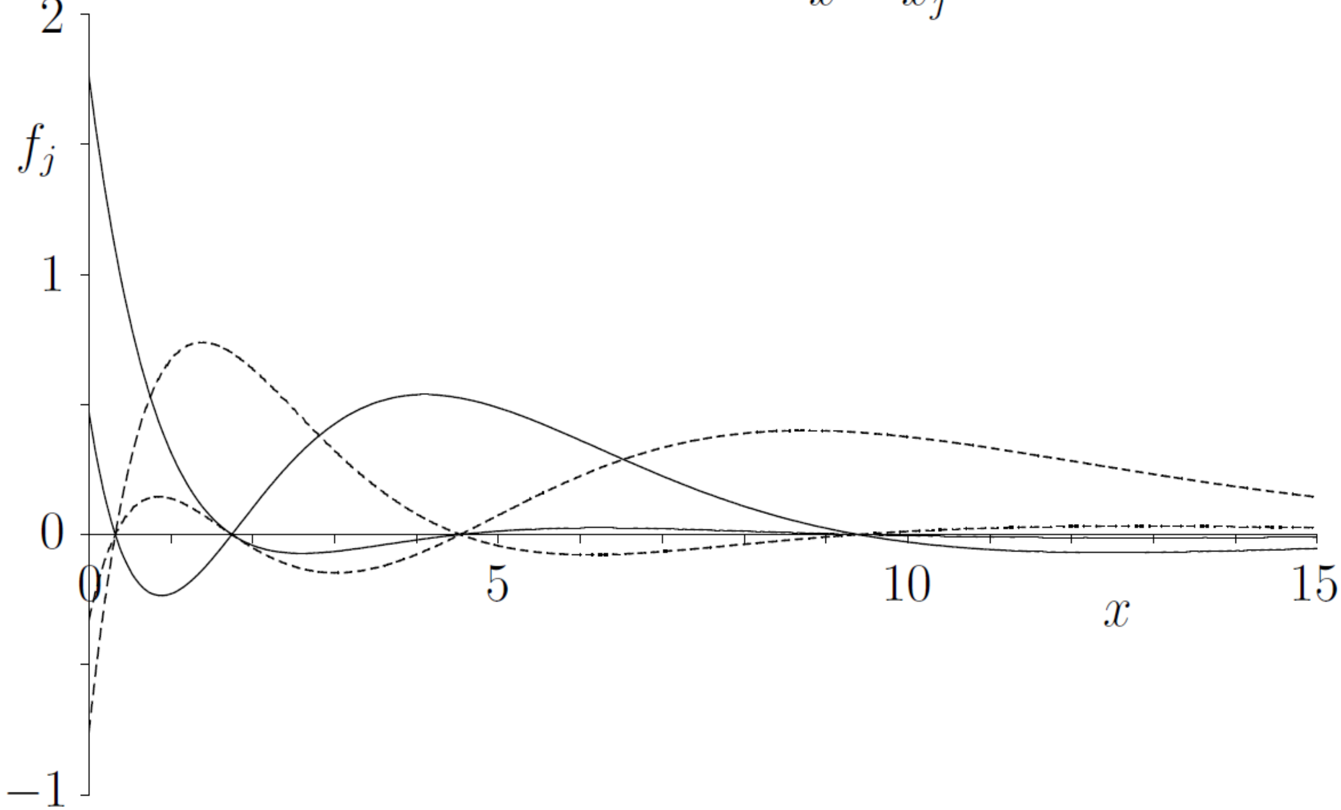
Lagrange-Laguerre mesh over $(0,\infty)$

$$L_N^\alpha(x_i) = 0$$

Lagrange-Laguerre functions

$$f_j(x) = (-1)^j x_j^{1/2} (h_N^\alpha)^{-1/2} \frac{L_N^\alpha(x)}{x - x_j}\, x^{\alpha/2} e^{-x/2}$$



Lagrange-Laguerre basis in external region:

$$\chi_j(r) = h^{-1/2} f_j[(r-a)/h]$$

- scale parameter *h* to be adjusted

Lagrange-mesh 'Hamiltonian minus Bloch operator' matrix

$$M_{\kappa ij}^{\mathrm{ext}(1,1)} = V(hx_i + a)\delta_{ij} \qquad M_{\kappa ij}^{\mathrm{ext}(2,2)} = [V(hx_i + a) - 2mc^2]\delta_{ij}$$

$$M_{\kappa ij}^{\mathrm{ext}(2,1)} = M_{\kappa ij}^{\mathrm{ext}(1,2)} = \hbar c \left[\frac{1}{h} \langle f_i | \frac{d}{dx} + \frac{1}{2}\delta(x) | f_j \rangle + \frac{\kappa}{hx_i + a}\delta_{ij} \right]$$

$$\langle f_i | \frac{d}{dx} + \frac{1}{2}\delta(x) | f_j \rangle = (-1)^{i-j} \frac{x_i + x_j}{2\sqrt{x_i x_j}\,(x_i - x_j)} \qquad i \neq j$$

$$\langle f_i | \frac{d}{dx} + \frac{1}{2}\delta(x) | f_i \rangle = 0$$

● No calculation of integrals → potential values at mesh points

Ground state of hydrogenic atoms with *N* = 2

$$\kappa = -1$$

$$x_{1,2} = 2\gamma \mp \sqrt{2\gamma} \qquad \gamma = \sqrt{\kappa^2 - \alpha^2 Z^2}$$

4 x 4 Lagrange-mesh Hamiltonian matrix

$$\boldsymbol{H}_{-1} = \left(\begin{array}{cc|cc} -\frac{2Z^2}{x_1} & 0 & -\frac{Z}{\alpha x_1} & -\frac{2Z}{\alpha}\sqrt{\frac{x_2}{x_1}}\frac{1}{x_2-x_1} \\ 0 & -\frac{2Z^2}{x_2} & -\frac{2Z}{\alpha}\sqrt{\frac{x_1}{x_2}}\frac{1}{x_1-x_2} & -\frac{Z}{\alpha x_2} \\ \hline -\frac{Z}{\alpha x_1} & -\frac{2Z}{\alpha}\sqrt{\frac{x_1}{x_2}}\frac{1}{x_1-x_2} & -\frac{2Z^2}{x_1} - \frac{2}{\alpha^2} & 0 \\ -\frac{2Z}{\alpha}\sqrt{\frac{x_2}{x_1}}\frac{1}{x_2-x_1} & -\frac{Z}{\alpha x_2} & 0 & -\frac{2Z^2}{x_2} - \frac{2}{\alpha^2} \end{array} \right)$$

Its third eigenvalue gives the exact energy for any *Z.*
The corresponding eigenvector gives the exact wave function.

Exact 3rd eigenvalue

$$E_{1s1/2} = -\frac{Z^2}{\gamma + 1}$$

3rd eigenvector

$$(\boldsymbol{p}^T_{1s1/2}, \boldsymbol{q}^T_{1s1/2}) = -\frac{1}{2}\sqrt{\frac{\gamma+1}{2\gamma}} \left(\sqrt{x_1}, \sqrt{x_2}, -\frac{Z\alpha\sqrt{x_1}}{\gamma+1}, -\frac{Z\alpha\sqrt{x_2}}{\gamma+1} \right)$$

$\rightarrow$ exact radial components

$$P_{1s1/2}(r) = -\sqrt{\frac{\gamma+1}{8\gamma}} [\sqrt{x_1}\, \hat{f}_1^{(\alpha')}(2Zr) + \sqrt{x_2}\, \hat{f}_2^{(\alpha')}(2Zr)] = \sqrt{\frac{(\gamma+1)Z}{\Gamma(2\gamma+1)}} (2Zr)^{\gamma} e^{-Zr}$$

$$Q_{1s1/2}(r) = -\frac{Z\alpha}{\gamma+1} P_{1s1/2}(r)$$

Exact mean value with Gauss quadrature

$$\langle r \rangle = h\, \frac{x_1^2 + x_2^2}{x_1 + x_2} = Z^{-1}\left(\gamma + \frac{1}{2}\right)$$