

**Solving Momentum-Space Coupled-Channels
Equations for Electron-Atom Scattering
Using a Rotated-Contour Method**

Anthony John Blackett

BSc (Hons)

This thesis is presented for the degree of Doctor of Philosophy
at Murdoch University

Division of Science, Murdoch University

March 2002

Declaration

I declare that this thesis is my own account of my research and contains as its main content work which has not previously been submitted for a degree at any tertiary educational institution.



Anthony John Blackett

Abstract

In the last twenty years, electron-atom scattering theory has witnessed significant theoretical developments. One of these advances is the use of the momentum-space convergent close-coupling approach to fully incorporate target atom continua. This theoretical framework is based on the momentum-space Lippmann-Schwinger equation, an integral form of the Schrödinger equation. Although the approach has been highly successful in its application to atomic scattering theory, computing numerical solutions is inherently difficult because the momentum-space LS equation is a singular integral equation. Standard numerical integration techniques are normally employed to solve the problem and as computing power has increased, calculations have improved. However, there remains the problem of the integral's singular nature, which demands complicated methods for selecting integration points, particularly near the energy-dependant singularity. The rotated-contour method uses a complex-variable approach that solves the momentum-space LS equation by integrating along a deformed contour in the complex momentum plane away from the singularities. This method has the potential for simplifying the numerical integrations associated with the close-coupling equations.

A rotated-contour method is first applied to a simple scattering model – electron scattering from the Yukawa potential. This gives some insight into the difficulties that arise when calculating potential matrix elements for complex momenta. The method is then applied to the s -wave model of the electron-hydrogen scattering problem and finally, the full

Abstract

problem. Existing FORTRAN software written to solve the momentum-space LS equations for electron-hydrogen scattering using standard techniques has been converted to C++. Extensive modification of the code has resulted in a flexible Windows-based program with a graphical user interface that runs on any modern computer using PC architecture. The program can calculate results using either a conventional method (no rotation) or a rotated-contour method.

Using a rotated-contour method to solve the momentum-space LS equations necessitates detailed knowledge of the analytic nature and singularity structure of the coupled-channels potentials. This is achieved through the extensive use of the computer symbolic algebra system Maple to compute closed-form solutions for the direct potentials and for a range of partial-wave direct and exchange potentials. It is found that logarithmic branch point singularities are present on the real momentum axis for an extensive class of partial-wave direct-potential matrix elements. The analysis reveals that a rotated-contour method cannot be applied to the full atomic scattering problem due to these analytic problems which are associated with the long-range nature of the Coulomb potential.

Contents

	Declaration	i
	Abstract	iii
	Contents	v
	List of Figures	xi
	List of Tables	xiii
	Acknowledgements	xv
1	Introduction	1
	1.1 Momentum-Space Coupled-Channels Equations	1
	1.2 Numerical Software	4
	1.3 Symbolic Computer Algebra	7
	1.4 Notation and Conventions	8
2	Atomic Scattering Amplitudes: A Computational Overview	11
	2.1 One-Channel T-Matrix and Scattering Amplitudes	12
	2.2 Solving the Lippmann-Schwinger Equation	15
	2.2.1 Partial-wave expansions	16
	2.2.2 Cauchy principal-value integral – regularisation	18
	2.2.3 Quadrature integration – matrix solution	20

2.3	Overview of Solving Coupled-Channels Equations	22
2.4	Calculating Potential Matrix Elements	25
2.4.1	Electron-electron direct matrix elements	27
2.4.2	Electron-core direct matrix elements	31
2.4.3	Electron-electron exchange matrix elements	33
2.4.4	Energy-dependent exchange matrix elements	34
2.5	Calculating Observable Quantities	36
2.6	Characterisation of the LS Kernels	36
2.6.1	Partial-wave potentials in closed form	37
2.6.2	Real-valued momentum formulations of LS kernels	39
3	Solving Momentum-Space LS Equations by Rotated Contours	45
3.1	The Rotated-Contour Method	46
3.1.1	An analytic example of the rotated-contour method	49
3.2	Contour Rotation Applied to the LS Equation	51
3.3	Mapping the LS Equation's Singularity Structure	54
3.3.1	Restrictions on the contour-rotation angle	58
4	Yukawa Scattering: Illustration of a Rotated-Contour Approach	61
4.1	Computing Yukawa-Potential Matrix Elements	63
4.1.1	Partial-wave expansion of the potential matrix	63
4.1.2	Analytic approach to evaluating potentials	64
4.1.3	Numerical integration for evaluating potentials	68

4.2	Solving the Lippmann-Schwinger Equation	72
4.2.1	Singularity-structure analysis for the Yukawa potential	72
4.2.2	Contour-rotation angle constraints	76
4.3	Numerical Solution	77
4.3.1	Potential matrix elements	78
4.3.2	Second-Born T-matrix elements	80
4.3.3	Full T-matrix elements	90
5	Analytic Structure of Potentials for s-Wave Model e-H Scattering	93
5.1	s-Wave Model Born-Series' Singularity Structures	94
5.1.1	Singularity structure for the direct $1s$ - $1s$ kernel	96
5.1.2	Singularity structure for the direct $1s$ - $2s$ ($2s$ - $1s$) kernel	99
5.1.3	Singularity structure for the direct $2s$ - $2s$ kernel	102
5.2	Contour-Rotation Angle Constraints	103
5.3	Analytic Continuation of Direct Potentials	104
5.3.1	$1s$ - $1s$ partial-wave direct potential in closed form	104
5.3.2	$1s$ - $2s$ partial-wave direct potential in closed form	105
5.3.3	$2s$ - $2s$ partial-wave direct potential in closed form	106
5.4	Analytic Continuation of Exchange Potentials	107
5.4.1	$1s$ - $1s$ partial-wave exchange potential in closed form	108
5.4.2	$1s$ - $2s$ partial-wave exchange potential in closed form	109
5.4.3	$2s$ - $2s$ partial-wave exchange potential in closed form	110

5.5	Evaluating Partial-Wave Exchange Integrals	111
5.5.1	Integrals for the energy-dependent exchange potential	112
5.5.2	Integrals for the two-electron exchange potential	115
6	Rotated-Contour CC(ns) Electron-Hydrogen Scattering Results	125
6.1	Program Structure and Methodology	125
6.1.1	Calculating s -wave direct potentials on a rotated contour . . .	127
6.1.2	Calculating exchange potentials on a rotated contour	129
6.2	Single-Channel e-H Elastic Scattering – CC(1s)	130
6.2.1	Direct potential for the $1s$ - $1s$ transition	131
6.2.2	Exchange potential for the $1s$ - $1s$ transition	134
6.2.3	CC(1s) T-matrix elements and differential cross sections . . .	136
6.3	Two-State Coupling e-H Scattering – CC(1s,2s)	140
6.3.1	Direct potentials for $2s$ - $2s$, $1s$ - $2s$ and $2s$ - $1s$ transitions	141
6.3.2	Exchange potentials for $2s$ - $2s$, $1s$ - $2s$ and $2s$ - $1s$ transitions . .	143
6.3.3	CC(1s,2s) T-matrix and differential cross sections	145
6.4	Three-State Coupling e-H Scattering – CC(1s,2s,3s)	146
7	Analytic Structure of General Potentials for e-H Scattering	149
7.1	Singularity Structures of Direct $1s$ - $2p$ Kernels	150
7.1.1	Analytic properties of the $1s$ - $2p_0$ direct potential	150
7.1.2	Analytic properties of the $1s$ - $2p_{\pm 1}$ direct potential	155
7.1.3	Analytic properties of general direct potentials	156

7.2	Analytic Structure of Partial-Wave Direct Potentials	157
7.2.1	Analytic structure of $1s-2p$ partial-wave direct potential	158
7.2.2	Numerical $1s-2p$ and $2p-1s$ partial-wave direct potential	162
7.2.3	Analytic structure of $2p-2p$ partial-wave direct potential	166
7.2.4	Numerical $2p-2p$ partial-wave direct potential	167
7.3	Partial-Wave Exchange Potentials	169
7.3.1	Analytic structure for $1s-2p$ exchange potential	170
7.4	Consideration of Modified Contours	175
8	Conclusions	179
8.1	Rotated-Contour Method	179
8.2	Computer Algebra Systems	182
8.3	Numerical Software Development in C++	184
A	Selected Useful Formulae	187
A.1	Wigner $3-j$ and $6-j$ Symbols	187
A.2	Clebsch-Gordan Coefficients	188
A.3	Legendre and Associated Legendre Polynomials	188
A.4	Spherical Harmonics	188
A.5	Integrals	190
A.6	Hypergeometric Functions	190

B	Potential Matrix Elements for Electron-Atom Scattering	191
B.1	Potential Matrix as a Partial-Wave Expansion	192
B.2	Partial-Wave Potential Matrix Elements	194
B.3	Direct-Potential Matrix Elements	195
B.3.1	Electron-core direct-potential matrix elements	196
B.3.2	Electron-electron direct-potential matrix elements	196
B.4	Exchange-Potential Matrix Elements	203
B.4.1	Energy-dependent exchange-potential matrix elements	205
B.4.2	Electron-electron exchange-potential matrix elements	207
C	Content of the CDROM	211
C.1	CDROM Overview	211
C.2	CDROM Contents	212
C.3	Computed Analytic Potentials	213
	References and Bibliography	217

List of Figures

Figure 2.1:	Basic atomic scattering experiment	13
Figure 2.2:	Direct potential and kernel for $1s$ - $1s$ e-H scattering	40
Figure 2.3:	Direct potential and kernel for $1s$ - $2s$ e-H scattering	41
Figure 2.4:	Direct potential and kernel for $2p$ - $1s$ e-H scattering	42
Figure 3.1:	Complex contours for deriving the rotated-contour method	47
Figure 4.1:	Real and imaginary parts of spherical Bessel $j_0(z)$	69
Figure 4.2:	Real and imaginary parts of spherical Hankels $h_0^{(1,2)}(z)$	71
Figure 4.3:	Singularity structure of potential matrix elements	74
Figure 4.4:	Contour-rotation angle convergence of VG_0V for $\mu/k = 5$	84
Figure 4.5:	Rotation convergence of VG_0V amplitudes for $\mu/k = 1$	87
Figure 4.6:	Contour-rotation angle convergence of VG_0V for $\mu/k = 1/5$	88
Figure 5.1:	Orientation of the momentum-transfer vector \mathbf{K}	95
Figure 5.2:	e-H Born-series $1s$ - $1s$ singularity structure	98
Figure 5.3:	e-H Born-series $1s$ - $2s$ singularity structure	101
Figure 5.4:	e-H Born-series $2s$ - $2s$ singularity structure	102
Figure 6.1:	TCrossWin interaction settings dialog box	126
Figure 6.2:	$1s$ - $1s$ half-off-shell partial-wave ($J = 0$) direct potential	132
Figure 6.3:	$1s$ - $1s$ half-off-shell partial-wave ($J = 0$) exchange potential	136
Figure 6.4:	$1s$ - $1s$ differential cross section for e-H scattering	140
Figure 6.5:	$2s$ - $2s$ half-off-shell partial-wave ($J = 0$) direct potential	141
Figure 6.6:	$1s$ - $2s$ half-off-shell partial-wave ($J = 0$) direct potential	142

List of Figures

Figure 6.7:	$2s$ - $1s$ half-off-shell partial-wave ($J = 0$) direct potential	142
Figure 6.8:	$2s$ - $2s$ half-off-shell partial-wave ($J = 0$) exchange potential .	143
Figure 6.9:	$1s$ - $2s$ half-off-shell $J = 0$ partial-wave exchange potential ..	144
Figure 6.10:	$2s$ - $1s$ half-off-shell $J = 0$ partial-wave exchange potential ..	144
Figure 6.11:	$1s$ - $1s$ and $1s$ - $2s$ differential cross sections	145
Figure 6.12:	$1s$ - $1s$, $1s$ - $2s$ and $1s$ - $3s$ differential cross sections	146
Figure 7.1:	Singularity structure of $1s$ - $2p_0$ e-H direct potentials	153
Figure 7.2:	Direct potential log function and its derivative	160
Figure 7.3:	Direct potential log function on rotated contour	161
Figure 7.4:	$2p$ - $1s$ half-off-shell partial-wave ($J = 0$) direct potential	165
Figure 7.5:	$1s$ - $2p$ half-off-shell partial-wave ($J = 0$) direct potential	165
Figure 7.6:	$2p$ - $2p$ direct potential log function and its derivatives	167
Figure 7.7:	$2p$ - $2p$ half-off-shell partial-wave ($J = 0$) direct potential	168
Figure 7.8:	$2p$ - $2p$ half-off-shell partial-wave ($J = 1$) direct potential	169
Figure 7.9:	$1s$ - $2p$ half-off-shell partial-wave ($J = 0$) exchange potential .	172
Figure 7.10:	$2p$ - $1s$ half-off-shell partial-wave ($J = 0$) exchange potential .	173
Figure 7.11:	$1s$, $2s$, $2p$ differential cross sections (exchange only)	174

List of Tables

Table 2.1:	$1s$ - $1s$ direct-potential matrix elements for e-H scattering	38
Table 4.1:	Potentials for electron-Yukawa scattering	79
Table 4.2:	VG_0V for electron-Yukawa potential scattering	83
Table 4.3:	T-matrix convergence for electron-Yukawa scattering	91
Table 6.1:	$1s$ - $1s$ partial-wave ($J=0$) direct potentials	131
Table 6.2:	$1s$ - $1s$ on-shell direct potential and second-Born T-matrix . . .	134
Table 6.3:	$1s$ - $1s$ partial-wave ($J=0$) exchange potentials	135
Table 6.4:	$1s$ - $1s$ on-shell potential and second-Born T-matrix	137
Table 6.5:	$1s$ - $1s$ on-shell T-matrix and V-matrix	138
Table 7.1:	$2p$ - $1s$ partial-wave ($J=0$) direct potentials	164

Acknowledgements

I must first give my appreciation and thanks to Professor Andris Stelbovics, my PhD supervisor, for his guidance and helpful support not only throughout this thesis, but through my entire undergraduate and postgraduate studies. Andris' depth of knowledge over a broad spectrum of scattering theory has been invaluable, and he has always been willing and able to provide expert help whenever it was required. His continued support in the face of apparently insurmountable problems gave me renewed vigour which ultimately resulted in the completion of this thesis.

My sincere gratitude goes to my wife Carol who has suffered immeasurably over the many years that it has taken to reach this conclusion of my studies. Without her continued support at home, completing this thesis would have been impossible. We can now look forward to enjoying our future together free of study and the lonely nights and weekends that have been an inescapable aspect of our life over the past thirteen years since starting my undergraduate studies as a part-time student.

My thanks also goes to Associate Professor Stephen Thurgate, who first directed me onto this path of study in physics, and his support throughout my studies is very much appreciated. I'm also indebted to Associate Professor Ken Harrison for his fascinating undergraduate course on the *Complex Variable*, and for listening to and answering my many questions concerning complex variable techniques. I would also like to extend my

Acknowledgements

appreciation for the contribution of moral support given by Professor Igor Bray in the latter stages of the thesis and for his willingness to help wherever possible.

My appreciation is also offered to Dr Bill Scott for his helpful discussions on Maple, its idiosyncrasies, and for his generous provision of a copy of maple7 at a most fortuitous time.

Appreciation is also given to Dr Chris Lund for his moral support and for the financial support that he gave in the form of work that allowed me to survive this difficult time.

I would also like to acknowledge my fellow students, Tony Shackleton and Philip Bartlett, for the many discussions we had on numerical and algebraic computing, and to Katrina Lyon and Dr Chris Lund for the use of their colour laser printer in the production of this thesis.

Finally, financial support for this work was provided primarily by the Australian Federal Government through the Australian Postgraduate Award Scheme and without which, this work would not have been undertaken.