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

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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.

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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

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.

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