APPLICATION OF L^2 METHODS IN ATOMIC SCATTERING

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

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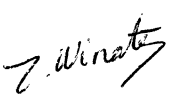
I declare that this thesis is my own account of my research and contains as its main content work which has not previously been submitted for a degree at any University.



Toto Winata

Dedicated

To my wife, Monita and my son, Radite

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ABSTRACT

An L^2 expansion of Yamani and Reinhardt [1975] which employs non-orthogonal, square integrable functions of Laguerre type is used to approximate Coulomb wave functions of continuum and bound states. The convergence of L^2 approximations to continuum and bound states is investigated in the hydrogenic case.

The connection between the L^2 approximation and pseudo states is derived by studying the completeness relation for the exact states and the quadrature approximations. Corresponding equivalent weights are shown to be related to a Gaussian quadrature derived from attractive-Coulomb Pollaczek polynomials. Gaussian quadrature rules that are satisfied are calculated numerically.

The use of pseudo states in the close-coupling equations is discussed especially in relation to the Poet [1978] model which gives a highly accurate solution for a simplified model of electron-hydrogen collisions in which only s-wave hydrogen target states are admitted. The convergence of channel potentials which contribute to the close-coupling equations is then examined and discussed. the convergence of pseudostate Born amplitudes is studied as a further test in obtaining a good pseudo-state set. In addition, the convergence rate of the L^2 approximation to the bound-bound, bound-free channel and free-free channel potentials is examined. The bound-bound, bound-free potentials are shown to converge geometrically while the free-free potentials have very slow convergence.

In order to examine the effect of convergence rates several detailed models are employed and compared with the full Poet calculations. Elastic, discrete inelastic, total ionisation and inelastic cross-sections are presented for the energy interval 1.0 to 3.5 Rydbergs. Triplet scattering is reproduced excellently. Singlet scattering displays minor pseudo-resonance structure for the largest (10 basis set) calculations. Weak coupling approximations are examined. They perform very well in triplet scattering but decidedly less well for the singlet channel.