Chapter 1

Introduction

1.1 Motivation and Aim

Theoretical electron-atom collision physics is an immensely rich and diversified field of study. The main goal is to model as accurately as possible the interaction of atoms with electrons (or positrons) and to confirm the predictions with experimental observables. One such model of electron-hydrogen scattering is the Temkin-Poet [1, 2] model and it has attracted a great deal of attention in recent years. This would at first seem surprising since, even though it retains enough complexity associated with the treatment of exchange and the continuum it ignores much of the essential physics of real electron-atom collisions by neglecting angular momentum coupling. Other methods, for example, convergent close coupling (CCC) [3, 4], intermediate energy R-Matrix (IERM) [5], R-Matrix with pseudo-states (RMPS) [6], and the second-order distorted-wave (DWB2) [7] have been highly successful in modelling general scattering experiments. The question is, then, if the Temkin-Poet model is not an accurate representation of electron scattering, why study it?

The answer lies in the fact that the model, due to its simplicity, provides a superb

testing ground for methods designed to solve the general electron-atom problem. The main advantage of having an exact solution of limited complexity is that other more general methods designed to solve the full problem can be tested in this restrictive case, and an idea of their accuracy obtained. The quality of the solution may then be used as a gauge for assessing the accuracy of the approximation before an attempt at applying it to a more realistic problem is made.

The Poet model is also sometimes called the "s-wave" model of electron-hydrogen scattering. In this method the interaction potential $1/r_{12}$ between the two electrons is replaced by $1/r_>$ where $r_>$ is the greater of the two electron-proton distances, facilitating a separation of variables. This simplification enabled Poet [1] to derive a set of equations for the elements of the scattering matrix which was considerably simpler than than those using other techniques to solve the Schrödinger equation. Poet applied the method using the S-matrix equations to obtain accurate cross sections for elastic and the excitation of the $2s$ and $3s$ states.

Callaway and Oza [8] used a pseudo-state method to calculate elastic and excitation cross sections for the 2s and 3s states and after averaging found good agreement with the exact results of Poet. Subsequently Callaway and Oza [9] used an extension of another later method proposed by Poet [10] and the optical theorem to estimate ionisation cross sections. More recently the CCC method [11] was applied to the Temkin-Poet problem to obtain convergent results in complete agreement Poet. After this successful demonstration of the CCC method Bray and Stelbovics [12] applied it to the full electron-hydrogen problem. The authors subsequently returned to the simplified model to obtain more detailed information than that given by Poet and, in addition to extending the range of energies, included ionisation and total cross sections [13]. Bartschat and Bray [14] also applied an RMPS method to electron-hydrogen scattering in the Temkin-Poet model and reported excellent

agreement to their CCC calculation for elastic, excitation, and total cross sections obtained at incident electron energies between 0 and 100 eV.

The Temkin-Poet model has often been used to test other methods prior to their application to the general problem. Wang and Callaway [15], for example, demonstrated the effectiveness and accuracy of their calculations for electron-hydrogen scattering for total angular momentum L=0 with close coupling and other direct numerical methods. Bhatia *et al* [16] applied a one-channel T-matrix variational principle to the spherically symmetric model of electron-hydrogen scattering to calculate total cross sections. They found no spurious structures and their results were in excellent agreement with Callaway and Oza [9]. Direct coordinate-space methods for solving the Schrödinger equation in the Temkin-Poet model have proved highly successful, too. Jones and Stelbovics [17], [18] implemented a finite-difference scheme to numerically integrate Schrödinger's equation subject to asymptotic boundary conditions and obtained results for elastic, inelastic and ionisation, accurate to one percent. This was the first time matching to asymptotic boundary conditions was shown to yield convergent ionisation amplitudes for a Coulomb three-body problem.

Investigations into the s-wave model for other target systems have been made (e.g. [19] and [20]), but such studies have not been as numerous as those for electron-hydrogen scattering. Despite the fact that the calculation of physical processes for electron scattering from positive ions is formally only slightly more complicated than scattering from neutral targets, the extra complexity coming from the target boundary conditions, substantial numerical difficulties nevertheless do exist. One problem associated with both R-matrix and close-coupling schemes, for example, is the appearance of pseudo-resonances (a series of unphysical resonances in the continuum) in the scattering cross sections. In the R-matrix method the elimination of such unphysical features is carried out by a process called T-matrix averaging.

Slim and Stelbovics [21] have provided a formal justification for this procedure. In the coupled channels method it is known that such features can be eliminated by use of an L^2 Laguerre basis. Initial calculations were carried out by Winata [22] to demonstrate the reduction in size of these features with size of the basis set in the Temkin-Poet model. The full demonstration of convergence in the CCC method was given later [11]. For ion targets, given that infinite series of Feshbach resonances are present below each inelastic threshold, the pseudo-resonant structure associated with any discretisation of the continuum is much more complicated near the ionisation threshold. Any method to obtain accurate cross sections should therefore be applied to the solution of the Temkin-Poet model for hydrogen-like ions. Bartschat and Bray [23] applied both the CCC and IERM methods to calculate excitation and ionisation cross sections for electron-helium ion scattering in the simplified s-wave model and noted the disappearance of pseudoresonant structure with increasing basis size. The same observation was noted earlier by Konovalov and McCarthy [24] who applied a J-matrix method to the Temkin-Poet model for electron-hydrogen scattering where it was found that no averaging was needed to obtain the converged results. Thus the Temkin-Poet model has proved very useful in uncovering numerical difficulties that would have undesirable effects when applied to the full scattering problem. Resolving these kinds of problems in a simplified model is the first step towards a better theory.

The power of the Temkin-Poet model should not be underestimated as there is much to be learned about the physics of scattering through the application of a simplified approach. It has been noted [25], for example, that since angular correlations are completely absent in the s-wave model, the excellent agreement between theory and experiment (cf. [26] and [27]) shows that the net effects of such angular correlations in the total ionisation cross section must average to zero over a wide range of energies.

In view of the importance of the Temkin-Poet model as a useful tool for theoretical development, further investigations are warranted since there are questions relating to aspects of the model that still pose fundamental and significant challenges. The first of these concerns the ionisation of hydrogen, particularly in the energy region immediately above the ionisation threshold. What makes the problem different from inelastic scattering are the conceptual and technical difficulties associated with the scattering boundary conditions for three free Coulomb particles. In 1953 Wannier[28] predicted that near the ionisation threshold the cross section for ionisation of a neutral atom by incident electrons should be proportional to E^k, where E is the excess energy above threshold and $k = 1.127$. Although based on purely classical analysis [29] (i.e., not derived from quantum mechanics), it has nevertheless provided a forum for much debate, experimentation and a great number of theoretical physics papers (e.g., [30] and [31]). While the Wannier threshold law appears to be now well established, its range of validity however has not been definitively determined by theory calculations. Recently the near-ionisation-threshold behaviour for the Temkin-Poet model has been discussed by Ihra and Macek and co-workers [32, 33]. They predicted an exponentially suppressed ionisation cross section in contrast to the Wannier prediction. One of the investigations carried out in this thesis will be a numerical study for the model with a view to establishing the validity of the Ihra-Macek scaling laws and the region of their applicability.

A further topic of interest for which only a few studies have been carried out [34] is the nature of the scaling laws for discrete inelastic transitions. Because of the accurate solutions we are able to generate, we can investigate them in detail. In particular, the near-ionisation threshold region should be of interest, the reason being that because ionisation is suppressed it is not unreasonable to expect that unusual behaviour of the inelastic cross sections may also occur.

Another interesting area concerns the modelling of electron scattering by hydrogen-like ions. Although it is similar to that of electron scattering by hydrogen in that both are described by the one-electron Hamiltonian, one must use Coulomb-wave rather than plane-wave boundary conditions for inelastic scattering. This adds an extra complexity to the problem with the appearance of so-called closed-channel or Feshbach resonances in the cross section arising from the temporary capture of an incident electron by the excited ion. Determining their energies and widths require special techniques to extract the eigenvalues of the scattering matrix. Again, because of the high accuracy of our methods we can provide definitive positions and widths for the Temkin-Poet model, thus providing a benchmark set of results for other methods.

The aim of this thesis is not only to obtain highly accurate solutions for a special case of electron scattering. Concomitant to the quantitative prediction of our computed cross sections is the interpretation of their observed behaviour, particularly where deviations from other published works are exhibited, and to endeavour to explain why such deviations exist.

1.2 Scattering Theory

1.2.1 Basic Principles

First, we briefly summarise the scattering process for a single particle moving in a potential field. A complete description of scattering is necessarily obtained by solving the time dependent Schrödinger equation

$$H|\Psi\rangle \;=\; i\hbar\frac{\partial}{\partial t}|\Psi\rangle. \tag{1.1}$$

The operator H, called the Hamiltonian, is the physical observable corresponding to the total energy of the system, given by

$$H = K + V \tag{1.2}$$

where K is the kinetic energy and V is the total potential energy. It is important to note that Eq. (1.1) does not have a unique solution unless it is solved with the appropriate boundary conditions. They describe the state of the system before and after a scattering process and depend on the experiment being performed. If the potential is independent of time, Eq. (1.1) has stationary state solutions of the form

$$\psi(\mathbf{r}, t) = e^{-iEt/\hbar}\psi_E(\mathbf{r}) \tag{1.3}$$

where $\Psi_E(r)$ satisfy the time independent Schrödinger equation [1]

$$\left[-\frac{1}{2}\nabla^2 + V(r) - E\right]\psi_E(\mathbf{r}) = 0. \tag{1.4}$$

We will use the time-independent formulation for the modelling of the scattering process.

[1] We assume atomic units where $\hbar = m = 1$

Asymptotically the scattering wavefunction will be a sum of incident and scattered waves

$$\psi(\mathbf{r}) \;=\; \psi_{in}(\mathbf{r}) + \psi_{sc}(\mathbf{r}) \underset{r\to\infty}{\sim} e^{i\mathbf{k}.\mathbf{r}} + f(\theta,\phi)\frac{e^{ikr}}{r} \tag{1.5}$$

where the momentum of the incident beam of particles is $k = \sqrt{2E}$ and for simplicity we assume only elastic scattering is possible.

Eq. (1.5) expresses the physical situation where an incident particle beam described by an incoming plane wave is scattered by a potential at $r = 0$ to produce a spherical wave directed radially outward from the scattering centre. The scattering amplitudes $f(\theta,\phi)$ give the relative strength of the scattered wave in the direction of $\mathbf{r}$, defined by the angles θ, ϕ relative to the scattering plane, and are generally complex functions of the scattering energy. As such they define the wavefunction in the collision region and hence embody all the experimental observables such as cross sections and transition amplitudes. It is therefore the basic function we seek to determine.

1.2.2 Electron-Atom Collisions

The above description of the scattering process is suitable for describing a scattering event in which neither the target nor projectile has any internal structure. However, in any realistic interaction such as the scattering of electrons by atoms or molecules several reactions may occur:

(i) The projectile is scattered without loss of energy. This is referred to as elastic scattering where only the momentum direction of the projectile is altered.

(ii) The projectile suffers a loss of energy leading to a change or rearrangement to the internal structure of the target. This is referred to as inelastic scattering where the transition from one state to another in the target is accompanied by a change in both the momentum and energy of the scattered particle.

(iii) The kinetic energy of the incident particle is sufficient enough to break up the internal composition of the target, leading to the ejection of one (or more) constituent particles.

Let us now consider the problem of scattering of an electron from a hydrogenic ion. We summarise the scattering formalism and define the relevant properties of the scattering process and the resulting S-matrix that will be used in the remainder of the thesis. The Schrödinger equation describing the interaction between an electron and atomic hydrogen (or hydrogenic ion of atomic number $Z \geq 2$) is given by

$$\left(-\frac{1}{2}\nabla_1^2 - \frac{1}{2}\nabla_2^2 - \frac{Z}{r_1} - \frac{Z}{r_2} + \frac{1}{|\mathbf{r_1} - \mathbf{r_2}|}\right)\Psi(\mathbf{r_1}, \mathbf{r_2}) = E\Psi(\mathbf{r_1}, \mathbf{r_2}) \tag{1.6}$$

in atomic units. Let us label the spin by the quantum number S. If we assume that the total spin and orbital angular momenta of the two electrons are conserved, the Pauli principle demands that the coordinate-space wave function have the symmetry property

$$\Psi^S(\mathbf{r_1}, \mathbf{r_2}) = (-1)^S \Psi^S(\mathbf{r_2}, \mathbf{r_1}) \tag{1.7}$$

where S=0 (singlet) or S=1 (triplet). For simplicity we will omit the explicit mention of the spin label S although it is to be assumed that all scattering amplitudes and S-matrix elements implicitly depend on it. Here $\mathbf{r_1}$ and $\mathbf{r_2}$ are the coordinates of the projectile and target electrons, respectively, with the origin of the coordinate system being the target nucleus. Let us consider the scattering process

$$\mathrm{e}^- + \mathrm{A(i)} \rightarrow \mathrm{e}^- + \mathrm{A(j)} \tag{1.8}$$

in which an electron is incident on a target atom in an initial eigenstate ψ_i with energy ϵ_i, followed by the subsequent emergence of an electron leaving the target atom in the final eigenstate ψ_j. From conservation of energy we have

$$\epsilon_{tot} = \frac{1}{2}k_i^2 + \epsilon_i = \frac{1}{2}k_j^2 + \epsilon_j. \tag{1.9}$$

For a neutral target we seek solutions to Eq.(1.6) having the asymptotic form

$$\Psi(\mathbf{r_1},\mathbf{r_2}) \underset{r_1\to\infty}{\sim} \psi_i(\mathbf{r_2})\, e^{i\mathbf{k_i}.\mathbf{r_1}} + \sum_j \psi_j(\mathbf{r_2})\, f_{ji}(\mathbf{k_j},\mathbf{k_i})\, \frac{e^{ik_j r_1}}{r_1} \tag{1.10}$$

where $\psi_i(\mathbf{r_2})e^{i\mathbf{k_i}.\mathbf{r_1}}$ describes the initial channel and $f_{ji}(\mathbf{k_j},\mathbf{k_i})$ is the scattering amplitude for a transition which leaves the target atom in the state ψ_j. This equation differs from Eq. (1.5) in that the scattering wavefunction contains contributions at infinity from all atomic states corresponding to open channels (i.e., those channels for which $k_j^2 \geq 0$). It should be noted that we have not specified ionisation boundary conditions at this stage; that is, the target electron remains bound to the atom. This particular contribution to the scattering will be addressed later. The remaining states, corresponding to closed channels ($k_j^2 < 0$) give decaying terms and do not contribute to the asymptotic form; however, they are important when the projectile electron is near the target, leading to the formation of resonances (intermediate short-lived bound states). For ion targets, the exponentials in Eq. (1.10) must be modified by including the logarithmic phase factors due to the distortion by the Coulomb field. Because the asymptotic form of Eq. (1.10) separates into sum of products in variables $\mathbf{r_1}$ and $\mathbf{r_2}$ it is reasonable to construct a method of solution for Ψ that utilises this fact.

The Temkin-Poet model is derived by considering only the total l=0 partial wave and, moreover, permitting only transitions between target states of s-symmetry. The scattering boundary condition obtained by the partial-wave decomposition of Eq. (1.10) can be written for the l=0 partial wave as

$$\psi(r_1,r_2) \underset{r_1\to\infty}{\sim} \psi_i(r_2)\, e^{-ik_i r_1} - \sum_{j\,\epsilon\, open} \psi_j(r_2)\, e^{ik_j r_1}\, S_{ji}. \tag{1.11}$$

Here S_{ji} are the S-matrix elements connecting all open channels. Since $|S_{ji}|^2$ is the probability of transition to a final state j from an initial state i, a sum over all open

channels must give

$$\sum_{j\ \epsilon\ open} |S_{ji}|^2 = 1. \tag{1.12}$$

If we have a hydrogenic ion as the target we replace the plane waves ($e^{\pm ikr}$) by Coulomb waves. The appropriate generalisation for this is to use the regular and irregular Coulomb functions (see appendix A) whose asymptotic forms for l=0 are given respectively by

$$F_0(\eta,\rho) \underset{r\to\infty}{\sim} \sin(kr - \eta \ln 2kr + \sigma_0) \tag{1.13}$$

$$G_0(\eta,\rho) \underset{r\to\infty}{\sim} \cos(kr - \eta \ln 2kr + \sigma_0) \tag{1.14}$$

where $\sigma_0 = \arg\Gamma(1+i\eta)$ is the Coulomb phase shift, $\eta = (z-1)/k$ and $\rho = kr$.

Choosing the combination

$$H_0^{\pm}(k,r) = G_0(kr,\eta) \pm iF_0(kr,\eta) \tag{1.15}$$

$$\underset{r\to\infty}{\sim} \exp \pm i(kr - \eta \ln 2kr + \sigma_0) \tag{1.16}$$

generates incoming (−) and outgoing (+) distorted plane waves for an electron incident on a ion. For a neutral atom we have $\eta = 0$ and we recover our familiar plane waves.

The partial cross sections for elastic and inelastic scattering are defined by

$$\sigma_{ji}^S = \frac{1}{k_j^2}\frac{2S+1}{4}\left|\delta_{ij} - S_{ij}^S\right|^2. \tag{1.17}$$

The total cross section is obtained by summing over all states accessible from state i and is given by the optical theorem

$$\sigma_{total} = \frac{2S+1}{2k_i^2}\Big(1 - Re(S_{ii})\Big). \tag{1.18}$$

The cross section averaged over singlet and triplet spin states is given by

$$\sigma_{av} = \frac{1}{4}\sigma_s + \frac{3}{4}\sigma_t. \tag{1.19}$$

1.2.3 Properties of the S-Matrix

We finish by noting some properties of the S-matrix which will be required later. From Eq. (1.12) it follows that the S-matrix is unitary:

$$SS^\dagger = S^\dagger S \;=\; 1 \tag{1.20}$$

and from time reversal invariance it also follows that the S-matrix is symmetric:

$$S_{ji} = S_{ij}. \tag{1.21}$$

Since the S-matrix S is unitary and symmetric, it may be diagonalised by a real orthogonal matrix R, where

$$\sum_q R_{iq} R_{qj} = \delta_{ji}. \tag{1.22}$$

If R^T is the transpose of R, we may write

$$S = R^T \bar{S} R \tag{1.23}$$

where $\bar{S}$ is diagonal

$$\bar{S}_{ji} = \delta_{ji} \exp(2i\Delta_j). \tag{1.24}$$

In terms of matrix elements

$$S_{ji} = \sum_l R_{jl} e^{2i\Delta_j} R_{il}. \tag{1.25}$$

The parameters Δ_j are called eigenphase shifts. Where only one channel is open the eigenphase shifts reduce to the ordinary phase shift δ, but where two or more channels are open the phase shift is given by the sum of eigenphases in each channel:

$$\delta(E) \;=\; \sum_j \delta_j(E). \tag{1.26}$$

Near a resonance the S-matrix is well approximated by [35]

$$S_{ji}(E) \;=\; S_{ji}^{bg} \;-\; \frac{i\gamma_j\gamma_i}{E - E_R + i\Gamma/2} \tag{1.27}$$

where S^{bg} is an energy-dependent background, Γ is the total width of the resonance and the γ are the partial widths for decay into an open channel.

A resonance is typically identified in the cross section where the phase shift undergoes a rapid increase through an odd multiple of $\frac{\pi}{2}$ about a narrow energy interval centred about the maximum of the peak. For a pure resonance described by a Lorentzian this corresponds to its full width at half maximum. The width of a resonance peak relates to the rate of decay of the resonant state. The resonance position E_R and width Γ are determined by parametrizing the Breit Wigner formula

$$\tan \Delta_l = \frac{\Gamma_0}{E_0 - E} + A(E). \tag{1.28}$$

and solving for the parameters E_0, Γ_0 and A over an energy region surrounding the resonance energy. Equivalently the resonance energy and width are given by:

$$\Gamma_0^{-1} = \left.\frac{d\Delta_l}{dE}\right]_{E=E_0} \tag{1.29}$$

$$\Gamma = \frac{2\Gamma_0}{1 + A^2} \tag{1.30}$$

$$\epsilon = \frac{\Gamma_0}{1 + A^2} \tag{1.31}$$

$$E_R = E_0 + \epsilon. \tag{1.32}$$

The term $A(E)$ represents the slowly varying Coulomb background and is linear or quadratic in energy.

The partial widths for decay into channel l from a resonant state ji is

$$\gamma_j = [R_{jl}]^2 \, \Gamma$$

$$\gamma_i = [R_{il}]^2 \, \Gamma \tag{1.33}$$

and, since R is orthogonal, have the property

$$\Gamma = \sum_j \mid \gamma_j \mid^2 . \tag{1.34}$$

1.3 Approximation Methods

There are several factors which make the electron-atom scattering problem more complicated than simple potential scattering:

(i) The first involves the exchange interaction due to exchange symmetry properties of the wavefunction of the "electron + atom" system with respect to interchange of its arguments. The scattering cross sections are therefore spin-dependent.

(ii) The second concerns excitation of the target. When a particle collides with a target that has some internal structure (e.g., an atom), inelastic scattering can occur. The onset of inelastic processes appears as a loss of probability flux from the incident beam, leading to excitation or ionisation of the target.

(iii) The third relates to electron-impact ionisation of an atom where one assumes that the incident electron recedes faster than the ionised electron. In the collinear geometry of the Temkin-Poet model (and assuming no exchange with the ionised electron takes place) the incident electron will still see the screened charge on the target atom.

The complexity of a particular method depends on how, or whether at all, it is capable of modelling each of these processes. Problems associated with the tractability of the problem also have to be addressed. For example, in any approach to solving the scattering problem by numerical means two fundamental issues arise:

(i) An N-body problem in general involves solving a 3(N-1) variables in coordinate space. To make the problem tractable, one attempts to solve the equation in a region where an approximate separation of variables is possible, or in a region where one variable becomes asymptotically larger than the others.

(ii) Since there are many possible final states in a collision, the total wavefunction is given by an infinite sum over discrete (bound) states and an integration over

the continuum, each term in the sum being weighted by the probability of a transition to that particular state. But, as a computer is a finite-state machine, any realistic calculation can only approximate this. The choice of representation, then, automatically imposes an unavoidable limitation on the form of the solution. As a result, any approximation is only reliable over a limited range of energies. The grouping of scattering theories to different energy regimes (viz., low, intermediate and high) is thus seen to arise more from theoretical considerations and less from the phenomenology characterising a particular scattering process.

Calculations of scattering amplitudes are generally of two types: perturbation series expansions based on the Born approximation and non-perturbative approaches based on the expansion of a trial wavefunction in a set of basis functions.

The Born series is a perturbation series expansion of the scattering wavefunction, or the scattering amplitude, in powers of the interaction potential. In the Born approximation the interaction between an incident particle and an atomic target is treated as a weak perturbation. This is valid at larger energies where the high speed of the projectile limits the momentum transferred in the collision; basically the scattered electron moves so quickly that neither it nor the target is strongly influenced by the electron potential. Exchange of the incident electron with the target is regarded as unlikely and the absence of any correlation in the motions of the two means that we can represent the system as an independent set of free particle and the target states. The Born approximation appears as the first term of the expansion of a collision parameter in powers of the interaction potential between a particle and an atom. The distorted wave Born approximation (DWBA) is an extension of the first Born approximation in which the incident wave plane wave is replaced by a distorted wave arising from the static projectile-atom interaction. Notable investigations using the DBWA approximation include three-body ionisation [36]

and (e,2e) calculations for hydrogen and helium [37].

A further refinement to DWBA theory enables target polarisation and flux loss due to inelastic scattering to be built into the theory by adding an additional contribution, obtained by iterating the defining equation once to generate a second-order approximation. This is known as the second-order distorted-wave Born approximation (DW2BA) and has been applied to electron-hydrogen scattering [7, 38, 39, 40] and electron-sodium [41] for which it has yielded reliable results in the intermediate and high energy ranges with significant improvement between theory and experiment over the first order approximation.

The R-matrix method is a variational approach to atomic scattering in which the numerical solution of the three-body Schrödinger equation in a finite, spherical region is matched to two-body boundary conditions in the exterior region to yield transition amplitudes. The inner region is made just large enough to envelope the atomic target states of interest. When the scattered electron is in the interior region it can be considered to form a complex with the atom and thus behaves very much like a bound state. In this region exchange and correlation effects are important and their contributions to the scattering amplitude are explicitly included in the scattering wavefunction. When the scattered electron is in the external region, however, electron exchange with the target is can be neglected and the scattered electron moves in the weak long-range potential of the target; the wavefunction is then represented by an asymptotic or perturbation expansion. The R-Matrix with pseudostates (RMPS) method improves convergence by including a large number of so-called "pseudostates". These states are not true eigenstates but are chosen to approximate the higher discrete states and continuum. This method has been applied both to electron-hydrogen scattering [6, 23, 42, 43] and to more complex systems including helium [44, 45], beryllium [46, 47] and boron [48] targets.

Another variation, the intermediate energy R-matrix (IERM) method, developed by Burke *et al* [5] and analysed by Scholz [49], uses different expansions in the internal and external regions, including bound and continuum states of the target in the internal region and a set of bound orbitals in the external region. This particular method has offered a stable numerical solution for electron scattering calculations [50, 51, 52, 53, 54] and is especially suited to calculations at intermediate energies where many continuum channels are open.

The close-coupling approximation is another non-perturbational method in which the total wavefunction of the system is represented as a superposition of the ground state and all excited state wave functions of the atom. The coefficients in this superposition are functions of the scattered electron coordinates and describe the interaction of the scattered electron with the atom. Expanding the Schrödinger equation in terms of these functions then converts it into a system of coupled integro-differential equations. The number of equations is infinite but can be approximated by replacing the system by a finite one and neglecting the rest.

In the coupled-channel optical method (CCO), first pioneered by McCarthy and Stelbovics [55], a finite set of channels (P space) are coupled explicitly while the remaining channels including the continuum (Q space) are treated via a complex nonlocal polarisation potential, facilitating the separation of direct and exchange contributions of the elastic channel from the smaller contributions due to coupling to excited states. The CCO method has been moderately successful for electron-hydrogen scattering [56, 57, 58, 59], electron-sodium scattering [57, 58], and electron-helium ion scattering [60].

Convergence is markedly improved by the addition of pseudostates although, as in the RMPS method, a by-product is the appearance of unphysical pseudoresonances.

Elimination of pseudoresonances is achieved by replacing sum over the discrete states and integration over the continuum by a finite sum using as set of special functions, the Laguerre functions, to diagonalise the target Hamiltonian. This method, developed by Bray and Stelbovics [3, 12], is known as the convergent close coupling (CCC) method as scattering amplitudes converge as the number of functions is increased. It is to date by far the most accurate method for describing electron scattering, yielding reliable cross sections for electron-helium ion ionisation [61], electron-helium ion [45] scattering and positron-hydrogen scattering [62], and quite remarkable agreement between theory and experiment for total ionisation cross section and spin symmetry measurements [13, 63].

The above summary serves to illustrate some of the more common approaches that have been used in theoretical atomic scattering over the last three decades. Whatever method we choose to solve a particular physical problem, however, its success lies ultimately in its validation by experiment. But even prior to its application to a realistic scattering problem, a method must at least be capable of reproducing the results of an established benchmark, if one exists. Hence the need for theoretical approaches like the Temkin-Poet model in aiding the development process.

We now turn to its discussion in the next chapter.