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Relativistic Inelastic Scattering Using a Logarithmic Grid

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This paper describes a method for solving a spherically symmetrical non-relativistic or relativistic inelastic scattering problem on a logarithmic grid over the whole radial distance. The relativistic problem involves the calculation of four coupled oscillatory wavefunctions. The oscillatory nature of the wavefunctions usually limits the step size of a numerical method; however it is shown how more slowly varying functions can be obtained enabling the calculation to be performed efficiently on a logarithmic grid.

1. INTRODUCTION

Comparatively few numerical methods have been used for the solution of optical potential problems. The earliest method used is an extension of the WKB transformation and avoids the numerical solution of differential equations determining the phase from the condition that the second derivative of the solution is zero at the classical turning point; details are given by Chen (1). Mizuno and Chen (2) have used a matrix Numerov method for the solution of the complex Schrodinger equation. These seem to be the only numerical methods used until Allison (3) produced a program for calculating non-relativistic absorption and elastic cross sections for electron scattering from neutral atoms. This program uses a Numerov method to perform an outward integration of the complex Schrodinger equation which is matched onto an asymptotic form obtained as a linear combination of spherical Bessel and Neuman functions. This asymptotic series restricts the use of the program to scattering from neutral atoms.

This paper describes the solution of optical potential problems on a logarithmic grid. The program is intended for the calculation of electron scattering from

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positive ions. Although the complex part of the potential is only short range the Coulomb tail of the real part of the potential necessitates the evaluation of the wavefunction over large radial distances. The method previously described by Mayers and Turner (4) for the calculation of single channel wavefunctions using a logarithmic grid does not generalise in a straightforward manner to larger systems of equations. Thus a slightly different technique is described here which it is expected will generalise to enable solution of the multi-channel scattering problem on a logarithmic grid.

The problem is outlined in Section 2 and the method in Section 3. A pair of equations referred to as coupling equations are obtained and solved on a logarithmic grid. The solution of the coupling equations is described in Section 4; Section 5 describes the matching of the inward and outward solutions of the optical potential problem to recover the desired wavefunctions and phase shifts. The paper is concluded with a short discussion in Section 6.

2. Relativistic Optical Potential Problem

The relativistic optical potential problem is described by the following pair of complex equations

$$\begin{aligned} P'(r) + k/rP(r) + f_c(r)\, Q(r) &= 0 \\ Q'(r) - k/rQ(r) - g_c(r)\, P(r) &= 0 \end{aligned} \tag{1}$$

where

$$\begin{aligned} g_c(r) &= 1/c(E - V_c(r)) = g(r) + ih(r) \\ f_c(r) &= g_c(r) + 2c = f(r) + ih(r) \\ V_c(r) &= V_1(r) + iV_2(r) \\ P(r) &= P_1(r) + iP_2(r) \\ Q(r) &= Q_1(r) + iQ_2(r) \\ h(r) &= -1/cV_2(r) \qquad i = \sqrt{-1} \end{aligned} \tag{2}$$

Equation (1) is solved subject to the following boundary conditions

$$P(0) = 0 \qquad P(r) \sim N \operatorname{Sin}(\Psi(r) + \phi) \qquad \text{as} \quad r \to \infty \tag{3}$$

where

$$\Psi(r) = \omega r + \eta \log(2\omega r)$$

$$\omega^2 = 2E + E^2/c^2$$

$$\eta = \tfrac{1}{2}Z/c\{((E + 2c^2)/E)^{1/2} + (E/(E + 2c^2))^{1/2}\} \qquad \text{if} \quad V(r) \to -Z/r$$

$$= 0 \qquad \text{if} \quad V(r) \to 0 \text{ faster than } O(1/r).$$

Suppose the complex phase shift is written as $\phi = \lambda + i\mu$. Then the four components of the wavefunctions given by Eqs. (2) have the following asymptotic form:

$$\begin{aligned} P_1(r) &\to N \operatorname{Cosh}(\mu) \operatorname{Sin}(\Psi(r) + \lambda) \\ P_2(r) &\to N \operatorname{Sinh}(\mu) \operatorname{Cos}(\Psi(r) + \lambda) \\ Q_1(r) &\to -1/N \operatorname{Cosh}(\mu) \operatorname{Cos}(\Psi(r) + \lambda) \\ Q_2(r) &\to 1/N \operatorname{Sinh}(\mu) \operatorname{Sin}(\Psi(r) + \lambda). \end{aligned} \tag{4}$$

It is often convenient to choose $N = (f(\infty)/g(\infty))^{1/4}$ for the normalisation of the solutions to Eqs. (1).

3. Method

Both the relativistic and non-relativistic optical potential scattering problems may be written in the form of a pair of first-order complex coupled ordinary differential equations

$$S' + a_1 S + a_2 T = 0 \tag{5a}$$

$$T' + a_3 T + a_4 S = 0. \tag{5b}$$

There is an obvious correspondence between the above equations and Eqs. (1). The non-relativistic problem can be obtained by choosing the above equations so that

$$\begin{aligned} a_1 &= 0 \\ a_2 &= D(r) \qquad T(r) = Y(r) \\ a_3 &= 0 \qquad S(r) = Y'(r) \\ a_4 &= -1. \end{aligned} \tag{6}$$

$D(r) = 2(E - V_c(r)) - l(l+1)/r^2$ in an obvious notation. If we add a complex multiple τ of Eq. (5b) to Eq. (5a) we can obtain the single first-order equation

$$(S + \tau T)' + \zeta(S + \tau T) = 0 \tag{7}$$

provided that the two following relations hold:

$$\begin{aligned} \zeta &= a_1 + \tau a_4 \\ \tau' + \zeta\tau &= a_2 + \tau a_3. \end{aligned} \tag{8}$$

Eliminating ζ between Eqs. (8) gives a first-order differential equation for τ,

$$\tau' + (a_1 - a_3)\,\tau + a_4 \tau^2 = a_2. \tag{9}$$

We calculate a smooth solution of Eq. (9) which will be referred to as the coupling equation. This means that the variable τ is analogous to the solution of the amplitude equations discussed by Mayers and Turner (4) and changes less rapidly than the oscillatory solution $S(r)$, $T(r)$ we wish to calculate. The coupling equation (9) is solved in the asymptotic region, where r is large and the solution continues inwards to about the classical turning point.

The solution to Eq. (7) is readily obtained from the complex exponential relation

$$\begin{aligned} S + \tau T &= Ne^{-\int \zeta \, dr} \\ N &= \text{constant.} \end{aligned} \tag{10}$$

In order to obtain an oscillatory solution from Eqs. (5a) and (5b), it can be seen that ζ must have a non-trivial imaginary part. This technique may also be used when the complex part of the potential is zero. In this case S, T, N are real, with only τ, ζ complex, and the solution may be obtained by equating real and imaginary parts on either side of Eq. (10). However in the general case we must calculate two different smooth solutions τ to Eq. (9). Equating the real and imaginary parts on either side of Eq. (10) for the two solutions to Eq. (9) leads to a 4×4 system of equations for the four components of the complex equations (5a) and (5b). During the remainder of this paper the method will be illustrated using the relativistic equations.

Suppose $\tau = \alpha - i\beta$, $\zeta = \xi + i\eta$ then for relativistic inelastic scattering equation (9) may be written

$$\begin{aligned} \alpha' + 2k/r\alpha - g(\alpha^2 - \beta^2) - 2h\alpha\beta &= f \\ \beta' + 2k/r\beta + h(\alpha^2 - \beta^2) - 2g\alpha\beta &= -h \\ \xi &= k/r - g\alpha - h\beta \\ \eta &= g\beta - h\alpha. \end{aligned} \tag{11}$$

It will be convenient to denote the two solutions we calculate to Eq. (11) by $\alpha_j, \beta_j, j = 1, 2$ which are used to calculate the functions $\xi_j, \eta_j, j = 1, 2$ defined above. Equations (10) yield the following fourth-order system of equations for the real and imaginary parts of the wavefunctions $P(r)$, $Q(r)$ at each radial grid point

$$\begin{bmatrix} 1 & 0 & \alpha_1 & \beta_1 \\ 0 & 1 & -\beta_1 & \alpha_1 \\ 1 & 0 & \alpha_2 & \beta_2 \\ 0 & 1 & -\beta_2 & \alpha_2 \end{bmatrix} \begin{bmatrix} P_1 \\ P_2 \\ Q_1 \\ Q_2 \end{bmatrix} = \begin{bmatrix} N_1 e^{-\int \xi_1} \operatorname{Sin}\left(\int \eta_1 + \theta_1\right) \\ N_1 e^{-\int \xi_1} \operatorname{Cos}\left(\int \eta_1 + \theta_1\right) \\ N_2 e^{-\int \xi_2} \operatorname{Sin}\left(\int \eta_2 + \theta_2\right) \\ N_2 e^{-\int \xi_2} \operatorname{Cos}\left(\int \eta_2 + \theta_2\right) \end{bmatrix}. \tag{12}$$

The constants N_i, θ_i, $i=1, 2$ are determined by matching the above solutions onto an outward integration of the radial equations (1) close to the classical turning point. This is described in Section 5.

4. Solution of the Coupling Equations

In the limit $r \to \infty$ where $h \to 0$ the relativistic coupling equations (11) have the following approximate smooth solutions

$$\alpha \approx k/rg \qquad \beta \approx \pm(fg - k^2/r)^{1/2}/g \tag{13}$$

The two smooth solutions of the coupling equations we calculate are obtained by starting in the asymptotic region from both the positive and negative β solutions. In the region where $h(r) \neq 0$ approximate analytical solutions to the coupling equations (11) may be obtained by solving the algebraic equations remaining after neglecting the α and β derivatives. Further details are given by Turner (5). This approximate solution may be used as an initial estimate for an iterative scheme for calculate a more accurate solution. This iterative scheme is similar to that used by Mayers and Turner (4) for the solution of the amplitude equations obtained from the relativistic scattering problem. However in this case the coupling equations have only quadratic non-linearities and the following asymptotic series proved to be the most convenient method for solving the coupling equations in the asymptotic region.

We substitute the following series into Eqs. (11)

$$\begin{aligned} \alpha(r) &= \tilde{\alpha}_0 + \sum_{j=1}^{\infty} \tilde{\alpha}_j / r^j \\ \beta(r) &= \tilde{\beta}_0 + \sum_{j=1}^{\infty} \tilde{\beta}_j / r^j. \end{aligned} \tag{14}$$

For large values of r the potential is assumed to be

$$V_c = V_1 + iV_2 = -Z/r.$$

It is then easy to obtain series expansions of α and β in powers of $1/r$, by substituting the expansions (14) into Eq. (11) and equating powers of $1/r$. These series begin with

$$\alpha(r) = \left(\frac{kc}{E}\right) 1/r + \cdots,$$

$$\beta(r) = \left(1 + \frac{2c^2}{E}\right)^{1/2} - \frac{Zc^2}{E^2}\left(1 + \frac{2c^2}{E}\right)^{-1/2} \frac{1}{r} + \cdots.$$

Successive coefficients can then easily be found from recurrence relations and for a given value of r the calculation stops when the terms in both series contribute less than a specified tolerance.

The solution of the coupling equations obtained above in the asymptotic region is continued inwards towards the classical turning point using a Newton-type iterative scheme. This solution may be evaluated on a logarithmic grid. The transformation $\rho = \log r$ of the independent variable is made and the coupling equations solved on a grid using equal step sizes in the ρ variable. For first-order equations this transformation is particularly easy and at each point on the logarithmic grid the following equations are solved:

$$\begin{aligned}
\alpha^{(n)'} + e_1^{(n-1)}\alpha^{(n)} + e_2^{(n-1)}\beta^{(n)} &= rf(r) - rg(r)(\alpha^{(n-1)^2} - \beta^{(n-1)^2}) \\
&\quad - 2rh(r)\,\alpha^{(n-1)}\beta^{(n-1)} \\
\beta^{(n)'} - e_2^{(n-1)}\alpha^{(n)} + e_1^{(n-1)}\beta^{(n)} &= -rh(r) + rh(r)(\alpha^{(n-1)^2} - \beta^{(n-1)^2}) \\
&\quad + 2rg(r)\,\alpha^{(n-1)}\beta^{(n-1)}
\end{aligned}$$

$n = 1, 2, 3, \ldots .$ (16)

$$\begin{aligned}
e_1^{(n-1)} &= 2(k - rg(r)\,\alpha^{(n-1)} - rh(r)\,\beta^{(n-1)}) \\
e_2^{(n-1)} &= 2(rg(r)\,\beta^{(n-1)} - rh(r)\,\alpha^{(n-1)}).
\end{aligned}$$

The acute prime denotes differentiation with respect to ρ.

Convergence of the iterative scheme in Eqs. (16) may be demonstrated by an analysis similar to that described in Section 4 of Mayers and Turner (4). Convergence locally is obtained over a few grid points before continuing the solution over the next group of grid points towards the classical turning point. The unconditionally stable trapezoidal rule is used to continue the asymptotic series solution inwards. The stability of higher order methods applied to the solution of Eqs. (16) may be established by using standard stability theory (see, e.g., Lambert (6)). For potentials with short range complex parts the following approximation

$$e_1^{(n-1)} \approx 0, \qquad e_2^{(n-1)} \approx 2rg(r)\,\beta^{(n-1)}$$

was found sufficient for determining the stability of higher order difference schemes applied to Eqs. (16). The above approximation neglects the complex part of the potential and this is usually valid in the region where fourth-order methods are liable to become unstable. Thus the integration of the coupling equations towards the classical turning point proceeds in the same way as that of the amplitude equations previously discussed by Mayers and Turner (4).

5. Matching Solutions and Phase Determination

Suppose at a given point $r = a$ close to the classical turning point the solutions $P_1(a)$, $P_2(a)$, $Q_1(a)$, $Q_2(a)$ have been obtained by outward integration of the

relativistic optical potential equations and $S_1(a)$, $S_2(a)$, $T_1(a)$, $T_2(a)$ are the real and imaginary parts of the solution of Eq. (7) at the same point. Choosing the lower limit of integration in Eqs. (12) to be the matching point $r=a$ enables these equations to be reduced to

$$\begin{bmatrix} 1 & 0 & \alpha_1(a) & \beta_1(a) \\ 0 & 1 & -\beta_1(a) & \alpha_1(a) \\ 1 & 0 & \alpha_2(a) & \beta_2(a) \\ 0 & 1 & -\beta_2(a) & \alpha_2(a) \end{bmatrix} \begin{bmatrix} S_1(a) \\ S_2(a) \\ T_1(a) \\ T_2(a) \end{bmatrix} = \begin{bmatrix} N_1 \operatorname{Sin}\theta_1 \\ N_1 \operatorname{Cos}\theta_1 \\ N_2 \operatorname{Sin}\theta_2 \\ N_2 \operatorname{Cos}\theta_2 \end{bmatrix}. \tag{17}$$

The inward and outward solutions can be joined since there exists a complex normalisation constant $M_1 + iM_2$ such that

$$\begin{aligned} P_1(a) + iP_2(a) &= (M_1 + iM_2)(S_1(a) + iS_2(a)) \\ Q_1(a) + iQ_2(a) &= (M_1 + iM_2)(T_1(a) + iT_2(a)). \end{aligned} \tag{18}$$

It is convenient to write the normalisation constant in the form

$$N_3 = (M_1^2 + M_2^2)^{1/2}, \qquad \operatorname{Cos}\theta_3 = M_1/N_3, \qquad \operatorname{Sin}\theta_3 = M_2/N_3.$$

We multiply the second of Eqs. (18) by $\alpha_j(a) - i\beta_j(a)$, $j=1, 2$ respectively and, using Eqs. (17), obtain the relations

$$\begin{aligned} W_j(a) &= N_3 N_j \operatorname{Sin}(\theta_j - \theta_3) \qquad j=1, 2, \\ X_j(a) &= N_3 N_j \operatorname{Cos}(\theta_j - \theta_3) \qquad j=1, 2, \end{aligned} \tag{19}$$

where

$$\begin{aligned} W_j(a) &= P_1(a) + \alpha_j(a)\, Q_1(a) + \beta_j(a)\, Q_2(a) \\ X_j(a) &= P_2(a) - \beta_j(a)\, Q_1(a) + \alpha_j(a)\, Q_2(a) \qquad j=1, 2. \end{aligned}$$

The left-hand side of Eqs. (19) is known at the point $r=a$ and $\tan(\theta_j - \theta_3)$, $j=1, 2$, is obtained by dividing Eqs. (19). This gives two relations for the three phases θj, $j=1, 3$. The third relation is obtained from consideration of the asymptotic form of the solution of the optical potential equations (1). Substituting Eqs. (4) into the left-hand side of Eqs. (12) in the asymptotic region where $\alpha_j(\infty)=0$, $\beta_j(\infty) = \pm(f(\infty)/g(\infty))^{1/2} = \pm N^2$, $j=1, 2$, gives the following relations:

$$\begin{aligned} N_1 &= Ne^{\mu} e^{\int^{\infty} \xi_1} \\ N_2 &= Ne^{-\mu} e^{\int^{\infty} \xi_1} \end{aligned} \tag{20}$$

$$\Psi(r)+\lambda=\int^{r_h}\eta_1\,dr+\theta_1$$

$$\Psi(r)+\lambda=-\left(\int^{r_h}\eta_2\,dr+\theta_2\right)$$

$$\theta_1+\theta_2=-\left(\int^{r_h}\eta_1+\eta_2\right)dr \tag{21}$$

where r_h is any point in the asymptotic region such that $h(r_h)$ is negligible.

It can be seen from Eqs. (11) that when $h(r)$ is negligible the two solutions of the coupling equations we calculate differ only in the sign of β. Thus in this region $\eta_1+\eta_2=0$ and the sum $\theta_1+\theta_2$ is determined from the above once r is sufficiently large that $h(r)$ is negligible. The phases θ_j, $j=1, 3$ are obtained from Eqs. (19) and (21). The determination of the normalisation constants N_1 and N_2 in Eq. (20) above requires the evaluation of the infinite range integrals of ξ_j, $j=1, 2$. From Eq. (11) and the asymptotic relation $\alpha\approx k/rg$ it can be seen that provided $h(r)\to 0$ faster than $O(1/r)$ the infinite range integrals remain finite as $r\to\infty$. In fact using the asymptotic series solution (14) the infinite range integral may be evaluated analytically from a sufficiently large radial distance. This is the main reason for using the asymptotic series solution at large radial distances instead of an iterative scheme similar to that previously described by Mayers and Turner (4).

All the N_j, θ_j, $j=1, 3$, may be eliminated between Eqs. (19) and (20) to provide the following expression for the absorption part of the phase shift

$$e^{2\mu}=\left[\frac{W_1(a)^2+X_1(a)^2}{W_2(a)^2+X_2(a)^2}\right]^{1/2}e^{\int^{\infty}\xi_1-\xi_2}. \tag{22}$$

The above provides a convenient evaluation of the imaginary part of the phase shift. Note that when $h(r)=0$ then $\xi_1=\xi_2$ and thus if only the phase shift is required and not the wavefunctions equation (22) may be evaluated by continuing the integration just until $h(r)$ becomes negligible.

6. Discussion

Approximate solutions to the coupling equations (11) may be obtained by solving the non-linear algebraic equations remaining after neglecting the derivatives of α, β. These approximate solutions may be used to define "smoother variable" transformations as previously described by Mayers and Turner (4). However it is the opinion of the authors that again the smoother variable equations offer little if any advantage over the coupling equations themselves.

Instead of multiplying Eq. (5b) by τ, a multiple of Eq. (5a) could equally have been added to Eq. (5b). This leads to an alternative pair of coupling equations instead of Eqs. (11). The two sets of coupling equations are apparently equivalent

with no significant difference in the convergence rates of the corresponding Newton iterations. This is not the case for the amplitude equations previously discussed by Mayers and Turner (4).

The initial power series was obtained assuming the imaginary part of the potential to be a constant near the origin. Thus for Eqs. (5a) and (5b) the following series expansions are used

$$S = \sum_{i=0}^{\infty} S_i^{(\gamma+i)}, \qquad T = \sum_{i=0}^{\infty} T_i r^{(\gamma+i)}.$$

S_i, T_i are complex coefficients obtained by equating the powers of r; γ is obtained from the indicial equation. There is one arbitrary complex constant, say S_0, to be chosen. However the solution obtained from the initial integration depends upon the relative magnitude of the real and imaginary part of S_0. For the inelastic scattering problem here it is appropriate to define S_0 to be real. In this case T_0 is also real and the wavefunctions S and T are only complex through the introduction of a non-zero imaginary part to the potential.

The logarithmic grid used in this paper enables easy integration to large radial distances as required for inelastic scattering from positive ions. In our program potentials with Coulomb and non-Coulomb real parts are handled identically but using different values for the coefficients in the same real asymptotic series. Chen and Peacher (7) describe a number of imaginary potentials which have been used during the testing of this program. The results obtained from the program for potentials with Coulomb real parts have been checked for consistency (i.e., changing the matching point of the inward and outward integrations), since there does not appear to be a readily available program for checking results. For the non-Coulomb complex potentials given by Chen and Peacher (7) the phase shifts evaluated using the method described here have been validated for a number of energies and angular momenta with results obtained from Allison's (3) code.

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