A Numerical Approach to the Solution of Coupled Equations Involved in Electron-Ion and Electron-Atom Scattering Problems

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A numerical procedure is outlined which treats the coupled equations involved in electron-ion scattering, as well as electron-atom scattering, within the close-coupling formalism. The coupled integrodifferential equations of the scattering problem are solved by a two-step process. First, the equations are separated into auxiliary equations which are then solved numerically in the interior region from zero out to some transformation point r_t. Any convenient numerical technique can be used to integrate the equations; in this work, a noniterative integral equation method is used. Next, the long-range potential terms are taken into account at r_t via an open-channel projection technique. This technique simply projects the reactance matrix to its asymptotic value. The numerical procedure is then tested by applying it to e–He$^+$ scattering. Finally, two specific disadvantages of the procedure related to the treatment of closed channels are discussed in detail.

I. INTRODUCTION

In previous work by Smith and Henry [1] and Rountree *et al.* [2], a numerical procedure using noniterative integral equation theory is discussed and applied to low-energy e$^-$ — H and e$^-$–O scattering within the close-coupling formalism. In previous work by Korff *et al.* [3–4], a similar numerical procedure using Numerov's method is discussed and applied to e$^-$–Na and e$^-$–Li scattering within the non-exchange close-coupling formalism. Both methods integrate a set of coupled equations out to a transformation point r_t, where the reactance matrix is projected to its asymptotic value [5]. Also, note that Karule [6] has extended the Percival–Marriott method [7] for use in electron–atom collision problems where the exchange terms are also treated using auxiliary equations, but another numerical technique is used to integrate the coupled equations.

Here a numerical procedure is outlined which treats the coupled equations involved in electron–ion, as well as electron–atom, scattering within the close-

coupling formalism. Since an integral equation method is to be used in solving the coupled equations in the interior region, it is necessary to extend it to the ion case. The projection technique is also extended to the ion case by simply evaluating a more general class of integrals that results when using Coulomb waves [8].

The numerical procedure is briefly presented in Section II; application of the procedure to e–He$^+$ scattering is given in Section III. In Section IV, two specific disadvantages of the numerical procedure are discussed in detail. A few concluding remarks are given in Section V.

II. OUTLINE OF THE NUMERICAL PROCEDURE

Since Coulomb waves rather than plane waves are used in the asymptotic boundary conditions imposed on the scattered electron in electron–ion scattering, the numerical procedure used to solved the coupled equations must account for these boundary conditions. The coupled equations can be integrated in the interior region (from zero out to the transformation point r_t) using any desired numerical technique such as that provided by integral equation theory or the Numerov method [7]. However, at r_t any long-range potential terms must be taken into account in obtaining the reactance matrix. An open-channel projection technique [1, 3] is used which approximates the reactance matrix at infinity using its value at r_t. Other techniques are reviewed by Burke and Seaton [7], such as those which involve linearly independent solutions to the coupled equations in the asymptotic region (i.e., the region where $r \geqslant r_t$).

In integral equation theory the boundary conditions are contained in the integral equations through the use of Green's functions. In the asymptotic region, it is clear that Green's functions which behave asymptotically as Coulomb waves, rather than plane waves, must be used. In Section A, the method of outward integration is outlined where Coulomb Green's functions are used. However, in Section B, an alternative procedure is discussed which uses a combination of free-space and Coulomb Green's functions. In Section C, an open-channel projection procedure is presented for use in the ion case, as well as the neutral case.

A. *Coulomb Green's Functions*

To illustrate the alterations that are necessary in using integral equation theory, we need only retain the direct potential in the coupled differential equations [7]. The resulting equations are

$$\left[\frac{d^2}{dr^2} - \frac{l_i(l_i + 1)}{r^2} + \frac{2z}{r} + k_i^2 \right] F_{ij}(r) = \sum_{n=1}^{N} V_{in}(r) F_{nj}(r), \tag{1}$$

where N is the total number of channels, l_i and k_i are the angular momentum and wave number for channel i, V is the direct-potential matrix, and z is the residual charge of the ion. Next, F is a square matrix, which represents the reduced radial part of the scattered-electron wave function. These equations have a solution with asymptotic forms

$$F_{ij}(r) \underset{r \to 0}{\sim} r^{l_i+1}$$

$$F_{ij}(r) \underset{r \to \infty}{\sim} \begin{cases} k_i^{-1/2}[\sin(\xi_i + \sigma_i)\, \delta_{ij} + \cos(\xi_i + \sigma_i)\, R_{ij}], & i \text{ open}, \\ d_{ij}e^{-\kappa_i r}(2\kappa_i r)^{z/\kappa_i} + \phi_{ij}(r), & i \text{ closed}, \end{cases} \qquad (2)$$

with

$$\xi_i = k_i r - l_i(\pi/2) + (z/\kappa_i)\ln(2\kappa_i r),$$

$$\sigma_i = \arg \Gamma(l_j + 1 - iz/\kappa_i), \qquad (3)$$

$$\kappa_i = |k_i|.$$

Note that R is the familiar open-channel reactance matrix and d is a matrix associated with the closed channels. The matrix ϕ is included in Eq. (2) to emphasize the possible existence of long-range terms that couple with the open channels to give rise to polarization effects [9].

The set of coupled differential equations in Eq. (1) can be straightforwardly cast into a set of coupled integral equations [1, 10]. If the Coulomb term $(2z/r)$ in Eq. (1) is retained in defining the Green's functions, we obtain the equation

$$\left[\frac{d^2}{dr^2} - \frac{l_i(l_i+1)}{r^2} + \frac{2z}{r} + k_i^2\right] G_i^{(\alpha)}(k_i r) = 0, \qquad \alpha = 1, 2, \qquad (4)$$

where $G_i^{(\alpha)}(k_i r)$ are referred to as Coulomb Green's functions. The associated boundary conditions are

$$G_i^{(1)}(k_i r) \underset{r \to 0}{\sim} r^{l_i+1}$$

$$G_i^{(1)}(k_i r) \underset{r \to \infty}{\sim} \begin{cases} k_i^{-1/2}\sin(\xi_i + \sigma_i), & i \text{ open}, \\ (2\kappa_i)^{-1/2}\, e^{+\kappa_i r}(2\kappa_i r)^{-z/\kappa_i}, & i \text{ closed}, \end{cases}$$

$$\qquad (5)$$

$$G_i^{(2)}(k_i r) \underset{r \to \infty}{\sim} \begin{cases} k_i^{-1/2}\cos(\xi_i + \sigma_i), & i \text{ open}, \\ -(2\kappa_i)^{-1/2}\, e^{-\kappa_i r}(2\kappa_i r)^{+z/\kappa_i}, & i \text{ closed}, \end{cases}$$

where ξ_i, σ_i, and κ_i are defined in Eq. (3). The set of unnormalized integral equations can now be written as

$$\psi_{ij}(r) = G_i^{(1)}(k_i r)\, H_{ij}^{(2)}(r) - G_i^{(2)}(k_i r)\, H_{ij}^{(1)}(r),$$

$$H_{ij}^{(2)}(r) = \delta_{ij} - \int_0^r G_i^{(2)}(k_i x) \left[\sum_n V_{in}(x)\, \psi_{nj}(x)\right] dx, \qquad (6)$$

$$H_{ij}^{(1)}(r) = - \int_0^r G_i^{(1)}(k_i x) \left[\sum_n V_{in}(x)\, \psi_{nj}(x)\right] dx,$$

where the normalized solution $F_{ij}(r)$ is obtained from the unnormalized solution $\psi_{ij}(r)$ by a simple matrix multiplication.

Let us briefly consider the open channel Green's functions. From Abramowitz and Stegun [11], the Green's functions can be expressed in terms of the regular solution F_l and the irregular solution G_l, namely,

$$G_i^{(1)}(k_i r) = k_i^{-1/2} F_{l_i}(k_i r),$$

$$G_i^{(2)}(k_i r) = k_i^{-1/2} G_{l_i}(k_i r). \qquad (7)$$

Note that the Wronskian relation $W[G_i^{(1)}, G_i^{(2)}] = +1$ was used in obtaining Eq. (7). The numerical generation of these functions is straightforward [12].

Let us next consider the closed channel Green's functions. From Abramowitz and Stegun [11], note that there are several solutions to the closed-channel version of Eq. (4), namely,

$$\frac{d^2 w}{dy^2} + \left[-\frac{1}{4} + \frac{\alpha}{4} + \frac{(\frac{1}{4} - \mu^2)}{y^2}\right] w = 0, \qquad (8)$$

where $y = 2\kappa r$, $\mu = l + \frac{1}{2}$, and $\alpha = z/k$. We can use the familiar Whittaker solutions $M_{\alpha,\mu}(y)$ and $W_{\alpha,\mu}(y)$ as long as $\Gamma(\frac{1}{2} + \mu - \alpha)$ is well defined. At the critical values

$$\tfrac{1}{2} + \mu - \alpha = -n, \qquad n = 0, 1, 2..., \qquad (9)$$

it is well known that $M_{\alpha,\mu}(y)$ and $W_{\alpha,\mu}(y)$ are linearly dependent functions; moreover, these critical values correspond to the familiar bound states in a Coulomb field with $z > 0$. It seems reasonable that the Whittaker solutions can be used successfully as long as κ^2 is not too close to the critical values. In an effort to avoid any numerical difficulty that could arise when κ^2 is near the critical values, an alternative approach that uses free-space Green's functions in the interior region is suggested in Section B. As a result, we can avoid using closed-channel Coulomb functions in the interior region.

Once all the necessary Green's functions are obtained, we proceed as follows. Integrate Eq. (6) from zero out to r_t in the usual manner. After forcing closed-channel boundary conditions (an approximation that is discussed in Section IV.A), we obtain $\psi(r_t)$ and $H^{(\alpha)}(r_t)$ for the open channels only. We define the open-channel reactance matrix at r_t as $R(r_t) = H^{(1)}(r_t) \cdot [H^{(2)}(r_t)]^{-1}$. Using the open-channel projection procedure to be discussed in Section C, we project $R(r_t)$ to its asymptotic value $R = R(\infty)$.

B. Coulomb and Free-Space Green's Functions

It is apparent that Coulomb Green's functions are necessary at the transformation point r_t. However, while integrating Eq. (6) from zero out to r_t, it is permissible to use free-space functions. In this manner we avoid using closed-channel Coulomb functions in the interior region. However, at r_t the amplitudes $H_f^{(\alpha)}(r_t)$, which are relative to free-space functions, must be transformed into the amplitudes $H_c^{(\alpha)}(r_t)$, which are relative to Coulomb functions. As a result, the projection of $R(r_t)$ can proceed as indicated at the end of Section A.

Suppose we have integrated Eq. (6) out to r_t where we obtain the open-channel matrices

$$\psi_f(r) = G_f^{(1)}(r)\,H_f^{(2)}(r) - G_f^{(2)}(r)\,H_f^{(1)}(r),$$

$$\psi_f{}'(r) = G_f'^{(1)}(r)\,H_f^{(2)}(r) - G_f'^{(2)}(r)\,H_f^{(1)}(r), \tag{10}$$

after the closed channel boundary conditions are forced [1]. In terms of Coulomb functions, we have Eq. (10) except the subscript f is replaced by the subscript c. By matching the two solutions at r_t, we have

$$\psi_f(r_t) = \psi_c(r_t),$$

$$\psi_f{}'(r_t) = \psi_c{}'(r_t), \tag{11}$$

which yields

$$\begin{bmatrix} H_c^{(2)}(r_t) \\ H_c^{(1)}(r_t) \end{bmatrix} = - \begin{bmatrix} G_c'^{(2)}(r_t) & G_c^{(2)}(r_t) \\ G_c'^{(1)}(r_t) & G_c^{(1)}(r_t) \end{bmatrix} \begin{bmatrix} \psi_f(r_t) \\ \psi_f{}'(r_t) \end{bmatrix} \tag{12}$$

having used the Wronskian relation $W[G_c^{(1)}, G_c^{(2)}] = +1$. All that remains in obtaining $H_c^{(\alpha)}(r_t)$ from Eq. (12) is to specify $G_c^{(\alpha)}(r_t)$ and $G_c'^{(\alpha)}(r_t)$. One way by which we can obtain these open-channel Coulomb Green's functions at r_t is to evaluate their respective asymptotic expansions given by Abramowitz and Stegun [11]. However, care must be taken to choose an adequate value of r_t to ensure proper convergence of the asymptotic expansions. To guarantee at least five-figure

TABLE I

The Specification of ρ for Various η and $l = 0$ Which Ensures
at Least 5-Figure Accuracy in G_c and G_c'

η	ρ
± 1.0	10
± 5.0	15
± 10.0	23
± 15.0	33
± 20.0	40

accuracy in $G_c^{(\alpha)}$ and $G_c'^{(\alpha)}$, Table I specifies an adequate value of $\rho = kr_t$ for various $\eta = z/k$ and $l = 0$ [13]. For higher values of l, it is sufficient to use the value $\rho_l = \rho_0 + \frac{1}{4}$. Having obtained $H_c^{(\alpha)}(r_t)$, we calculate the reactance matrix R using the projection procedure to be discussed in the next section.

C. Projection Procedure

The objective of this procedure is to take the reactance matrix $R(r_t)$ and project it to its asymptotic value R. The procedure corrects for any long-range potential terms which are neglected in calculating $R(r_t)$.

As discussed by Smith and Henry [1], a projection equation for the amplitudes can be obtained, namely,

$$\begin{bmatrix} H_c^{(1)} \\ H_c^{(2)} \end{bmatrix} = \begin{bmatrix} I + C^{(1,1)} & C^{(1,2)} \\ C^{(2,1)} & I + C^{(2,2)} \end{bmatrix} \begin{bmatrix} H_c^{(1)}(r_t) \\ H_c^{(2)}(r_t) \end{bmatrix}, \tag{13}$$

where $C^{(a,b)}$ are square matrices which are proportional to the integrals

$$D_{ij}^{(\alpha,\beta)} = \int_{r_t}^{\infty} G_i^{(\alpha)}(k_i x)\, G_j^{(\beta)}(k_j x)\, V_{ij}(x)\, dx. \tag{14}$$

As discussed in Korff et al. [3], an alternative projection procedure is presented, which can be shown to be equivalent to Eq. (13) to first order in $D_{ij}^{(\alpha,\beta)}$. Whichever procedure is used, both must calculate the integral $D_{ij}^{(\alpha,\beta)}$ given in Eq. (14).

Let us now consider the manner in which the integral $D_{ij}^{(\alpha,\beta)}$ is evaluated. If we denote the asymptotic form of the direct potential as

$$V_{ij}(x) = \sum_{\lambda=1} a_{ij}^{(\lambda)}/x^{\lambda+1} \tag{15}$$

and express the Green's functions in terms of their asymptotic expansions [11]

$$G_i^{(\alpha)}(k_i r) = k_i^{-1/2} \sum_{m=1}^{\infty} \{S_m^{(\alpha)} \sin(\xi_i + \sigma_i) + C_m^{(\alpha)} \cos(\xi_i + \sigma_i)\}, \qquad (16)$$

then we can express $D_{ij}^{(\alpha,\beta)}$ in terms of the basic integral

$$L(k, N, \eta, r_t) = \int_{r_t}^{\infty} e^{ikx} \frac{dx}{x^{N+i\eta}}, \qquad (17)$$

where

$$k = \pm(k_i \pm k_j),$$
$$\eta = \pm(\eta_i \pm \eta_j), \qquad (18)$$
$$N = 2, 3, 4,...,$$

and $\eta_i = -z/k_i$. When evaluating $D_{ij}^{(\alpha,\beta)}$ with asymptotic expansions for the open-channel Green's functions, care must be taken to ensure the convergence of the integrated sum to within a specified accuracy. The values of $\rho = kr_t$ given in Table I are sufficient to guarantee five significant figures.

To evaluate the basic integral, we let

$$L(k, N, \eta, r_t) = r_t^\nu x^{-\nu} \Gamma(\nu, x), \qquad (19)$$

with

$$\nu = 1 - N - i\eta,$$
$$x = -ikr_t, \qquad (20)$$
$$\Gamma(\nu, x) = \int_x^{\infty} t^{\nu-1} e^{-t} dt.$$

According to Luke [14], we have

$$\Gamma(\nu, x) = x^{\nu-1} e^{-x} F(1 - \nu, 0, x), \qquad (21)$$

where $F(1 - \nu, 0, x)$ can be evaluated using continued fractions. From Eqs. (19) and (21) we obtain the equation

$$L(k, N, \eta, r_t) = r_t^\nu x^{-1} e^{-x} F(1 - \nu, 0, x). \qquad (22)$$

The convergence of the continued fraction expansion is governed by the parameter $y = kr_t$. For $y \leqslant y_0 = 2$, it is found that the convergence is not as rapid as desired. Hence, let us proceed as follows when $y \leqslant y_0$. We take

$$L(k, N, \eta, r_t) = L(k, N, \eta, r_0) + M(k, N, \eta, r_0, r_t), \qquad (23)$$

where

$$M(k, N, \eta, r_0, r_t) = \int_{r_t}^{r_0} e^{ikx} \frac{dx}{x^{N+i\eta}}$$

$$(24)$$

$$= k^{N-1+i\eta} \int_{y}^{y_0} \frac{e^{iu}}{u^{N+i\eta}} \, du.$$

Using $e^{iu} = \sum_{l=0}^{\infty} (iu)^l/l!$, we obtain the series expansions

$$M(\eta \neq 0) = k^{N-1+\eta} \sum_{l=0}^{\infty} \frac{i^l}{l! \, (l+1-N-i\eta)} \, [y_0^{l+1-N-i\eta} - y^{l+1-N-i\eta}],$$

$$M(\eta = 0) = k^{N-1} \sum_{\substack{l=0 \\ l \neq N-1}}^{\infty} \frac{i^l}{l! \, (l+1-N)} \, [y_0^{l+1-N} - y^{l+1-N}]$$

$$+ \frac{i^{N-1}}{(N-1)!} \, [\ln y_0 - \ln y]. \tag{25}$$

In summary, we evaluate the basic integral directly from Eq. (22) using continued fractions provided $y = kr_t > y_0 = 2$. For $y \leqslant y_0$, we use Eq. (23) where $L(k, N, \eta, r_0)$ is evaluated using continued fractions and $M(k, N, \eta, r_0, r_t)$ is evaluated using the series expansions given in Eq. (25).

Finally, in evaluating all the necessary basic integrals required to specify the projection matrix in Eq. (13), we use recurrence relations on $L(k, N, \eta, r_t)$. For instance, after using integration by parts, we obtain

$$L(k, N, \eta, r_t) = \frac{e^{ikr_t} r_t^{1-N-i\eta}}{N-1+i\eta} + \frac{ik}{(N-1+i\eta)} \, L(k, N-1, \eta, r_t) \quad (26)$$

for upward recurrence and

$$L(k, N, \eta, r_t) = - \frac{e^{ikr_t} r_t^{-N-i\eta}}{ik} + \frac{(N+i\eta)}{ik} \, L(k, N+1, \eta, r_t) \tag{27}$$

for downward recurrence. We start at $N = N_0$ and evaluate $L(k, N_0, \eta, r_t)$ as outlined in the preceding paragraph. From N_0 we recur downward to $N = 2$ and upward to $N = N_{max}$ (for example, $N_{max} = 100$). If we take (numerically established)

$$M = \text{INT}(\mid k \mid r_t),$$

$$N_0 = \begin{cases} M, & M \geqslant 2, \\ 2, & M < 2, \end{cases} \tag{28}$$

where INT(x) chooses the closest integer to x, the recurrence procedure can proceed without much significant figure loss.

In summary, we see that continued fractions, series expansions, and recurrence relations combine to yield a complete specification of the basic integral used in expressing the projection matrix in Eq. (13). Moreover, note two important facts. First, this procedure for evaluating the projection matrix for the ion case ($z \neq 0$) is also valid for the atom case ($z = 0$). Second, this procedure is designed to work even for high angular momentum (for example, $l = 50$). Refer to Appendix I for the evaluation of σ_i.

III. APPLICATION TO e⁻–He⁺ SCATTERING

In application of the numerical procedure via integral equation theory, let us consider the ^1S partial wave for the $e^- + He^+$ scattering problem within the close-coupling formalism. We can solve the equations given by Percival and Seaton [15], where the continuum functions are not orthogonalized to the He⁺ atomic orbitals. Alternatively, we can constrain the continuum functions to be orthogonal to the atomic orbitals and variationally include the necessary correlation functions to completely account for the constraints [7]. The two procedures are found to yield the same eigenphases to within 0.2 % for energies from $k^2 = 2.0$ Ry to 5.0 Ry using a 1s–2s–2p expansion. Consequently, only the results obtained using the Percival–Seaton equations will be quoted.

Here is a brief outline of this section. First, the open-channel projection procedure is tested for increasing values of the transformation point r_t. Second, the ^1S partial-wave contribution to the cross-sections $Q(1s–1s)$, $Q(1s–2s)$, and $Q(1s–2p)$ is studied as more hydrogenic states are included in the close-coupling

TABLE II

The Unprojected and Projected Eigenphases for $k^2 = 3.2$ and 5.0 at Two Values of r_t Using a 3-State Expansion

r_t	A	B	C	D
90.81	0.152(+1)	0.155(+1)	0.112(+1)	0.112(+1)
	0.316	0.320	0.299	0.298
	−0.709	−0.741	−0.146(−1)	−0.198(−1)
151.61	0.153(+1)	0.155(+1)	0.112(+1)	0.112(+1)
	0.317	0.319	0.298	0.298
	−0.722	−0.741	−0.166(−1)	−0.198(−1)

expansion. Third, a specific example is given that should help motivate the use of free-space Green's function in the interior region.

First, let us consider the use of the open-channel projection procedure when using a $1s$–$2s$–$2p$ expansion. In Table II, the eigenphases at the transformation points $r_t = 90.81$ and 151.61 are given for the incident electron energies $k^2 = 3.2$ and 5.0. Columns A and B contain the unprojected and projected eigenphases for $k^2 = 3.2$. Columns C and D similarly contain eigenphases for $k^2 = 5.0$. From an observation of Table II, we see that the unprojected results do progress toward the projected results as r_t increases. We can also make the significant observation that the dipole potential which couples the degenerate channels, does not affect the projected results as much as in the e^-–H case [1]. In the hydrogen case, for example, a value of r_t as large as 500 was required to converge the projected cross-section to within 0.1 %, at an energy just above the $n = 2$ threshold. It would appear that the degenerate dipole coupling does not dominate at large distances in e^-–He^+ scattering. This behavior can easily be attributed to the idea that the effect of the degenerate dipole coupling is being measured against a dominating Coulomb term.

TABLE III

Cross-Sections in units of πa_0^2 (with phase shifts in brackets) for the 3-state, 6-state, and 8-state calculations. Rows (a–c) give the $Q(1s$-$1s)$, $Q(1s$-$2s)$, and $Q(1s$-$2p)$ cross-sections, respectively, for the ^1S partial wave

k^2(Ry)		Q(3-state)		Q(6-state)		Q(8-state)		Q(BT)
3.20	(a)	.297(−1)	.320	.315(−1)	.332	.318(−1)	.334	—
	(b)	.936(−2)	−.743	.744(−2)	−.530	.733(−2)	−.522	.616(−2)
	(c)	.405(−2)	1.55	.337(−2)	−1.47	.332(−2)	−1.46	.322(−2)
3.24	(a)	.292(−1)	.316	.313(−1)	.333	.316(−1)	.335	—
	(b)	.920(−2)	−.709	.667(−2)	−.485	.656(−2)	−.477	.540(−2)
	(c)	.425(−2)	1.52	.308(−2)	−1.48	.303(−2)	−1.47	.309(−2)
5.00	(a)	.158(−1)		.163(−1)		.166(−1)		N.A.
	(b)	.306(−2)		.288(−2)		.273(−2)		
	(c)	.421(−2)		.380(−2)		.370(−2)		

Let us next consider the 3-state $(1s$–$2s$–$2p)$, the 6-state $(+3s$–$3p$–$3d)$ and the 8–state $(+4s$–$4p)$ results at $k^2 = 3.2$, 3.24, and 5.0. We compare the excitation cross sections with the correlation (BT) results of Burke and Taylor [16] where applicable. The BT excitation cross-sections are obtained using a 3-state expansion plus explicit two-electron correlation terms. Next we note that the 3-state results agree to within 0.2 % with the tabulated 3-state results of Burke *et al.* [17]. The

6-state results are found to agree to at least within 1.0 % with the graphical 6-state results of Ormonde et al. [18]. Table III gives these cross-sections in units of πa_0^2, where Rows (a–c) contain the $Q(1s–1s)$, $Q(1s–2s)$ and $Q(1s–2p)$ cross-sections, respectively. First, note that as the number of states (n) increases, the elastic cross-section increases while the inelastic cross-sections decrease toward the BT excitation results. Also, at the energy $k^2 = 5.0$. the changes in the cross-sections become smaller as n increases. In any case, this trend toward the BT results indicates that the addition of more atomic He+ states into the close-coupling expansion will lead to rather slow convergence. However, this conclusion is not strictly correct. Since the cross-sections don't necessarily have to change monotonically as more terms are included in the total wave function, it is not apparent that the BT excitation cross-sections are "better." It would have been more appropriate to compare the individual phase shifts because of the bounds they satisfy below the $n = 3$ threshold. With this thought in mind, we note that the change in the cross-section $Q(n$-state) from $n = 6$ to $n = 8$ is small. Perhaps, if more atomic He+ states are included in the close-coupling expansion, the convergence may not be too slow.

Finally, consider a specific example that should help motivate the use of free-space Green's functions during the integration of the coupled equation in the interior region (from zero out to r_i). Recall that there exists bound states for a Coulomb field with $z > 0$. They occur for He+ $(z = +1)$ at the critical energies (refer to Eq. (9))

$$\kappa_{i,m}^2 = [l_i + m]^{-2} Ry, \qquad m = 1, 2, 3,.... \qquad (29)$$

In particular, there are an infinite number of Coulomb bound states. Therefore, if we attempted to map the series of ¹S resonances that exist between the $n = 2$ and

TABLE IV

A study of the first five ¹S resonance positions just below
the $n = 3$ threshold. Column (a) contains the
resonance positions calculated by Burke and Taylor [16].
Column (b) contains the critical values taken relative
to the $n = 3$ threshold

	a	b
1.	3.294	3.31
2.	3.368	—
3.	3.440	3.44
4.	3.479	3.49
5.	3.489	3.52

$n = 3$ thresholds of He$^+$, the use of closed-channel Coulomb Green's could be numerically hazardous, especially if the resonance positions are near the critical energies. Let us then compare the positions of the critical energies taken relative to the $n = 3$ threshold with the positions of the resonances. From quantum defect theory [19], recall that the Coulomb term is the principle factor in supporting some of these resonances. Therefore, we should expect the critical energies to be close to some of the resonance positions. In Table IV, column (a), observe the theoretical energy positions of the first five ^1S resonances just below the $n = 3$ threshold given by Burke and Taylor [16]. By subtracting the critical energies 1/4, 1/9, 1/16, and 1/25 from the $n = 3$ threshold energy of 3.556, the results in column (b) are obtained. Note the unsurprising result that some of the resonance positions lie quite close to the critical energies.

In order to test the use of free-space Green's functions for energies near a resonance, let us consider calculating the position and width of the first ^1S resonance just below the $n = 3$ threshold. First, the reactance matrix R is diagonalized by an orthogonal transformation U. The phase shifts δ_i are then defined by

$$[U^T R U]_{ij} = \delta_{ij} \tan \delta_i .$$

Next, the sum of the phase shifts $\delta(k^2)$ is fitted to the resonance formula[16]

$$\delta(k^2) = a + bk^2 + \tan^{-1} [\tfrac{1}{2}\Gamma/(E_r - k^2)],$$

where a and b are simple constants, Γ and E_r are the width and position, respectively, of the first resonance, and the effects of other nearby resonances are

energies on each side of the resonance position, application of the resonance formula yields $\Gamma = .636(-2)$ and $E_r = 3.293$. In comparison with the 6-state results of Ormonde *et al.* [18], they obtain $\Gamma = .632(-2)$ and $E_r = 3.293$, which are in good agreement with the present results.

IV. DISADVANTAGES OF THE NIEM

In this section, let us discuss two specific disadvantages of the numerical procedure presented here. Both disadvantages are related to the treatment of the closed channel components of the unnormalized solution $\psi(r)$ given in Eq. (6). The first problem can occur when the closed-channel boundary conditions are forced with a premature drop of the closed channels. The second problem can occur if some of the closed-channel Green's functions grow (exponentially) too rapidly for increasing r.

A. *First Disadvantage*

The first problem associated with the closed channels can occur even when the closed channel Green's functions do not grow rapidly. We integrate $\psi(r)$ of Eq. (6) from zero out to a point r_c where the closed channels are dropped after setting $\psi_{co}(r)$ (i.e., i closed and j open) to zero with the use of an appropriate matrix multiplication [1]. However, as indicated in the boundary conditions in Eq. (2), there can exist back-coupling to the open channels which give rise to long-range polarization effects.

Consider the illustrative example of e⁻–O scattering for the ^4P partial wave where only the ground state s-wave channel is open (i.e., no d-wave) and any excited state channels are closed [2]. When $V_{1j}(r) \sim_{r\to\infty} a_{1j}/r^2$ (where $j \neq 1$), there exists dipole coupling from the closed channels to the open channel in the form of the usual dipole polarization term α/r^4. It is apparent that dropping closed channels before the polarization term is negligible could lead to a substantial error, especially at very low energy. However, it is quite possible that we cannot integrate the closed channels out far enough because of the growth of the solution.

TABLE V

For the ^4P partial wave of e–O scattering, we obtain the corrected (Q_c) and uncorrected (Q_u) cross-sections in units of πa^2_0 with phase shifts in parentheses. Using the corrected phase shifts, we calculate $\beta = k \cot(\eta)$; we fit β with the modified Blatt–Jackson formula to obtain γ

$k^2(Ry)$	$Q_u(\eta_u)$	$Q_c(\eta_c)$	β	γ
3.0(−1)	3.92(−.726)	3.90(−.724)	—	—
2.0(−1)	4.13(−.591)	4.11(−.588)	—	—
1.0(−1)	4.33(−.415)	4.30(−.413)	—	—
1.0(−2)	4.47(−.130)	3.63(−.117)	—	—
1.0(−3)	4.48(−.0410)	2.57(−.0311)	−1.02	−0.98
1.0(−4)	4.48(−.0130)	2.11(−.00890)	−1.12	−1.12
1.0(−5)	4.48(−.00410)	1.95(−.00271)	−1.17	−1.17
1.0(−6)	4.48(−.00130)	1.90(−.000844)	−1.18	−1.18

To illustrate this particular problem further, consider the effect of the polarization term $V_{\rm pol} = -5.19/r^4$ on the usual static exchange results for the ^4P partial wave of e⁻–O scattering. With only the ground state s-wave channel present, we integrate $\psi(r)$ from zero out to $r_c = 10.56$. At this point, we introduce the polarization term into the direct potential. Carrying the integration out to the point $r_t = 50.373$, we project the reactance matrix to its asymptotic value. We label the cross-section

Q_c. For a comparison, we can neglect the polarization term V_{pol} to obtain the cross-section Q_u. From Table V, we see that as k^2 decreases, the polarization term does become more important, as expected. However, for $k^2 \geqslant 0.1$ we see that the polarization term has little effect, indicating that shorter-ranged potential terms may be more important. In summary, we see that neglect of the polarization potential at r_c can introduce serious error into the final results, especially at very low energy.

Next let us check the low-energy behavior of these results against the modified Blatt–Jackson formula as given by O'Malley, Spruch, and Rosenberg [20]. For $l = 0$, the formula is

$$k \cot(\eta) = -\frac{1}{a} + \frac{\pi\alpha}{3a^2} k + \frac{2\alpha}{3a} k^2 \ln\left(\frac{\alpha k^2}{16}\right) + \cdots, \qquad (30)$$

where "a" is the scattering length and $\alpha = 5.19$ is the dipole polarizability. For the last four energies in Table V, the quantities $\beta_i = k_i \cot(\eta_i)$ are calculated using the corrected phase shifts η_c. The values β_i are then fitted with the r.h.s. of Eq. (30) to obtain the results γ_i. As we can see in Table V, the fitted results γ_i agree well with the calculated results β_i especially at very low energy. Note that $a_c = 0.838$ for the corrected results as compared with $a_u = 1.30$ for the uncorrected results. This indicates that the scattering length is dependent on the dipole polarizability α, as expected [20].

In order to avoid this particular problem, the closed channels must be handled more appropriately. A familiar technique [6, 7] is to obtain linearly independent asymptotic solutions of the coupled equations at r_t. These solutions are integrated inward to an intermediate point r_m, where the inward and outward solutions are appropriately matched. In this manner, the effect of the closed channels in the asymptotic region can be retained in any given calculation. Moreover, the closed-channel part of $F(r)$ is matched to its correct asymptotic form as given in Eq. (2). When using an asymptotic expansion, care must be taken to use a value of r_t that will ensure its convergence. For example, it is well known [7] that when the channel energy separations become too small, poor convergence results for the expansion suggested by Burke and Schey [21]. In an attempt to avoid such convergence problems, it may be possible to obtain the asymptotic solutions via a projection technique similar to the open-channel technique discussed in Section C, but appropriately modified to handle closed channels [22].

B. Second Disadvantage

Let us now consider the second problem. Note that an inward and outward integration technique is intended to avoid the numerical difficulties that result from the growth of solutions originating from any closed channels and exchange

terms [7]. However, we shall see that the inward and outward solutions cannot always be matched at an interior point r_m, especially if r_t and $\kappa_i{}^2$ are large (for example, $r_t = 35.0$ and $\kappa_i{}^2 = 5.0$ Ry.) To illustrate this point clearly, we consider the coupled equations given in Eq. (1) with $z = 0$ for numerical simplicity. First, an integral equation theory is used to study the origin of the difficulty. Second, a numerical example is provided which confirms the conclusions of the study.

The normalized solution $F_{ij}(r)$ of Eq. (1) can be written as

$$F_{ij}(r) = \Delta_i \delta_{ij} G_i^{(1)}(k_i r) + G_i^{(2)}(k_i r) \int_0^r G_i^{(1)}(k_i x)\, S_{ij}(x)\, dx$$

$$+ G_i^{(1)}(k_i r) \left[C_{ij} - \int_0^r G_i^{(2)}(k_i x)\, S_{ij}(x)\, dx \right], \tag{31}$$

where

$$C_{ij} = \int_0^\infty G_i^{(2)}(k_i x)\, S_{ij}(x)\, dx,$$

$$S_{ij}(x) = \sum_n V_{in}(x)\, F_{nj}(x), \tag{32}$$

$$\Delta_i = \begin{cases} 1, & i \text{ open,} \\ 0, & i \text{ closed.} \end{cases}$$

Note that the unnormalized solution $\psi_{ij}(r)$ of Eq. (6) results when we omit the constant C_{ij}. As an result, the solution contains closed-channel components that grow exponentially. However, at $r = r_m$ this behavior is taken out by matching to an inward solution. Therefore, we are effectively subtracting out any exponential growth as in the integral equation for $F_{ij}(r)$. For example, with i closed the r.h.s. of Eq. (31) becomes

$$F_{ij}(r) \underset{r \to \infty}{\sim} G_i^{(2)}(k_i r)\, d_{ij} + \phi_{ij}(r), \tag{33}$$

where d and ϕ are matrices given in Eq. (2). Assuming dipole coupling between the open and closed channels, the bracketed term in Eq. (31) can be shown to have the asymptotic form [9]

$$C_{ij} - \int_0^r G_i^{(2)}(k_i x)\, S_{ij}(x)\, dx = \int_r^\infty G_i^{(2)}(k_i x)\, S_{ij}(x)\, dx \underset{r \to \infty}{\sim} e^{-\kappa_i r}\phi_{ij}^{(1)}(r), \tag{34}$$

where $\phi^{(1)}$ contributes to ϕ in Eq. (33). We see that after some point r_d^{out}, the subtraction becomes erroneous due to significant figure loss on a computer. Therefore, if we attempted matching for $r_m > r_d^{\text{out}}$, we could not subtract out the exponential growth. In attempting to avoid this problem, we integrate inward to a match point $r_m < r_d^{\text{out}}$.

We can also write the normalized solution $F_{ij}(r)$ as

$$F_{ij}(r) = \Delta_i \delta_{ij} G_i^{(1)}(k_i r) + G_i^{(1)}(k_i r) \int_r^\infty G_i^{(2)}(k_i x)\, S_{ij}(x)\, dx$$

$$+ G_i^{(2)}(k_i r) \left[D_{ij} - \int_r^{r_a} G_i^{(1)}(k_i x)\, S_{ij}(x)\, dx \right], \tag{35}$$

where

$$D_{ij} = \int_0^{r_a} G_i^{(1)}(k_i x)\, S_{ij}(x)\, dx, \tag{36}$$

$$r_a = \begin{cases} \infty, & i \text{ open}, \\ r_t, & i \text{ closed}. \end{cases}$$

If we neglect D_{ij}, we obtain an unnormalized solution for use during the inward integration starting at $r = r_t$. After defining the linearly independent solutions, we can use an asymptotic expansion [21] (or perhaps a general projection technique [22]) to obtain the initial values at r_t which are needed to begin the inward integration of the solutions. As we integrate the unnormalized solutions inward, we see that the integral (for i closed)

$$I_{ij}(r) = \int_r^{r_t} G_i^{(1)}(k_i x) \sum_n V_{in}(x)\, \psi_{nj}(x)\, dx \tag{37}$$

can become quite large, depending on the values of r_t and κ_i. As a result, this term will introduce a growth into the incoming solutions. At the match point r_m, we subtract out this behavior by matching to the outward solution. From Eq. (35), the matching effectively performs the subtraction (for i closed)

$$D_{ij} - I_{ij}(r) \underset{r \to 0}{\sim} 0. \tag{38}$$

Since both D_{ij} and I_{ij} can be quite large, we see that at some point r_d^{in}, the subtraction yields erroneous results due to significant figure loss on a computer. It is apparent that the matching cannot yield accurate results if $r_d^{in} > r_d^{out}$ in a given calculation.

To confirm these observations numerically, and to obtain some idea of what to expect in similar calculations, consider a two-channel example problem. Let us solve Eq. (1) with $l_1 = 0$, $l_2 = 1$, $k_1^2 = k^2 = 1.0$, $k_2^2 = -\kappa^2$, and $z = 0$. The direct potential is taken to be

$$V_{11}(r) = V_{22}(r) = 0,$$
$$V_{12}(r) = V_{21}(r) = -2(1 - e^{-r})^4/r^2, \tag{39}$$

which exhibits dipole coupling between the channels [7]. At a point r_t, we obtain the initial values for three linearly independent solutions $v_{i\beta}$ (where $i = 1, 2$ and $\beta = 1, 2, 3$), using an expansion technique suggested by Burke and Schey [21]. We use Numerov's method to integrate the three solutions inward from $r = r_t$ to $r = r$. Next we integrate two linearly independent solutions $u_i(r)$ outward also

are obtained using the approximate solution

$$u_{i\alpha}(r) = \delta_{i\alpha} G_i^{(1)}(k_i r), \tag{40}$$

which is adequate for small values of r. At the match point r_m, we take

$$F_i^{\text{out}}(r) = \sum_{\alpha=1}^{2} u_{i\alpha}(r)\, b_\alpha ,$$

$$\tag{41}$$

$$F_i^{\text{in}}(r) = \sum_{\beta=1}^{3} v_{i\beta}(r)\, a_\beta ,$$

where $a_1 = 1.0$ and $a_2 = R$. Note that R is the single-channel reactance matrix. We match at $r = r_m$ by requiring

$$F_i^{\text{out}}(r_m) = F_i^{\text{in}}(r_m),$$

$$\tag{42}$$

$$F_i'^{\text{out}}(r_m) = F_i'^{\text{in}}(r_m).$$

For a given κ^2 and r_t, we shall examine the constants b_1, b_2, a_2, a_3 for various match points r_m. In Table VI, we tabulate the constants for $\kappa^2 = (1.0\text{–}5.0)$, for $r_t = 25.0$, and for the matching range $r_m = (5.0, 9.0, 11.0, 15.0, 20.0)$. We see that for $\kappa^2 = 1.0$, the single-channel reactance matrix $R = a_2$ is stable across the entire matching range. As κ^2 increases, the constant R becomes less stable across the matching range. Moreover, observe that r_d^{out} decreases and r_d^{in} increases as κ^2 increases. As we expected, the outward integration cannot proceed beyond some point r_d^{out} and the inward integration cannot proceed beyond some point r_d^{in}, in order to obtain an adequate value for the constant R.

Next, let us examine the effect of increasing r_t. From Eq. (35), we expect that the inward solution will experience more growth as r_t increases. We will find this aspect to be true numerically as can be seen from the behavior of a_3 as r_t increases. With an increase in the growth of the inward solution, we shall see that r_d^{in} does become larger.

Let us examine the results for $r_t = 30.0$ and $r_t = 35.0$ in Tables VII and VIII, respectively. First, note that the value of r_d^{in} does increase as r_t increases. As a result, we see that no match is possible for $\kappa^2 = 5.0$ and $r_t = 35.0$. Next, even if

TABLE VI

For various κ^2 with $r_t = 25.0$, the constants b_1, b_2, a_2, a_3 are examined for various match points r_m

$\kappa^2(Ry)$		$r_m = 5.0$	$r_m = 9.0$	$r_m = 11.0$	$r_m = 15.0$	$r_m = 20.0$
1.0	b_1	.995	.995	.995	.995	.995
	b_2	.193	.193	.193	.193	.193
	a_2	.490(−1)	.490(−1)	.490(−1)	.490(−1)	.490(−1)
	a_3	.116(+6)	.116(+6)	.116(+6)	.116(+6)	.222(+6)
2.0	b_1	.998	.998	.998	.998	.998
	b_2	.904(−1)	.904(−1)	.904(−1)	.904(−1)	.904(−1)
	a_2	.364(−1)	.364(−1)	.364(−1)	.364(−1)	.368(−1)
	a_3	.121(+10)	.121(+10)	.121(+10)	.121(+10)	.456(+12)
3.0	b_1	.999	.999	.999	.999	.104(+1)
	b_2	.553(−1)	.553(−1)	.553(−1)	.553(−1)	.573(−1)
	a_2	.291(−1)	.291(−1)	.291(−1)	.290(−1)	.133
	a_3	.161(+13)	.161(+13)	.161(+13)	.161(+13)	−.146(+17)
4.0	b_1	.100(+1)	.999	.999	.997	−.105
	b_2	.382(−1)	.382(−1)	.382(−1)	.381(−1)	−.402(−2)
	a_2	.239(−1)	.243(−1)	.243(−1)	.259(−1)	−.230(+1)
	a_3	.737(+15)	.737(+15)	.737(+15)	.738(+15)	−.148(+21)
5.0	b_1	.891	.100(+1)	.100(+1)	.102(+1)	−.778(−2)
	b_2	.251(−1)	.282(−1)	.282(−1)	.288(−1)	−.220(−3)
	a_2	.457	.208(−1)	.208(−1)	.466(−2)	−.227(−1)
	a_3	.640(+17)	.170(+18)	.170(+18)	.172(+18)	−.161(+23)

the constants are stable over some limited range, we may not be able to adequately construct the wave function $F_i(r)$, even around the match point r_m. For example, with $r_t = 30.0$ and $\kappa^2 = 3.0$, we see that the constants are stable between $r_m = 9.0$ and $r_m = 11.0$. However, if the wave function $F_i^{out}(r)$ and $F_i^{in}(r)$ are tabulated and compared for a few points about $r_m = 9.0$, the $i = 2$ components disagree completely, while the $i = 1$ components agree to only one significant figure.

We have seen that the breakdown of the outward and inward integration procedure originates from the closed-channel growth of the solutions. In an effort to avoid the growth, let us consider the following procedure. As discussed in

TABLE VII

For various κ^2 with $r_t = 30.0$, the constants b_1, b_2, a_2, a_3 are examined for various match points r_m

$\kappa^2(Ry)$		$r_m = 5.0$	$r_m = 9.0$	$r_m = 11.0$	$r_m = 15.0$	$r_m = 20.0$
1.0	b_1	.995	.995	.995	.995	.995
	b_2	.193	.193	.193	.193	.193
	a_2	.490(−1)	.490(−1)	.490(−1)	.490(−1)	.490(−1)
	a_3	.702(+7)	.702(+7)	.702(+7)	.702(+7)	.713(+7)
2.0	b_1	.998	.998	.998	998	.998
	b_2	.904(−1)	.904(−1)	.904(−1)	.904(−1)	.904(−1)
	a_2	.364(−1)	.364(−1)	.364(−1)	.364(−1)	.368(−1)
	a_3	.787(+12)	.787(+12)	.787(+12)	.787(+12)	.124(+13)
3.0	b_1	.100(+1)	.999	.999	.999	.104(+1)
	b_2	.550(−1)	.553(−1)	.553(−1)	.553(−1)	.573(−1)
	a_2	.725(−1)	.291(−1)	.291(−1)	.290(−1)	.133
	a_3	.621(+16)	.608(+16)	.608(+16)	.608(+16)	−.818(+16)
4.0	b_1	.679(+1)	.993	.999	.997	−.105
	b_2	.213	.379(−1)	.382(−1)	.381(−1)	−.402(−2)
	a_2	−.143(+1)	.274(−1)	.242(−1)	.259(−1)	−.230(+1)
	a_3	.506(+19)	.120(+20)	.119(+20)	.120(+20)	−.147(+21)
5.0	b_1	.384(+3)	.360	.100(+1)	.102(+1)	−.778(−2)
	b_2	.944(+1)	.102(−1)	.282(−1)	.288(−1)	−.220(−3)
	a_2	−.109(+1)	.374	.209(−1)	.466(−2)	−.227(−1)
	a_3	.609(+22)	.110(+23)	.978(+22)	.973(+22)	−.642(+22)

Section IV.A, the closed channels can be dropped after setting (rotating) the closed–open part of the outward solution to zero with the use of an appropriate matrix multiplication. However, this procedure can be applied at successive points during the integration of Eq. (1) to prevent any closed-channel growth. This "rotation" procedure was previously used by Gordon [23], Secrest [24], and White and Hayes [25]. We apply the procedure by noticing that

$$\psi(r) = F(r) \cdot C \qquad (43)$$

is also a solution of Eq. (1). Therefore, we can integrate Eq. (1) outwards while

TABLE VIII

For various κ^2 with $r_t = 35.0$, the constants b_1, b_2, a_2, a_3 are examined for various match points r_m

$\kappa^2(Ry)$		$r_m = 5.0$	$r_m = 9.0$	$r_m = 11.0$	$r_m = 15.0$	$r_m = 20.0$
1.0	b_1	.995	.995	.995	.995	.995
	b_2	.193	.193	.193	.193	.193
	a_2	.490(−1)	.490(−1)	.490(−1)	.490(−1)	.490(−1)
	a_3	−.315(+9)	−.315(+9)	−.315(+9)	−.315(+9)	−.315(+9)
2.0	b_1	.100(+1)	.998	.998	.998	.998
	b_2	.928(−1)	.904(−1)	.904(−1)	.904(−1)	.904(−1)
	a_2	−.599(−1)	.364(−1)	.364(−1)	.364(−1)	.368(−1)
	a_3	−.186(+15)	−.133(+15)	−.133(+15)	−.133(+15)	−.132(+15)
3.0	b_1	.673(+3)	.982	.999	.999	.104(+1)
	b_2	.202(+2)	.544(−1)	.553(−1)	.553(−1)	.573(−1)
	a_2	.225(+1)	.368(−1)	.291(−1)	.290(−1)	.133
	a_3	.427(+20)	−.246(+19)	−.262(+19)	−.262(+19)	−.520(+18)
4.0	b_1	−.116(+5)	−.773	.101(+1)	.997	−.105
	b_2	−.325(+3)	−.283(−1)	.385(−1)	.381(−1)	−.402(−2)
	a_2	.449(−1)	.820(−1)	.549(−2)	.259(−1)	−.230(+1)
	a_3	−.590(+22)	−.369(+21)	−.135(+23)	−.875(+22)	−.358(+24)
5.0	b_1	.261(+7)	−.125(+4)	.956	.102(+1)	−.778(−2)
	b_2	.641(+5)	−.354(+2)	.271(−1)	.288(−1)	−.220(−3)
	a_2	.180(−1)	.650	.294(−1)	.482(−2)	−.227(−1)
	a_3	−.584(+25)	.244(+27)	−.138(+25)	−.111(+26)	−.219(+26)

rotating the solution $F(r)$ at various points using Eq. (43). Then the outward solution is matched with the exterior (inward) solution at $r = r_m$.

In application to the present example problem, we can choose the matrix C so that

$$\psi = \begin{pmatrix} F_{11} & F_{11} \\ 0 & F_{11} \end{pmatrix} \tag{44}$$

at each rotation point. Using $r_m = 20.0$ and $r_t = 25.0$, the rotation procedure was tested for energies from $\kappa^2 = 1.0$ to $\kappa^2 = 5.0$. The constant $a_2 = R$ obtained using

this procedure agreed for all cases with the stable results given in Table VI, column $r_m = 11.0$. Therefore, we see that the rotation procedure works quite well for the special case where there are no exchange terms. However, when exchange terms are present, the exchange auxiliary equations are changed by the rotation procedure. Therefore, it is not apparent that the growth in the total solution can be avoided using the rotation procedure, when exchange terms are present.

V. SUMMARY AND CONCLUDING REMARKS

A discussion was given on a numerical approach to be used in electron–ion scattering, as well as electron–atom scattering, within the close-coupling formalism. First, we considered the use of integral equation theory for the solution of the coupled equations from zero out to the transformation point r_t. Second, an open-channel projection procedure was developed to obtain the reactance matrix. The procedure is designed to work for either the ion or neutral case and even for high angular momentum. Lastly, we considered specific disadvantages of the numerical procedure presented here.

In conclusion, we see that a numerical approach with outward and inward integration can work efficiently as long as the closed-channel wave numbers $\kappa_i{}^2$ and the point r_t (where the inward integration is begun) are not too large. However, in the event that they are large, the numerical approach can yield erroneous results. It is apparent that we must use a numerical approach, which is stable for these cases, or use another formalism which avoids the use of closed channels to introduce correlation and polarization effects.

APPENDIX I

Let us briefly consider the evaluation of $\sigma = \arg \Gamma(l + 1 - iz/\kappa)$. If we let $f = l - iz/\kappa$, then $\sigma = \arg \Gamma(1 + f)$. According to Luke [14], we have

$$\Gamma(1 + f) = A(f) \sum_{k=0}^{n-1} g_k H_k(f),$$

where

$$
\begin{aligned}
&n = 16, \\
&A(f) = (2\pi)^{1/2} (f + 11/2)^{f+1/2} e^{-(f+11/2)}, \\
&H_0(f) = 1, \\
&H_k(f) = \frac{f(f - 1) \cdots (f - k + 1)}{(f + 1)(f + 2) \cdots (2 + k)},
\end{aligned}
\tag{43}
$$

and the coefficients g_k are tabulated values. Noting that $\text{Im}(\ln \Gamma(1 + f)) = \arg \Gamma(1 + f) = \sigma$, we obtain σ once we have evaluated $\Gamma(1 + f)$ via Eq. (43). As pointed out by Luke [14], for sufficiently large values of $|f|$ (for example, $|f| = 10$), use of the asymptotic expansion for $\Gamma(1 + f)$ would be more efficient. In Abramowitz and Stegun [11], the asymptotic expansion for $\text{Im}(\ln \Gamma(iy))$ is given. With the use of the continuation formula $\Gamma(1 + f) = f\Gamma(f)$, we obtain

$$\Gamma(l + 1 + iy) = \alpha \Gamma(iy)$$

so that

$$\sigma = \text{Im}(\ln \alpha) + \text{Im}(\ln \Gamma(iy)). \qquad (44)$$

Hence, we can obtain σ using Eq. (43) if $|f| \leqslant 10$ and using Eq. (44) if $|f| > 10$.

ACKNOWLEDGMENTS

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