terms of the measured polarization. Because the corrections are small we simply multiply the correction factors and ignore the difference between P, P_s, and P_m' in the correction terms:

$$P_m = \left(\frac{k_{\parallel} - k_{\perp}}{k_{\parallel} + k_{\perp}}\right)\left(\frac{1-\epsilon}{1-\epsilon P}\right)\left(\frac{1-3\delta}{1-\delta P}\right) P \ . \qquad \text{(A5)}$$

*Work supported in part by the National Science Foundation under Contract No. GP-20696.

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PHYSICAL REVIEW A VOLUME 7, NUMBER 5 MAY 1973

Noniterative Integral-Equation Approach to Scattering Problems*

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(Received 21 August 1972)

A procedure which allows for both open and closed channels with exchange and orthogonality is formulated for a multichannel scattering process. Noniterative integral-equation theory is used to solve the coupled integrodifferential equations of the scattering problem from zero out to some transformation point where the reactance matrix is projected out to its asymptotic value by using a matrizant technique. The method is applied to a two-channel model which has some of the features of a $1s$-$2p$ approximation for e-H scattering.

I. INTRODUCTION

In recent publications,[1-6] several expansion or numerical procedures have been employed for studying low-energy electron-atom scattering within the close-coupling formalism. The principal difference between the expansion and numerical methods is the technique employed in solving the resultant coupled integrodifferential equations. Smith *et al.*[1] used a direct approach which consists of only numerical integration techniques. The expansion methods solve the scattering equations by using matrix techniques. In the present work, we suggest an alternative direct procedure that maintains a high degree of numerical accuracy and stability without sacrificing a rapid execution time on a computer.

A noniterative integral-equation method (NIEM) as applied to direct potentials is well known.[7] However, the utility of the technique has not been recognized until recently. In a series of papers,[8-11] the NIEM has been reviewed and extended somewhat to treat the solution of a nonrelativistic scattering problem.

In the present work, we present a modified and more compact formalism that treats, completely, a multichannel scattering problem in which direct-, exchange-, and orthogonality-potential terms are included. The formalism is discussed in Sec. II, and application is made to a model problem in Sec. III. Section IV contains a brief discussion.

II. FORMALISM

In this section we present the NIEM as applied to a multichannel scattering problem. The equations that arise in the close-coupling formalism[1] of an electron-complex atom scattering problem may be described by the coupled integrodifferential

equations

$$\left(\frac{d^2}{dr^2} - \frac{l_i(l_i+1)}{r^2} + k_i^2\right) F_{ij}(r) = \sum_n [V_{in}(r) + W_{in}(r)] F_{nj}(r) + \sum_\lambda \delta_{l_i l_\lambda} M_\lambda^{ij} P_\lambda(r), \quad i,j = 1,2\ldots,N, \quad (1)$$

where N is the number of channels, l_i and k_i are the angular momentum and wave number for channel i, $\underline{V}$ and $\underline{W}$ are direct- and exchange-potential matrices, and $P_\lambda(r)$ is the reduced radial part of the atomic electron orbital associated with the label λ. The $\underline{M}$ are the undetermined Lagrange multipliers that ensure that the incident-electron wave function is orthogonal to all the bound states λ of the atom. $\underline{F}$ is a square matrix, which represents the reduced radial part of the electron wave function, with j denoting the incident channel and i the outgoing channel. We allow for the possibility that a channel can be open or closed.

The exchange potential for this problem can be described, in general, by the expression

$$\sum_n W_{in}(r) F_{nj}(r) = \sum_{\alpha_i}{}' B_i^{(\alpha_i)} Y_t(P_{\rho_i}, F_{nj}; r) P_{\rho_n}(r), \quad (2)$$

with

$$Y_t(A,B;r) = \frac{1}{r^{t+1}} \int_0^r A(x) B(x) x^t dx + r^t \int_r^\infty \frac{A(x)B(x)}{x^{t+1}} dx,$$

where

$$t_{\min} \le t \le t_{\max},$$

$$t_{\min} = \mathrm{Max}(|l_{\rho_i} - l_n|, |l_{\rho_n} - l_i|),$$

$$t_{\max} = \mathrm{Min}(l_{\rho_i} + l_n, l_{\rho_n} + l_i),$$

and l_{ρ_i} is the angular momentum associated with the atomic state ρ_i. The prime on the summation in Eq. (2) denotes a sum over only exchange terms and, thus, the composite index is defined as $\alpha_i = (t, i, n, \rho_i, \rho_n)$, and $B_i^{(\alpha_i)}$ are the exchange potential coefficients. All values of t consistent with the indicated lower and upper limits are included in the sum over α_i. The exchange terms cited here are not separable and, therefore, require a different treatment to that of Sams and Kouri.[8-12]

The integral solution of Eq. (1) is

$$F_{ij}(r) = \Delta_i \delta_{ij} G_i^{(1)}(k_i r) + G_i^{(2)}(k_i r) \int_0^r G_i^{(1)}(k_i x) S_{ij}(x)\, dx - G_i^{(1)}(k_i r) \int_0^r G_i^{(2)}(k_i x) S_{ij}(x)\, dx + G_i^{(1)}(k_i r) \times \int_0^\infty G_i^{(2)}(k_i x) S_{ij}(x)\, dx, \quad (3)$$

with

$$\Delta_i = \begin{cases} 1, & i \text{ open} \\ 0, & i \text{ closed}, \end{cases} \quad (4)$$

where S is the source term on the right-hand side of Eq. (1), and $G_i^{(\alpha)}(k_i r)$ are the appropriate Green's functions that are defined as real diagonal matrices[13]

$$G_i^{(1)}(k_i r) = \begin{cases} k_i^{1/2} r\, j_{l_i}(k_i r), & i \text{ open} \\ (2\kappa_i)^{1/2} r a_{l_i}(\kappa_i r), & i \text{ closed} \end{cases}$$

$$G_i^{(2)}(k_i r) = \begin{cases} k_i^{1/2} r y_{l_i}(k_i r), & i \text{ open} \\ \dfrac{-(2\kappa_i)^{1/2}}{\pi} r b_{l_i}(\kappa_i r), & i \text{ closed}, \end{cases} \quad (5)$$

where $j_l(x)$ and $y_l(x)$ are spherical Bessel and Neumann functions, $a_l(x)$ and $b_l(x)$ are appropriately defined modified spherical Bessel and Neumann functions, and the closed-channel modified wave number is $\kappa_i = |k_i|$. The boundary conditions associated with the scattering problem are satisfied with the following Green's functions:

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

$$G_i^{(1)}(k_i r) \underset{r\to\infty}{\sim} \begin{cases} k_i^{-1/2} \sin(k_i r - l_i \tfrac{1}{2}\pi), & i \text{ open} \\ (2\kappa_i)^{-1/2} e^{\kappa_i r}, & i \text{ closed} \end{cases} \quad (6)$$

$$G_i^{(1)}(k_i r) \underset{r\to\infty}{\sim} \begin{cases} -k_i^{-1/2} \cos(k_i r - l_i \tfrac{1}{2}\pi), & i \text{ open} \\ -(2\kappa_i)^{-1/2} e^{-\kappa_i r}, & i \text{ closed}. \end{cases}$$

Furthermore, note that the index j in Eq. (3) not only denotes the incident channel, but also the different independent solutions corresponding to channel i.

Another solution $\underline{\psi}$ to Eq. (1) is defined by neglecting the normalization term as in variable-phase theory[5]

$$\psi_{ij}(r) = G_i^{(1)}(k_i r) H_{ij}^{(2)}(r) - G_i^{(2)}(k_i r) H_{ij}^{(1)}(r),$$
$$H_{ij}^{(2)}(r) = \delta_{ij} - \int_0^r G_i^{(2)}(k_i x) S_{ij}(x)\, dx, \quad (7)$$
$$H_{ij}^{(1)}(r) = -\int_0^r G_i^{(1)}(k_i x) S_{ij}(x)\, dx.$$

In contrast, Sams and Kouri[8] retain the normalization term. If all the channels are open, the asymptotic boundary conditions on $\underline{\psi}$ and $\underline{F}$ are

$$\psi_{ij}(r) \underset{r\to\infty}{\sim} k_i^{-1/2} [A_{ij} \sin(k_i r - l_i \tfrac{1}{2}\pi) + B_{ij} \cos(k_i r - l_i \tfrac{1}{2}\pi)], \quad (8)$$
$$F_{ij}(r) \underset{r\to\infty}{\sim} k_i^{-1/2} [\delta_{ij} \sin(k_i r - l_i \tfrac{1}{2}\pi) + R_{ij} \cos(k_i r - l_i \tfrac{1}{2}\pi)],$$

where A_{ij} and B_{ij} are the asymptotic limits of the functions $H_{ij}^{(2)}(r)$ and $H_{ij}^{(1)}(r)$, respectively, and R_{ij} is the reactance matrix. Since $\underline{\psi}$ is a solution of Eq. (1), the linear combination

$$\phi_{ij}(r) = \sum_n \psi_{in}(r) A_{nj}^{-1} \quad (9)$$

is also a solution of Eq. (1). Noticing that $\underline{\phi}$ and $\underline{F}$ also satisfy the same boundary conditions, we can conclude that they are identical by uniqueness. Therefore, the reactance-matrix elements R_{ij} can

be determined from knowledge of the asymptotic behavior of the unnormalized function $\underline{\psi}$ from the equation

$$R_{ij}=\sum_n B_{in}A_{nj}^{-1}. \tag{10}$$

Next, we allow for closed channels. Unlike Sams and Kouri,[10] we do not explicitly solve open- and closed-channel equations. For a closed channel i, the solution $\psi_{ij}(r)$ grows exponentially, while the true solution $F_{ij}(r)$ decays asymptotically. From the structure of Eq. (7), the solution ψ_{ij} depends only on the knowledge of ψ_{nj} for all n. Therefore, in order to recover the open-open part of F_{ij}, we must force the closed-channel boundary conditions on the closed-open part of ψ_{ij}, and again force the open-channel boundary conditions on the open-open part of ψ_{ij}. In particular, for a two-channel problem, we can set ψ_{21} to zero by placing $\underline{\psi}$ into upper triangular form.[14]

The unnormalized solution of Eq. (7) may be rewritten as

$$\psi_{ij}(r)=\delta_{ij}G_i^{(1)}(k_ir)+\int_0^r G_i^{(2,1)}(r|x)\left(\sum_n[V_{in}(x)+W_{in}(x)]\psi_{nj}(x)+\sum_\lambda \delta_{l_il_\lambda}M_\lambda^{ij}P_\lambda(x)\right)dx, \tag{11}$$

with

$$G_i^{(2,1)}(r|x)=G_i^{(2)}(k_ir)G_i^{(1)}(k_ix)-G_i^{(1)}(k_ir)G_i^{(2)}(k_ix).$$

The exchange term may be rewritten so that Eq. (11) becomes

$$\psi_{ij}(r)=\delta_{ij}G_i^{(1)}(k_ir)+\int_0^r G_i^{(2,1)}(r|x)\left[\sum_n V_{in}(x)\psi_{nj}(x)+\sum_{\alpha_i}{}' B_i^{(\alpha_i)}P_{\rho_n}(x)\left(\frac{1}{x^{t+1}}\int_0^x P_{\rho_i}(y)\psi_{nj}(y)y^t\,dy\right.\right.$$
$$\left.\left.-x^t\int_0^x\frac{P_{\rho_i}(y)\psi_{nj}(y)}{y^{t+1}}\,dy\right)+\sum_\lambda\delta_{l_il_\lambda}M_\lambda^{ij}P_\lambda(x)+\sum_{\alpha_i}{}' B_i^{(\alpha_i)}P_{\rho_n}(x)x^t\int_0^\infty\frac{P_{\rho_i}(y)\psi_{nj}(y)}{y^{t+1}}\,dy\right]dx. \tag{12}$$

The solution to (11) can be written as

$$\psi_{ij}(r)=\psi_{ij}^{(0)}(r)+\sum_{m\alpha_m}\psi_{im}^{(\alpha_m)}(r)C_{mj}^{(\alpha_m)}, \tag{13}$$

with

$$C_{ij}^{(\alpha_i)}=\begin{cases}\displaystyle\int_0^\infty\frac{P_{\rho_i}(y)\psi_{nj}(y)\,dy}{y^{t+1}}, & \alpha_i=1,2,\ldots,N_E(i)\\ M_\lambda^{ij}\delta_{l_il_\lambda}, & \alpha_i=N_E(i)+1,\ldots,N_E(i)+N_0(i)\end{cases} \tag{14}$$

$$\psi_{im}^{(\alpha)}(r)=\delta_{\alpha0}\delta_{im}G_i^{(1)}(k_ir)+\int_0^r G_i^{(2,1)}(r|x)\left[\sum_n V_{in}(x)\psi_{nm}^{(\alpha)}(x)+\sum_{\alpha_i}{}' B_i^{(\alpha_i)}P_{\rho_n}(x)\left(\frac{1}{x^{t+1}}\int_0^x P_{\rho_i}(y)\psi_{nm}^{(\alpha)}(y)y^t\,dy\right.\right.$$
$$\left.\left.-x^t\int_0^x\frac{P_{\rho_i}(y)\psi_{nm}^{(\alpha)}(y)}{y^{t+1}}\,dy\right)\right]dx+\delta_{im}B_m^{(\alpha)}\int_0^r G_m^{(2,1)}(r|x)D_m^{(\alpha)}(x)\,dx, \tag{15}$$

and

$$B_i^{(\alpha)}=\begin{cases}0, & \alpha=0\\ B_i^{(\alpha_i)}, & \alpha=\alpha_i=1,2,\ldots,N_E(i)\\ 1 & \text{otherwise}\end{cases}$$

$$D_i^{(\alpha)}=\begin{cases}0, & \alpha=0\\ P_{\rho_n}(x)x^t, & \alpha_i=1,2,\ldots,N_E(i)\\ P_\lambda(x), & \alpha_i=N_E(i)+1,\ldots,N_E(i)+N_0(i)\end{cases}$$

where $N_E(i)$ is the number of exchange terms in channel i, and $N_0(i)$ is the number of orthogonality terms. For a given pair (m,α_m), we can generate a column vector $\psi_{im}^{(\alpha_m)}$ using Eq. (15). Similarly, another column vector $\psi_{im}^{(\alpha'_m)}$ can be generated for a given pair (m,α'_m). If $D_m^{(\alpha_m)}=D_m^{(\alpha'_m)}$, then the corresponding column vectors are related by

$$\psi_m^{(\alpha_m)}=\frac{B_m^{(\alpha_m)}}{B_m^{(\alpha'_m)}}\psi_m^{(\alpha'_m)}. \tag{16}$$

In addition, computation time can be saved by making the observation that the auxiliary function $\psi^{(\alpha)}$ can be evaluated without any matrix inversions.[8]

The constraint condition that determines the constants M_λ^{ij} is

$$\delta_{l_il_\lambda}\int_0^\infty P_\lambda(x)\psi_{ij}(x)\,dx=0. \tag{17}$$

We impose the constraint that the radial function must be orthogonal to all the atomic orbitals. We further introduce the quantity

$$E_i^{(\alpha_i)}(r)=\begin{cases}P_{\rho_i}(r)/r^{t+1}, & \alpha_i=1,2,\ldots,N_E(i)\\ P_\lambda(r), & \alpha_i=N_E(i)+1,\ldots,N_E(i)+N_0(i)\end{cases} \tag{18}$$

so that Eqs. (18) and (14) may be combined to yield

$$\Delta_{\alpha_i} C_{ij}^{(\alpha_i)}=\int_0^\infty E_i^{(\alpha_i)}(y)\psi_{nj}(y)\,dy, \tag{19}$$

with

$$\Delta_{\alpha_i}=\begin{cases}1, & \alpha_i=1,2,\ldots,N_E(i)\\ 0 & \text{otherwise.}\end{cases}$$

Substituting Eq. (13) into Eq. (19) yields a set of simultaneous equations to be solved for the constants $C_{ij}^{(\alpha i)}$, namely,

$$\Delta_{\alpha_i} C_{ij}^{(\alpha i)}=D_{ij}^{(\alpha i,0)}+\sum_{m\beta_m} C_{mj}^{(\beta_m)} D_{im}^{(\alpha i,\beta_m)}, \tag{20}$$

with

$$D_{ij}^{(\alpha i,\beta)}=\int_0^\infty E_i^{(\alpha i)}(y)\psi_{nj}^{(\beta)}(y)\,dy, \quad \beta=0,\beta_j. \tag{21}$$

Noting that the exchange and orthogonality terms exhibit the short-range behavior of the atomic electron orbitals, we have that the upper limit of the integral in Eq. (19) is basically the range of these orbitals.

The unnormalized solution $\underline{\psi}$ can be determined at a transformation point r_t by integrating the homogeneous solution $\underline{\psi}^{(0)}$ and the particular solutions $\underline{\psi}^{(\alpha)}$ of Eq. (15) from zero to r_t. This value of r is the point at which the integrals involving exchange and orthogonality terms have converged. Once the auxiliary functions are obtained, the constants $D_{ij}^{(\alpha i,\beta)}$ are simply determined from Eq. (21). Then, the constants $C_{ij}^{(\alpha i)}$ are computed by matrix inversion from Eq. (20). Hence, the solution $\underline{\psi}(r_t)$ may be determined from Eq. (13). Note that any further contribution to $\underline{\psi}(r)$ for $r>r_t$ comes only from the direct potential $\underline{V}(r)$. Knowing $\underline{\psi}(r_t)$, $\underline{H}^{(1)}(r_t)$, and $\underline{H}^{(2)}(r_t)$, we may either continue integrating $\psi(r)$ to a point where the potential vanishes, or we may "project" the H matrices to their asymptotic value by a technique given below. Finally, we obtain the reactance matrix from Eq. (10).

The projection procedure comes from noting that

$$\frac{d\underline{Z}_{pj}}{dr}(r)=\begin{pmatrix}\dfrac{dH_{ij}^{(1)}}{dr}(r)\\[2ex] \dfrac{dH_{ij}^{(2)}}{dr}(r)\end{pmatrix}$$

$$=-\begin{pmatrix}G_i^{(1)}(k_ir)\sum\limits_n V_{in}(r)\psi_{nj}(r)\\[2ex] G_i^{(2)}(k_ir)\sum\limits_n V_{in}(r)\psi_{nj}(r)\end{pmatrix} \tag{22}$$

where $p=1,2,\ldots,2N$, and $r>r_t$.

Substituting Eq. (7) into Eq. (22) yields

$$\frac{d\underline{Z}_{pj}}{dr}(r)=\sum_{q=1}^{2N} M_{pq}(r)Z_{qj}(r),$$

$$M_{pq}(r)=G_{\bar{p}}^{(\alpha_p)}(k_{\bar{p}}r)\,G_{\bar{q}}^{(\beta_q)}(k_{\bar{q}}r)\,V_{\bar{p}\bar{q}}(r)(-1)^{\beta_q},$$

with

$$\bar{p}=\begin{cases}p, & p\le n\\ p-n, & p>n\end{cases} \qquad \alpha_p=\begin{cases}1, & p\le n\\ 2, & p<n\end{cases}$$

$$\bar{q}=\begin{cases}q, & q\le n\\ q-n, & q>n\end{cases} \qquad \beta_q=\begin{cases}2, & q\le n\\ 1, & q>n\end{cases}.$$

Integration of Eq. (22) yields

$$\underline{Z}(\infty)=\underline{Z}(r_t)+\int_{r_t}^\infty \underline{M}(r)\cdot\underline{Z}(r)\,dr,$$

$$\underline{Z}(r)=\underline{Z}(r_t)+\int_{r_t}^r \underline{M}(x)\cdot\underline{Z}(x)\,dx,$$

which may be combined to yield

$$\underline{Z}(\infty)=\left[\underline{I}+\int_{r_t}^\infty \underline{M}(r)\,dr\right]\cdot\underline{Z}(r_t)$$
$$+\int_{r_t}^\infty \underline{M}(r)\cdot\int_{r_t}^r \underline{M}(x)\cdot\underline{Z}(x)\,dx\,dr. \tag{23}$$

If the last term in Eq. (23) is neglected,[15,16] we obtain the simple projection equation

$$\underline{Z}(\infty)=\underline{S}(\infty,r_t)\cdot\underline{Z}(r_t),$$
$$\underline{S}(\infty,r_t)=\underline{I}+\int_{r_t}^\infty \underline{M}(r)\,dr, \tag{24}$$

where the reactance-matrix projection equation is obtained from Eqs. (7), (8), (10), and (24):

$$\underline{R}(\infty)=\left[\underline{S}^{(1,1)}\cdot\underline{R}(r_t)+\underline{S}^{(1,2)}\right]\cdot\left[\underline{S}^{(2,1)}\cdot\underline{R}(r_t)+\underline{S}^{(2,2)}\right]^{-1} \tag{25}$$

with

$$\underline{S}=\begin{bmatrix}\underline{S}^{(1,1)} & \underline{S}^{(1,2)}\\ \underline{S}^{(2,1)} & \underline{S}^{(2,2)}\end{bmatrix}$$

and

$$\underline{R}(r_t)=\underline{H}^{(1)}(r_t)\cdot\underline{H}^{(2)}(r_t)^{-1}. \tag{26}$$

If the asymptotic form of the direct potential is substituted into Eq. (24), the resulting matrix $\underline{S}$ may be evaluated in terms of the standard incomplete sine and cosine functions.

From the reactance-matrix projection equation (25), we see that the corrections applied to $R_{ij}(r_t)$ are asymmetric for $i\neq j$. Therefore, for some scattering problems, the long-range behavior of the direct potential especially near threshold may cause the projection procedure to be inaccurate if the value chosen for r_t is too small. It may be necessary to choose a larger value for r_t so that the symmetry and convergence of the reactance matrix are acceptable.

III. APPLICATION TO A MODEL PROBLEM

The formalism discussed in Sec. II is applied to a model two-channel problem described by the coupled equations

$$\left(\frac{d^2}{dr^2} - \frac{l_i(l_i+1)}{r^2} + k_i^2\right) F_{ij}(r) = \sum_n V_{in}(r)F_{nj}(r) + 2Y_0(P_i,F_{ij};\, r)P_i(r) + M_{ij}P_i(r)\,, \tag{27}$$

where

$$V_{11}(r) = -2(1+1/r)e^{-2r}\,,$$

$$V_{22}(r) = 24/r^3 - (\tfrac{1}{4}r^2 + \tfrac{3}{2}r + \tfrac{11}{2} + 14/r + 24/r^2 + 24/r^3)e^{-r}\,,$$

$$V_{12}(r) = V_{21}(r) = -\frac{\sqrt{2}}{3}\left[\frac{256}{81r^2} - e^{-3r/2}\left(\frac{4}{3}r + \frac{32}{9} + \frac{128}{27r} + \frac{256}{81r^2}\right)\right]\,,$$

$$l_1 = 0, \quad l_2 = 1\,.$$

The level splitting is chosen to be 0.75 Ry, so that $k_1^2 = k_2^2 + 0.75$. This model is a truncated version of a $1s$-$2p$ approximation for e-H scattering. The model contains (i) long-range off-diagonal dipole coupling, (ii) one exchange term in each channel, and (iii) one orthogonality term in each channel.

The unnormalized solution to Eq. (27) is

$$\psi_{ij}(r) = \delta_{ij}G_i^{(1)}(k_ir) + \int_0^r dx\, G_i^{(2,1)}(r\,|\,x)\left[\sum_n V_{in}(x)\psi_{nj}(x) + 2P_i(x)\int_0^r \left(\frac{1}{x} - \frac{1}{y}\right)P_i(y)\psi_{ij}(y)\,dy\right]$$

$$+ (2C_{ij} + M_{ij})\int_0^r dx\, G_i^{(2,1)}(r\,|\,x)P_i(x)$$

$$= \psi_{ij}^{(0)}(r) + \sum_m \psi_{im}^{(1)}C_{mj} + \sum_m \psi_{im}^{(2)}M_{mj}\,, \tag{28}$$

where the auxiliary functions are defined as

$$\psi_{ij}^{(\alpha)}(r) = \delta_{\alpha 0}\delta_{ij}\,G_i^{(1)}(k_ir) + \int_0^r dx\, G_i^{(2,1)}(r\,|\,x)\left[\sum_n V_{in}(x)\,\psi_{nj}^{(\alpha)}(x) + 2P_i(x)\int_0^x dy\left(\frac{1}{x} - \frac{1}{y}\right)P_i(y)\,\psi_{ij}^{(\alpha)}(y)\right]$$

$$+ \delta_{ij}(2\delta_{\alpha 1} + \delta_{\alpha 2})\int_0^r dx\, G_i^{(2,1)}(r\,|\,x)P_i(x)\,. \tag{29}$$

Note that the inhomogeneous terms for $\alpha = 1$ and $\alpha = 2$ differ only by a factor of 2, so that their auxiliary functions are related as

$$\psi_{ij}^{(1)}(r) = 2\psi_{ij}^{(2)}(r)\,. \tag{30}$$

The exchange constant is

$$C_{ij} = \int_0^\infty P_i(y)\psi_{ij}(y)y^{-1}\,dy$$

$$= C_{ij}^{(0)} + \sum_m C_{im}^{(1)}C_{mj} + \sum_m C_{im}^{(2)}M_{mj}\,, \tag{31}$$

with

$$C_{ij}^{(\alpha)} = \int_0^\infty P_i(y)\,\psi_{ij}^{(\alpha)}(y)y^{-1}\,dy\,,$$

and the orthogonality constant is determined by

$$0 = M_{ij}^{(0)} + \sum_m M_{im}^{(1)}C_{mj} + \sum_m M_{im}^{(2)}M_{mj}\,, \tag{32}$$

with

$$M_{ij}^{(\alpha)} = \int_0^\infty P_i(y)\,\psi_{ij}^{(\alpha)}(y)\,dy\,.$$

We solve Eq. (27) by the NIEM method as follows.

(i) Obtain the auxiliary functions given in Eq. (29) by using a convenient integration scheme. We use the trapezoidal rule with a variable step size, to integrate the equations.[8] The power of the method comes from the fact that, as pointed out by Sams and Kouri,[8] the solution at a given value of r depends only on previously calculated values of r. For example, in Eq. (29) we replace the integrals by quadrature sums,

$$\psi_{ij}^{(\alpha)}(r_m) = \delta_{\alpha 0}\,\delta_{ij}\,G_i^{(1)}(k_jr_m) + \sum_{k=1}^{m}\omega_k G_i^{(2,1)}(r_m\,|\,r_k)$$

$$\times\left(\sum_n V_{in}(r_k)\,\psi_{nj}^{(\alpha)}(r_k) + 2P_i(r_k)\sum_{l=1}^{k}\omega_l(r_k^{-1} - r_l^{-1})\right.$$

$$\left.\times P_i(r_l)\,\psi_{ij}^{(\alpha)}(r_l) + \delta_{ij}\,(2\delta_{\alpha 1} + 2\delta_{\alpha 2})\,P_i(r_k)\right),$$

where ω_k are the weights of the quadrature scheme. Now we have that there is zero contribution to the summations over k and l from the terms $k = m$ and $l = k$, respectively. Thus, the right-hand side of

this equation does not involve the unknown functions at r_m.

(ii) Solve for the constants C_{mj} and M_{mj}. Since the constants $C_{ij}^{(\alpha)}$ and $M_{ij}^{(\alpha)}$ are determined in step (i), C_{mj} and M_{mj} are obtained by solving the set of simultaneous equations given in Eqs. (31) and (32).

(iii) Compute the reactance matrix $\underline{R}(r_t)$ and step out to $\underline{R}$. From the information gained in steps (i) and (ii), the unnormalized solution $\underline{\psi}(r)$ given in Eq. (27) can be computed at some transformation point r_t. The matrix $\underline{R}(r_t)$ is then computed from Eq. (26) using $\underline{H}^{(1)}(r_t)$ and $\underline{H}^{(2)}(r_t)$ of Eq. (7), and this matrix is projected to its asymptotic value using Eq. (25).

We solve Eq. (27) by another numerical procedure in order to obtain solutions that may be used as a standard against which results from the NIEM may be judged. The numerical solutions are obtained by integrating the equations outwards and inwards by Numerov's method, with subsequent matching to obtain a final continuous solution. The asymptotic expansion method of Burke and Schey[17] is used to determine the reactance maxtrix. A combination of these methods has been outlined by Smith *et al.*[1]

Table I gives reactance-matrix elements that agree with the numerical standard within 0.2%. Above and below threshold, a transformation point of $r_t = 30$ was found to yield acceptable symmetry and stability, except for $E = 0.749$ and $E = 0.751$, where a value of $r_t = 60$ was required.

TABLE I. Reactance-matrix elements at energies below and above threshold. Column (NIEM) presents results calculated using the NIEM; (Standard) lists the values obtained from another numerical procedure.

E (Ry)		NIEM	Standard
0.1	R_{11}	−1.471	−1.471
0.2	R_{11}	−3.937	−3.935
0.5	R_{11}	3.287	3.288
0.7	R_{11}	1.870	1.871
0.749	R_{11}	1.718	1.718
0.751	R_{11}	1.713	1.713
	R_{12}	0.0071	0.0071
	R_{22}	−0.166	−0.166
0.80	R_{11}	1.572	1.572
	R_{12}	0.240	0.240
	R_{22}	−2.738	−2.740
1.0	R_{11}	1.273	1.273
	R_{12}	−0.193	−0.193
	R_{22}	0.686	0.686
1.5	R_{11}	0.891	0.891
	R_{12}	−0.220	−0.220
	R_{22}	0.440	0.440

IV. SUMMARY AND DISCUSSION

We have presented a computational procedure for obtaining accurate solutions to the coupled integro-differential equations which describe a multichannel scattering process. The true solutions to the equations are obtained from unnormalized solutions by forcing the boundary conditions associated with the scattering problem. The unnormalized solutions can be obtained in the interaction region, where exchange and orthogonality are important, by a simple technique analogous to the homogeneous and particular solutions of differential-equation theory. A procedure projecting the reactance matrix out to its asymptotic value has been presented.

The NIEM presented here can be readily extended to scattering problems where the dominant asymptotic potentials are Coulombic by using Coulomb Green's functions.

ACKNOWLEDGMENTS

Special thanks are extended to Dr. D. J. Kouri for his assistance in the initial steps of this work. We also wish to thank S. P. Rountree and C. A. Weatherford for their many conversations. We also are grateful for the computing facilities provided by the LSU Computer Research Center.

*Supported by the Office of Naval Research under Contract No. N00014-69-A-0211-0004.

†Research will constitute a portion of a thesis to be submitted to LSU in partial fulfillment of the requirements for the Ph.D. degree in Physics.

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