A “canonical functions” approach to the solution of two coupled differential equations of scattering theory
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Abstract. — The system of two coupled Schrödinger differential equations (CE) arising in the close-coupling description of electron-atom scattering is considered. A « canonical functions » approach is used. This approach replaces the integration of CE for the eigenvector with unknown initial values by the integration of CE for « canonical » functions having well-defined initial values at an arbitrary origin \( r_0 \) \( (0 < r_0 < \infty) \). The terms of the reactance matrix are then deduced from these canonical functions. The results are independent from the choice of \( r_0 \). It is shown that many conventional difficulties in the numerical application are avoided, mainly that of the choice of the starting boundary variable \( r_s \sim 0 \) which is automatically determined. The results of the present method are compared to those of other methods and show excellent agreement with previous accurate results.

1. Introduction.

Scattering problems of molecules, atoms, electrons, etc. are commonly formulated in terms of coupled differential equations of the form [1]

\[
[\mathbf{I}(d^2/dr^2 - \ell(\ell + 1)/r^2) + \mathbf{K}^2 - \mathbf{U}(r)] \mathbf{Y}(r) = 0
\]

where the \( p \times p \) square matrix \( \mathbf{Y} \) is composed of solutions \( Y_{nm} \) for the channel \( n \) with wavenumber \( K_n \) and angular momentum number \( \ell \), \( \mathbf{U}(r) \) is a \( p \times p \) matrix, \( \mathbf{I} \) is the unit matrix, \( r \) is the radial variable.

Acceptable solutions of (1) must be continuous together with their first derivatives and must obey the boundary conditions

\[
\mathbf{Y}(0) = 0
\]

\[
\mathbf{Y}(r) = \mathbf{I}_n \mathbf{A} - \mathbf{N} \mathbf{B} \quad \text{as} \quad r \to \infty
\]

Here \( \mathbf{I} \) and \( \mathbf{N} \) are diagonal matrices given by

\[
J_{nm} = \delta_{nm} K_n^{1/2} r_j t_n(K_n r)
\]

\[
N_{nn} = \delta_{nn} K_n^{1/2} r_j t_n(K_n r)
\]
where \( J_t(x) \) and \( \eta_t(x) \) are spherical Bessel and Neumann functions respectively [2], \( \delta_{nm} \) is the Kronecker delta.

The constant matrices \( A \) and \( B \) formed in (3) are sufficient to determine the « reactance » matrix \( \mathbf{R} = \mathbf{B} \cdot \mathbf{A}^{-1} \) from which all scattering cross sections for the problem can be calculated [3].

In the last two decades, considerable progress has been made in the development of numerical methods for the solution of (1) (see for example Refs [4-12]); an excellent review is given by Thomas et al [13] The numerical determination of \( \mathbf{R} \) may be outlined as follows an integrator (like that of Numerov [14]) is used starting at an initial point \( r_s \sim 0 \) where the boundary condition (2) is satisfied, and stepping on until a sufficiently « large » value \( r_f \) where the other boundary condition (3) is satisfied. The matching of the computed matrix \( \mathbf{Y} \) with its asymptotic form (3) allows one to deduce the reactance matrix \( \mathbf{R} \).

As mentioned by Bayliss et al [12], straightforward application of most methods gives results sensitive to the point \( r_s \). If \( r_s \) is too small, the solutions may become unstable; if \( r_s \) is large the solutions are inaccurate.

The aim of this work is to show that the « canonical functions » method already used for the radial Schrödinger equation [15, 16] allows one to avoid the difficulty mentioned above. For clarity, the extension of the canonical functions method to the present problem is outlined in the next section for the two channel problem. This method is then tested against a conventional application.

2. The canonical functions method.

For the two channel case, the coupled equations (1) can be written

\[
\begin{align*}
Y_1''(r) + [K_1^2 - U_1(r) - C(r)] Y_1(r) &= V(r) Y_2(r) \\
Y_2''(r) + [K_2^2 - U_2(r) - C(r)] Y_2(r) &= V(r) Y_1(r)
\end{align*}
\]

where \( C(r) = \ell (\ell + 1)/r^2 \), \( V(r) \) is the « coupling » potential. The boundary conditions (2)-(3) can be written

\[
\begin{align*}
Y_i(r_s) &= 0 \quad \text{with} \quad r_s \sim 0, \quad i = 1, 2 \\
Y_i(r_f) &= F_i(r_f) \quad \text{with} \quad r_f \sim \infty, \quad i = 1, 2
\end{align*}
\]

with

\[
F_i(r) = K_i^{1/2} r[A_i J_t(K_i, r) + B_i \eta_t(K_i, r)], \quad i = 1, 2.
\]

Each of the two equations (4) may be written

\[
Y''(r) = f(r) y(r) + s(r)
\]

and may be treated separately as a linear nonhomogeneous second order differential equation. It is equivalent to the Volterra second kind integral equation [17]

\[
y(r) = y(r_0) + (r - r_0) y'(r_0) + \int_{r_0}^{r_{0}} (r - r') f(r') y(r') \, dr' + \int_{r_0}^{r} (r - r') s(r') \, dr'
\]

\( r_0 \) being an arbitrary « origin » \( (0 < r_0 < \infty) \).
When we write (B) for both $Y_1$ and $Y_2$ we find the coupled integral equations

$$
Y_1(r) = Y_1(r_0) + (r - r_0) Y'_1(r_0) + \int_{r_0}^{r} (r - r') [f_1(r') Y_1(r') + V(r') Y_2(r')] \, dr'
$$

(9.1)

$$
Y_2(r) = Y_2(r_0) + (r - r_0) Y'_2(r_0) + \int_{r_0}^{r} (r - r') [f_2(r') Y_2(r') + V(r') Y_1(r')] \, dr'
$$

(9.2)

The solution $Y_i(r)$ of this system may be considered as the limit of the successive approximations

$$
Y_i^{(0)}(r) = Y_i(r_0) + (r - r_0) Y'_i(r_0)
$$

$i = 1, 2$

$$
Y_i^{(1)}(r) = Y_i^{(0)}(r) + \int_{r_0}^{r} (r - r') [f_i(r') Y_i^{(0)}(r') + V(r') Y_j^{(0)}(r')] \, dr' \quad i = 1, 2 \quad j = 3 - i
$$

$$
Y_i^{(2)}(r) = Y_i^{(1)}(r) + \int_{r_0}^{r} (r - r') [f_i(r') Y_i^{(1)}(r') + V(r') Y_j^{(1)}(r')] \, dr'
$$

and so on. We find finally that the solutions $Y(r)$ can be written

$$
Y_1(r) = Y_1(r_0) \alpha_{11}(r) + Y_1'(r_0) \beta_{11}(r) + Y_2(r_0) \alpha_{12}(r) + Y_2'(r_0) \beta_{12}(r)
$$

(10.1)

$$
Y_2(r) = Y_1(r_0) \alpha_{21}(r) + Y_1'(r_0) \beta_{21}(r) + Y_2(r_0) \alpha_{22}(r) + Y_2'(r_0) \beta_{22}(r)
$$

(10.2)

The functions $\alpha_{ij}$, $\beta_{ij}$ have well determined values at $r_0$; these are

$$
\alpha_{ij}(r_0) = \beta_{ij}(r_0) = \delta_{ij}, \quad \alpha_{ij}'(r_0) = \beta_{ij}'(r_0) = 0.
$$

(11)

These functions are particular solutions of the coupled differential equations (4). This is clear when we substitute in (4) $Y_1$ and $Y_2$ by their expressions (10) and when we identify the coefficients of (the arbitrary constants) $Y_i(r_0)$ and $Y'_i(r_0)$. We find

$$
\alpha_{11}^i(r) = f_1(r) \alpha_{11}(r) + V(r) \alpha_{21}(r)
$$

(12.1)

$$
\alpha_{21}^i(r) = f_2(r) \alpha_{21}(r) + V(r) \alpha_{11}(r)
$$

(12.2)

with similar systems for the couples $(\beta_{11}, \beta_{21})$, $(\alpha_{12}, \alpha_{22})$ and $(\beta_{12}, \beta_{22})$. Here $f_1(r)$ and $f_2(r)$ are given by

$$
f_i(r) = K_i^2 - U_i(r) - C(r), \quad i = 1, 2
$$

The system (12) allows the direct computations of $\alpha_{11}$ and $\alpha_{21}$ since their initial values are known (Eq (11), similar systems allow the determination of other couples $(\beta_{11}, \beta_{21})$, $(\alpha_{12}, \alpha_{22})$ and $(\beta_{12}, \beta_{22})$. The functions $\alpha_{ij}$ and $\beta_{ij}$ present an advantage over the functions $Y_i$ solutions of the system (4) since the initial values $Y_i(r_0)$ and $Y'_i(r_0)$ are not completely known even at $r_0 = 0$. For this reason we call $\alpha_{ij}$ and $\beta_{ij}$ the «canonical functions» of the given system (4).

These canonical functions allow the determination of $Y_i(r_0)$ and $Y'_i(r_0)$ and furthermore of $Y_i(r)$.

By using the first boundary condition (at $r = 0$), the expressions (10) of $Y_i(r)$ lead to the relations

$$
0 = Y_1(r_0) \alpha_{11}(0) + Y'_1(r_0) \beta_{11}(0) + Y_2(r_0) \alpha_{12}(0) + Y'_2(r_0) \beta_{12}(0)
$$

(13.1)

$$
0 = Y_1(r_0) \alpha_{21}(0) + Y'_1(r_0) \beta_{21}(0) + Y_2(r_0) \alpha_{22}(0) + Y'_2(r_0) \beta_{22}(0).
$$

(13.2)
These relations allow one to have the two constants $Y_i'(r_0)$ in terms of the two others $Y_i(r_0)$, and to write

$$Y_1'(r_0) = Y_1(r_0) L_{11} + Y_2(r_0) L_{12} \quad (14.1)$$
$$Y_2'(r_0) = Y_1(r_0) L_{21} + Y_2(r_0) L_{22} \quad (14.2)$$

where

$$L_{11} = \begin{vmatrix} \alpha_{11}(0) & \beta_{12}(0) \\ \alpha_{21}(0) & \beta_{22}(0) \end{vmatrix} /D$$
$$L_{12} = \begin{vmatrix} \alpha_{12}(0) & \beta_{12}(0) \\ \alpha_{22}(0) & \beta_{22}(0) \end{vmatrix} /D$$
$$L_{21} = \begin{vmatrix} \alpha_{11}(0) & \beta_{11}(0) \\ \alpha_{21}(0) & \beta_{21}(0) \end{vmatrix} /D$$
$$L_{22} = \begin{vmatrix} \alpha_{12}(0) & \beta_{11}(0) \\ \alpha_{22}(0) & \beta_{21}(0) \end{vmatrix} /D$$

with

$$D = - \begin{vmatrix} \beta_{11}(0) & \beta_{12}(0) \\ \beta_{21}(0) & \beta_{22}(0) \end{vmatrix}$$

By making use of (14), the expressions (10) of the solutions $Y_i(r)$ become

$$Y_1(r) = Y_1(r_0) \gamma_1(r) + Y_2(r_0) \delta_1(r) \quad (16.1)$$
$$Y_2(r) = Y_1(r_0) \gamma_2(r) + Y_2(r_0) \delta_2(r) \quad (16.2)$$

where $\gamma_i$ and $\delta_i$ are related to $\alpha_{ij}$ and $\beta_{ij}$ by

$$\gamma_i(r) = \alpha_{ii}(r) + L_{11} \beta_{11}(r) + L_{21} \beta_{12}(r), \quad i = 1, 2 \quad (17.1)$$
$$\delta_i(r) = \alpha_{12}(r) + L_{12} \beta_{11}(r) + L_{22} \beta_{12}(r), \quad i = 1, 2 \quad (17.2)$$

We notice here too that the functions $\gamma_i(r)$ and $\delta_i(r)$ are particular solutions of the system (4) since they are (according to (17)) linear combinations of $\alpha_{ij}, \beta_{ij}$. Their initial values are deduced from (17) we write

$$\gamma_1(r_0) = 1, \quad \delta_1(r_0) = 0, \quad \gamma_2(r_0) = 0, \quad \delta_2(r_0) = 1 \quad (18.1)$$
$$\gamma_1'(r_0) = L_{11}, \quad \delta_1'(r_0) = L_{12}, \quad \gamma_2'(r_0) = L_{21}, \quad \delta_2'(r_0) = L_{22} \quad (18.2)$$

and

$$\gamma_i''(r) = f_1(r) \gamma_1(r) + V(r) \gamma_2(r) \quad (19.1)$$
$$\gamma_i''(r) = f_2(r) \gamma_2(r) + V(r) \gamma_1(r) \quad (19.2)$$
$$\delta_i''(r) = f_1(r) \delta_1(r) + V(r) \delta_2(r) \quad (20.1)$$
$$\delta_i''(r) = f_2(r) \delta_2(r) + V(r) \delta_1(r) \quad (20.2)$$

Thus $\gamma_i(r)$ and $\delta_i(r)$ are again canonical functions well determined by equations (18)-(20).

By imposing the second boundary condition (3), i.e., by using (16) and (5.2), one gets

$$F_1(r_f) = Y_1(r_0) \gamma_1(r_f) + Y_2(r_0) \delta_1(r_f) \quad (21.1)$$
$$F_2(r_f) = Y_1(r_0) \gamma_2(r_f) + Y_2(r_0) \delta_2(r_f) \quad (21.2)$$

$F_i(r_f)$ being given by (6). These are two relations between $Y_1(r_0)$, $Y_2(r_0)$ and the unknowns.
$A_1$, $B_1$, $A_2$, $B_2$ leading to the reactance $R$. These unknowns are obtained by giving to $(Y_1(r_0), Y_2(r_0))$ two couples of arbitrary values.


According to the theory presented above, the determination of the solution $Y_i(r)$ of the coupled equations (4) where the initial values are not known, is reduced to that of the other functions having well determined initial values at an arbitrary origin $r_0$, i.e., the canonical functions $(\alpha_{i1})$, $(\alpha_{i2})$, $(\beta_{i1})$, $(\beta_{i2})$ with $i = 1, 2$.

The computation of these functions for $r \leq r_0$ allows that of other canonical functions $\gamma_i$ and $\delta_i$ with $i = 1, 2$. This computation for $r \geq r_0$ allows the determination of $A_i$, $B_i$ (Eq. (16)) and consequently that of $R$.

Thus the whole effort is reduced to the successive use of one single operation, this is the integration of the coupled equations

$$y_i^1 + [K_i^2 - U_1(r) - C (r)] y_1 = V (r) y_2$$  \hspace{1cm} (22 1)

$$y_i^2 + [K_i^2 - U_2(r) - C (r)] y_2 = V (r) y_1$$  \hspace{1cm} (22.2)

where all the coefficients are known, and where the initial values $y_i(r_0)$ and $y'_i(r_0)$ are always given: (i) by (11) when $y_i$ stands for $\alpha_{i1}$, then for $\alpha_{i2}$, $\beta_{i1}$ and $\beta_{i2}$; (ii) by (18) when $y_i$ stands for $\gamma_i$ and $\delta_i$. So one single algorithm is needed for all the steps of the problem.

In order to test the present method we consider the following problem: the calculation of the reactance matrix $R$ for electron-hydrogen scattering in the «strong-coupling approximation» where only the first and the second atomic stages ($l = 0$) are included in the eigenfunction expansion with exchange neglected [18].

The potentials $U_1$, $U_2$ and $V$ are given by

$$U_1 = 2 - (1 + 1/r) \exp (-2 r)$$

$$U_2 = - 2 (1/r + 3/4 + r/4 + r^2/8) \exp (-r)$$

$$V = 4 \sqrt{2}/27 (2 + 3 r) \exp (-1.5 r).$$

The wavenumbers are fixed at $K_1 = 1$ and $K_2 = 0.5$ a.u.

Table I. — Computed values of reactance matrix terms $A_1$, $B_1$, $A_2$, $B_2$ by the present method compared to those by Chandra [1, 9], by Mohamed [18], and by Apagyi et al. [20]. The wavenumbers are fixed at $K_1 = 1$ and $K_2 = 0.5$ a.u.

<table>
<thead>
<tr>
<th></th>
<th>$A_1$</th>
<th>$B_1$</th>
<th>$A_2$</th>
<th>$B_2$</th>
</tr>
</thead>
<tbody>
<tr>
<td>Chandra</td>
<td>1 138853</td>
<td>0.3854753</td>
<td>0.3854697</td>
<td>- 0.3256686</td>
</tr>
<tr>
<td>Mohamed (a)</td>
<td>1.138839</td>
<td>0.3854565</td>
<td>0.3854490</td>
<td>- 0.3256349</td>
</tr>
<tr>
<td>Mohamed (b)</td>
<td>1.138996</td>
<td>0.3855010</td>
<td>0.3855010</td>
<td>- 0.3256568</td>
</tr>
<tr>
<td>Apagyi (c)</td>
<td>1.1530019</td>
<td>0.3871720</td>
<td>0.3871420</td>
<td>- 0.3189450</td>
</tr>
<tr>
<td>Apagyi (d)</td>
<td>1 1530147</td>
<td>0.3871970</td>
<td>0.3871970</td>
<td>- 0.3187691</td>
</tr>
<tr>
<td>Present method</td>
<td>1 1530146</td>
<td>0.38719696</td>
<td>0.38719696</td>
<td>- 0.31876919</td>
</tr>
</tbody>
</table>

(a) Mohamed method used with a local tolerance $\varepsilon = 10^{-4}$

(b) Mohamed method used with a local tolerance $\varepsilon = 10^{-8}$

(c) Apagyi method used with a basis size $N = 10$

(d) Apagyi method used with a basis size $N = 20$
This problem is well indicated to test the present method since it was already treated by Chandra [19] using a fixed step de Vogelaere's method, then by Mohamed [18] using the same method with variable steps, and more recently by Apagyi et al. [20] using a variational technique. In Table I the terms $A_1$, $B_1$, $A_2$, $B_2$ of the reactance matrix computed by the present method are compared to those obtained by the previous works.

We note that our results are in agreement with the others, we consider this as a first confirmation of the present method. The results by Apagyi given in the fifth line are the limits of $A_1$, $B_1$, $A_2$, $B_2$ when the basis size $N$ increases from $N = 2$ to $N = 20$ (see Tab. III of Ref [18]). Our results are in excellent agreement with those of Apagyi with $N = 20$; we consider this agreement as a further confirmation of the present method. We note finally that we obtain $A_2 = B_1$ which is predicted by the theory [20] The difference $A_2 - B_1$ decreases with $N$ in the Apagyi work from $6 \times 10^{-2}$ for $N = 2$ to $8 \times 10^{-9}$ for $N = 20$.

Our computations are done on a home computer (the New Brain AD, giving 8 significant figures). The program is quite simple since it uses one single routine, i.e., the numerical integration of a system of two coupled differential equations with given coefficients and given initial values (a listing is available from the authors upon request).

The details of the numerical treatment will be published elsewhere. However, we note here that the boundary points $r_s$ and $r_t$ are not imposed in our program; they are obtained automatically by (i) looking to the constant limit of $\alpha_{11}(r)/\beta_{11}(r)$ (or $\alpha_{21}(r)/\beta_{21}(r)$) when $r \to 0$, to obtain $r_s$; and (ii) by looking to the convergence of the terms $A_i$, $B_i$ of the reactance matrix $R$ when $r \to \infty$ to obtain $r_t$. We note also that the integration of the differential equation may be done, within the present scheme, by using any integrator. That used for the present application is the variable step version [21] of the «integrals superposition» difference equation [22] proved to be highly accurate [23].

4. Discussion.

In order to study the validity of the numerical application of the present method, we notice that this method makes no use of any theoretical approximation, nore of any a priori assumption like that usually used in the choice of $r_s$ and $r_t$, the starting point $r_0$ and the final point $r_f$ are, here, automatically determined by the boundary conditions as it was shown in section 2.

Since the numerical treatment of the present method is reduced to one single routine (the integration of the system [22] with given coefficients and given initial values), the unique sources of error are those of the numerical integration of the system [22].

The numerical integration is sensitive to the chosen integrator and to the step-size strategy. The integrator used here is the «integral superposition» (IS) difference equation [22-23].

The main numerical difficulty appearing here lies in the singularity of the potentials $(U_1$ and $U_2$) in the vicinity of $r \to 0$, on one hand, and in the necessity of the integration of the system in this vicinity (as indicated in the introduction) on the other hand.

We face this situation, as we did for a singular potential in a single channel [24] by using the variable-step version of the «integral superposition difference equations» [21]. We give in Table II as example the quantities $L_{11}$, $L_{12}$, $L_{21}$, $L_{22}$ (Eqs (15)) deduced from the canonical functions $a_{ij}$, $b_{ij}$ and computed for $K_1 = 1$ a.u., $K_2 = 0.5$ a.u., starting at $r_0 = 1$ and integrating backwards towards $r_0 \to 0$. We notice that the automatic determination of the step-size in each interval, allows one to approach the origin $r = 0$ (to any imposed accuracy), simply by looking to the stability (when $r \to 0$) of the computed functions.

Another illustration of the simplicity of the present method is presented in Table III, where we give the terms $A_1$, $B_1$, $A_2$, $B_2$ of the reactance matrix $R$. These terms are deduced from the
Table II. — *Computed values (at several values of \( r < 1 \) of the quantities \( L_{11}, \ L_{12}, \ L_{21}, \ L_{22} \) deduced from the canonical functions \( \alpha_{ij}, \ \beta_{ij} \) (Eqs. (15)), and used as initial values for the computation of the reactance matrix elements.\)

<table>
<thead>
<tr>
<th>( r )</th>
<th>( L_{11} )</th>
<th>( L_{12} )</th>
<th>( L_{21} )</th>
<th>( L_{22} )</th>
</tr>
</thead>
<tbody>
<tr>
<td>0.767 ( ^a )</td>
<td>4.1582105</td>
<td>0.019421007</td>
<td>0.019421007</td>
<td>4.1340494</td>
</tr>
<tr>
<td>0.327</td>
<td>1.0226503</td>
<td>0.071945593</td>
<td>0.071945593</td>
<td>0.92288978</td>
</tr>
<tr>
<td>0.127</td>
<td>0.38968764</td>
<td>0.12217359</td>
<td>0.12217359</td>
<td>0.21119275</td>
</tr>
<tr>
<td>0.044</td>
<td>0.0599000016</td>
<td>0.16729176</td>
<td>0.16729176</td>
<td>-0.19134879</td>
</tr>
<tr>
<td>0.013</td>
<td>-0.11278618</td>
<td>0.19787078</td>
<td>0.19787078</td>
<td>-0.41383629</td>
</tr>
<tr>
<td>0.003</td>
<td>-0.18290949</td>
<td>0.21179547</td>
<td>0.21179547</td>
<td>-0.50680657</td>
</tr>
<tr>
<td>0.5(- 3) ( ^b )</td>
<td>-0.20326702</td>
<td>0.21600709</td>
<td>0.21600709</td>
<td>-0.53406899</td>
</tr>
<tr>
<td>0.5(- 4)</td>
<td>-0.20724818</td>
<td>0.21683973</td>
<td>0.21683973</td>
<td>-0.53941574</td>
</tr>
<tr>
<td>0.2(- 5)</td>
<td>-0.20752484</td>
<td>0.21689770</td>
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<td>-0.53978748</td>
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<tr>
<td>0.6(- 7)</td>
<td>-0.20763839</td>
<td>0.21692150</td>
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<tr>
<td>0.13(- 7)</td>
<td>-0.20767751</td>
<td>0.21692970</td>
<td>0.21692970</td>
<td>-0.53999262</td>
</tr>
<tr>
<td>0 12(- 7)</td>
<td>-0.20768748</td>
<td>0.21693178</td>
<td>0.21693178</td>
<td>-0.54000603</td>
</tr>
</tbody>
</table>

\( ^a \) The integration is started at \( r = 1 \) The steps are successively computed by the « variable-step integrals-superposition » difference equations [21].

\( ^b \) 0.5(- 3) stands for \( 0.5 \times 10^{-3} \)

Table III — *Computed elements \( A_1, \ B_1, \ A_2, \ B_2 \) of the reactance matrix \( R \) at several values of \( r > 1 \)

<table>
<thead>
<tr>
<th>( r )</th>
<th>( A_1 )</th>
<th>( B_1 )</th>
<th>( A_2 )</th>
<th>( B_2 )</th>
</tr>
</thead>
<tbody>
<tr>
<td>1.233 ( ^a )</td>
<td>0.92512638</td>
<td>0.50674237</td>
<td>0.50674237</td>
<td>-1 6588524</td>
</tr>
<tr>
<td>2.206</td>
<td>1.0966815</td>
<td>0.41862183</td>
<td>0.41862183</td>
<td>-1 4204144</td>
</tr>
<tr>
<td>5.410</td>
<td>1.1352786</td>
<td>0.40148657</td>
<td>0.40148657</td>
<td>-0.35697847</td>
</tr>
<tr>
<td>9.481</td>
<td>1.1527700</td>
<td>0.38793510</td>
<td>0.38793510</td>
<td>-0.32347088</td>
</tr>
<tr>
<td>14.137</td>
<td>1.1530114</td>
<td>0.38719181</td>
<td>0.38719191</td>
<td>-0.31883044</td>
</tr>
<tr>
<td>16.415</td>
<td>1.1530141</td>
<td>0.38719946</td>
<td>0.38719946</td>
<td>-0.31877888</td>
</tr>
<tr>
<td>18.856</td>
<td>1.1530149</td>
<td>0.38719700</td>
<td>0.38719700</td>
<td>-0.31876926</td>
</tr>
<tr>
<td>21.184</td>
<td>1.1530150</td>
<td>0.38719702</td>
<td>0.38719702</td>
<td>-0.31876914</td>
</tr>
<tr>
<td>23.507</td>
<td>1.1530150</td>
<td>0.38719702</td>
<td>0.38719702</td>
<td>-0.31876900</td>
</tr>
<tr>
<td>24.652</td>
<td>1.1530150</td>
<td>0.38719702</td>
<td>0.38719702</td>
<td>-0.31876899</td>
</tr>
</tbody>
</table>

\( ^a \) The integration is started at \( r = 1 \) The steps are successively computed by the « variable-step integrals-superposition » difference equations [21].

The computation of the canonical function \( \gamma_i, \ \delta_i \ (i = 1, 2) \) (Eqs. (16)) started at \( r_0 = 1 \) and stepping on towards \( r \rightarrow \infty \). \( r_1 \) is reached when \( A_1, \ B_1, \ A_2, \ B_2 \) become constants.

One may note that in both integrations (for \( r < r_0 \), and for \( r > r_0 \)) the number of intervals
Table IV — Dependence of computed elements $A_i$, $B_i$ of the matrix $R$ upon the variable step-size $h = h(e)$, where the local tolerance $e$ is made to vary.

<table>
<thead>
<tr>
<th>$e$</th>
<th>$A_1$</th>
<th>$B_1$</th>
<th>$A_2$</th>
<th>$B_2$</th>
</tr>
</thead>
<tbody>
<tr>
<td>$10^{-3}$</td>
<td>-1.1691259</td>
<td>-0.38913309</td>
<td>-0.38913309</td>
<td>0.31114486</td>
</tr>
<tr>
<td>$10^{-4}$</td>
<td>1.1548922</td>
<td>0.38742101</td>
<td>0.38742101</td>
<td>-0.31787312</td>
</tr>
<tr>
<td>$10^{-5}$</td>
<td>1.1533287</td>
<td>0.38723442</td>
<td>0.38723442</td>
<td>-0.31861915</td>
</tr>
<tr>
<td>$10^{-6}$</td>
<td>1.1530291</td>
<td>0.38719869</td>
<td>0.38719869</td>
<td>-0.31876227</td>
</tr>
<tr>
<td>$10^{-7}$</td>
<td>1.1530174</td>
<td>0.38719730</td>
<td>0.38719730</td>
<td>-0.31876785</td>
</tr>
<tr>
<td>$10^{-8}$</td>
<td>1.1530146</td>
<td>0.38719696</td>
<td>0.38719696</td>
<td>-0.31876919</td>
</tr>
</tbody>
</table>

effectively used is quite limited (~20). This allows one to deduce that no significant round-off error was generated.

The present variable-step strategy was already tested against the eigenvalue problem for the radial equation [21] and showed high accuracy (equivalent to the computer precision). We give in Table IV an example of the influence of the local tolerance $e$ on the computed terms of the reactance matrix. We notice the stability of these values when $e$ approaches the computer precision.

Table V. — Computed values of the reactance matrix terms $A_1$, $B_1$, $A_2$, $B_2$ by the present method compared to those $A_1(N)$, $B_1(N)$, $A_2(N)$, $B_2(N)$ by Apagyi et al [20], for several values of the basis size $N$.

<table>
<thead>
<tr>
<th>$N$</th>
<th>$A_1(N)$</th>
<th>$B_1(N)$</th>
<th>$A_2(N)$</th>
<th>$B_2(N)$</th>
</tr>
</thead>
<tbody>
<tr>
<td>4</td>
<td>1.1490601</td>
<td>0.3820256</td>
<td>0.3851256</td>
<td>-0.3432615</td>
</tr>
<tr>
<td>8</td>
<td>1.1527882</td>
<td>0.3873718</td>
<td>0.3872978</td>
<td>-0.3192054</td>
</tr>
<tr>
<td>12</td>
<td>1.1530122</td>
<td>0.3872067</td>
<td>0.3871988</td>
<td>-0.3188105</td>
</tr>
<tr>
<td>16</td>
<td>1.1530148</td>
<td>0.3871968</td>
<td>0.3871965</td>
<td>-0.3187697</td>
</tr>
<tr>
<td>20</td>
<td>1.1530147</td>
<td>0.3871970</td>
<td>0.3871970</td>
<td>-0.3187691</td>
</tr>
<tr>
<td>Present method</td>
<td>1.1530146</td>
<td>0.38719696</td>
<td>0.38719696</td>
<td>-0.31876919</td>
</tr>
</tbody>
</table>

These convincing results are emphasized by the comparison of the reactance matrix elements obtained here with those of the excellent work by Apagyi and Ladanyi [20]. We give in Table V our $A_i$, $B_i$ matrix elements compared to those $A_1(N)$, $B_1(N)$ obtained by Apagyi and Ladanyi using a «least-squares variational method involving only square integrable test functions» [20], $N$ being the number of the test functions. According to Abdel-Raouf [25], when $N$ increases this method becomes «free» of anomalies. Note that our results are the limits of those by Apagyi-Ladanyi when $N$ increases.

We notice finally in Table I the discrepancy between our results (and those by Apagyi-Ladanyi) and those by Mohamed [18] (and by Chandra [9]). We assume that the reasons of this discrepancy are mainly (i) the starting point used by Mohamed is $r_0 \sim 0.03$, it is only
~ 0.00000001 in our work, (ii) the final point used by Mohamed is \( r_f \approx 13.7 \), it is of about 25 in our work, (iii) the integrator used by Mohamed is the de Vogelaere's integrator (a fourth order one), it is equivalent to the fourth-order Runge-Kutta integrator [9], much less accurate than our «integrals superposition» integrators [23].

5. Conclusion.

The «canonical functions» method, already used with success for the diatomic eigenvalues problem [15] and the phase shift problem [16], is extended here to the system of coupled differential equations arising in some scattering problems, and mainly to the determination of the reactance matrix \( R \) of the two-state close-coupling approximation of the electron-atom scattering.

It is shown that the canonical functions approach reduces the determination of the system solution (with unknown initial values) to that of the system with known initial values. Many conventional difficulties are thus avoided, we mention namely those related to the solution initial values and the linear combination of solutions, and those related to the numerical determination of the boundary regions.

The generalization of the present approach to the \( N \)-channel problem, and to other scattering problems is undertaken.

References

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