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Log-Derivative Method for Two-Potential Scattering Problems

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The log-derivative method of Johnson is generalized to solve inhomogeneous equations for scattering. Two versions of the method—applicable to half-collision and to two-potential inelastic collision problems, respectively—are presented. Both versions are tested for accuracy and convergence on simple one channel problems. The connection between the log-derivative and the R-matrix propagation methods is discussed in some theoretical and practical aspects.

1. INTRODUCTION

Two potential descriptions of scattering processes gives rise to many computationally involved problems in the present day investigations [1–4]. One can observe [4–6] a growing interest in algorithms for solving inhomogeneous equations arising from these investigations. The most reasonable way of developing such algorithms seems to be an adaptation of the techniques already established and proved in scattering calculations. The present paper is intended to contribute to this adaptation.

Before specifying the particular goals it is necessary to give a description of problems to be considered. Two potential problems are usually formulated in such a way that one potential is weak and therefore the transition matrix for processes governed by it can be determined perturbatively. In the first order of the perturbation theory elements of the transition matrix are given by integrals involving the weak potential and the wave functions describing initial and final states of the system under consideration.

Depending on the type of the initial state one can distinguish two cases of the two potential problems:

(I) Half-collision problems, e.g., the problems arising from the recently proposed description of a wide class of photodissociation processes [3] (it is characteristic for the half-collision problem that the system is initially in a bound state);

(II) Many channel scattering problems which are initially treated as com-

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pletely or partially decoupled and then a perturbative procedure is applied for their recoupling.

The well-known distorted wave or distorted-wave Born approximations and the recent corrected-coupled-state approximation [7, 8] should be quoted as examples here.

The approximate transition matrices for these cases are related to the following two point boundary value problems for system of differential equations,

$$\left[\frac{d^2}{dx^2} + B(x)\right]\psi(x) = V(x)\,\psi_\alpha(x), \tag{1}$$

$$\psi(x) \xrightarrow[x\to 0]{} 0, \tag{1a}$$

$$\psi(x) \xrightarrow[x\to\infty]{} \begin{cases} n(x)\mathscr{T} & \text{in case (I),} \\ m(x) - n(x)\mathscr{T} & \text{in the case (II).} \end{cases} \tag{1b}$$

The homogeneous part of these equations takes the usual form of coupled channel scattering equations with B representing the strong potential and including additionally channel energies and centrifugal terms. The weak potential occurs in the inhomogeneity term as the matrix V. $\psi_\alpha(x)$ in this term stands for a bound state function, $\psi_b(x)$, in case (I) ($\alpha = b$-bound) or for a scattering wavefunction, $\psi_0(x)$, in case (II) ($\alpha = 0$). $\psi_0(x)$ satisfies Eq. (1) with V set equal to zero and the boundary conditions: (1a) and

$$\psi_0(x) \xrightarrow[x\to\infty]{} m(x) - n(x)\,\mathscr{T}_0; \tag{1c}$$

m and n are diagonal matrices of linearly independent solutions of Eq. (1) in the asymptotic region where both potentials vanish. Depending on the form of these solutions $\mathscr{T}$ and $\mathscr{T}_0$ stand for the partial wave components of the transition or reactance matrices [9].

Now, it seems appropriate to comment on the present status in adapting to the above problems the existing scattering methods. Since these comments are not intended as an exhaustive review of the subject we will confine ourselves to the invariant imbedding methods.

There are three papers which propose invariant imbedding algorithms for solving inhomogeneous equations related to the half-collision problems. Two of them, i.e., the paper by Schneider and Taylor [5] and the earlier one by Kulander and Light [4], give algorithms which are generalizations of the R-matrix propagation method [10–12]. So, these algorithms fall into the category of the approximate potential procedures [13]. The complementary category of the approximate solution procedures represents the algorithm of the paper by Singer, Freed, and Band [6].

While the popularity of the R-matrix propagation method is a good recommendation for the proposed generalized versions of this method, the usefulness of the approximate solution algorithm is not so evident. Although there are no doubts

about the overall adequacy of the approximate solution approach to half-collision equations, the particular realization of this approach, i.e., the Singer method, does not seem to be optimal.

The Singer method consists in a numerical integration of the first order differential equations for the transition matrices. One of these equations is essentially known from the earlier applications of the invariant imbedding technique to scattering theory [14, 15]. Standard algorithms, such as the Runge–Kutta algorithm, are proposed for the integration. Being applicable to equations of general form, they cannot be expected to be very efficient in cases of definite properties.

No invariant imbedding method has been proposed so far for the problems defined in case (II) above. Probably this is due to the fact that computational investigations of coupled inhomogeneous equations for this case have been only started in connection with the project intended to correct the coupled state approximation [7, 8]. The algorithm currently used was developed from the method of Sams and Kouri [16]. This method was found [17] to be very efficient in some scattering calculations but as an example of the solution following technique [13] it is not stable when applied to coupled equations problems.

The first goal of this paper is an approximate-solution method for solving half-collision problems. It is different from the algorithm of Singer *et al.* [6] in two essential points:

(1) Instead of the scattering matrices $\mathscr{T}$ and $\mathscr{T}_0$ (defined as functions of the scattering coordinate, x) the matrix L is used as the invariant imbedding propagator of solutions of the system of differential equations. The properties of this propagator for homogeneous equations were discussed previously [18, 19]. Here this discussion will be extended to take into account an inhomogeneity in the system of equations. Due to the use of the matrix L the realization of the invariant imbedding technique becomes simpler already at initial analytical stage.

(2) The matrix L and some quantities related to it are accumulated for subsequent sectors of integration range according to appropriate recurrence relations. In the limit of zero-length sectors, these relations become differential equations [18, 20] which correspond to those integrated in the Singer method. One of these equations is nonlinear. In consequence of using the recurrence relations in the new algorithm only the original linear differential equations must be integrated to find approximate expressions for the sought quantities in small sectors.

It is almost obvious that because of the above differences the proposed algorithm should be more efficient than the existing algorithm of the same type.

The second goal of this paper is an invariant imbedding algorithm applicable in case (II) of the two-potential problems. Correcting various dimensionality-reducing approximations in a perturbative way seems to be an approach of promising implications for future investigations of collision systems too complex to be treated within the full coupled channel approximation. In view of this fact any attempt to provide a useful tool for these investigations is, in our opinion, worth undertaking.

Both proposed algorithms are closely related to the log-derivative method of Johnson [21, 22].

The analytical background for their derivation is given in Section 2. The L-matrix formulation of the two-potential problems presented there reveals some similarities to the formulation based on the matrix R [10–12]. A discussion of this connection and of its practical implications is given in the Appendix. Details of the discretization procedure employed in the derivation of the algorithms are described in Section 3. The last section is devoted to an estimation of the new algorithms. It is illustrated in part by numerical tests.

2. L-Matrix Formulation of Two-Potential Problems

The starting point is the standard propagation relation for solutions of the system of N linear second order differential equations in an interval $[x', x'']$,

$$\begin{pmatrix} \psi(x'') \\ \dot{\psi}(x'') \end{pmatrix} = \Omega(x'', x') \begin{pmatrix} \psi(x') \\ \dot{\psi}(x') \end{pmatrix} + \int_{x'}^{x''} \Omega(x'', x) \begin{pmatrix} 0 \\ \phi(x) \end{pmatrix} dx. \tag{2}$$

Ω is the $2N \times 2N$ Cauchy matrix [23] with blocks denoted as $\Omega = \left(\begin{smallmatrix} \Omega_1 & \Omega_2 \\ \Omega_3 & \Omega_4 \end{smallmatrix}\right)$; $\phi(x)$ stands for the inhomogeneous part in the system of equations, and the overdots denote derivatives with respect to x. A simple rearrangement of (2) leads to the relation

$$\begin{pmatrix} \dot{\psi}(x') \\ \dot{\psi}(x'') \end{pmatrix} = L(x', x'') \begin{pmatrix} \psi(x') \\ \psi(x'') \end{pmatrix} + \begin{pmatrix} Q(x', x'') \\ T(x', x'') \end{pmatrix}; \tag{3}$$

which defines the propagator $L = \left(\begin{smallmatrix} L_1 & L_2 \\ L_3 & L_4 \end{smallmatrix}\right)$,

$$L = \begin{pmatrix} -\Omega_2^{-1}\Omega_1 & \Omega_2^{-1} \\ \Omega_3 - \Omega_4\Omega_2^{-1}\Omega_1 & -\Omega_4\Omega_2^{-1} \end{pmatrix}; \tag{4}$$

and two additional quantities, Q and T, occurring only in the case of inhomogeneous equations,

$$Q(x', x'') = -\Omega_2^{-1}(x'', x') \int_{x'}^{x''} \Omega_2(x'', x)\, \phi(x)\, dx, \tag{5a}$$

$$T(x', x'') = \int_{x'}^{x''} [\Omega_4(x'', x) - \Omega_4(x'', x')\, \Omega_2^{-1}(x'', x')\, \Omega_2(x'', x)]\, \phi(x)\, dx. \tag{5b}$$

In the case when the inhomogeneity depends on a solution of the corresponding homogeneous equations which vanishes at the point x', i.e., when $\phi(x) = V(x)\, \psi_0(x)$ with $\psi_0(x') = 0$, one can exploit the relation

$$\psi_0(x) = \Omega_2(x, x')\, \dot{\psi}_0(x') = \Omega_2(x, x')\, L_2(x', x'')\, \psi_0(x''), \tag{6}$$

and rewrite the definitions of Q and T in the form

$$Q(x', x'') = Q^{-}(x', x'')\,\psi_0(x''), \tag{7a}$$

$$T(x', x'') = T^{-}(x', x'')\,\psi_0(x''). \tag{7b}$$

The new matrices Q^{-} and T^{-} are independent of the value of ψ_0 at the point x''. They can be found before this values is established. Thus, it becomes possible in this case to evaluate the inhomogeneous term for the system of equations simultaneously with the process of solving these equations.

The propagator L and the quantities Q and T satisfy the following recurrence relations;

$$\begin{pmatrix} L_1(x', x'') & L_2(x', x'') \\ L_3(x', x'') & L_4(x', x'') \end{pmatrix} = \begin{pmatrix} L_1(x', y) & 0 \\ 0 & L_4(y, x'') \end{pmatrix} + \begin{pmatrix} L_2(x', y) & 0 \\ 0 & L_3(y, x'') \end{pmatrix} L(x', y, x'') \begin{pmatrix} L_3(x', y) & 0 \\ 0 & L_2(y, x'') \end{pmatrix}, \tag{8}$$

$$\begin{pmatrix} Q(x', x'') \\ T(x', x'') \end{pmatrix} = \begin{pmatrix} Q(x', y) \\ T(y, x'') \end{pmatrix} + \begin{pmatrix} L_2(x', y) & 0 \\ 0 & L_3(y, x'') \end{pmatrix} L(x', y, x'') \begin{pmatrix} T(x', y) \\ Q(y, x'') \end{pmatrix}, \tag{9}$$

where y is a point in the interval $[x', x'']$ and $L(x', y, x'')$ denotes the $2N \times 2N$ block matrix constructed according to the formulas:

$$L(x', y, x'') = \begin{pmatrix} -1 & 1 \\ -1 & 1 \end{pmatrix} l(x', y, x''),$$

$$l(x', y, x'') = [L_4(x', y) - L_1(y, x'')]^{-1}.$$

The relation for the propagator L has been already published [18] and shown to result from the recurrence property of the standard propagator $\Omega(x'', x')$,

$$\Omega(x'', x') = \Omega(x'', y)\,\Omega(y, x') \qquad \text{for} \quad y \in [x', x'']. \tag{10}$$

The recurrence relations for the Q and T quantities result, of course, from the same property of the matrix Ω. They can be derived either directly from Eqs. (5a), (5b), and (10) or from the relation (8) after rewriting the definitions (5a) and (5b) in terms of the propagator L;

$$Q(x', x'') = -L_2(x', x'') \int_{x'}^{x''} L_2^{-1}(x, x'')\,\phi(x)\,dx, \tag{11a}$$

$$T(x', x'') = L_3(x', x'') \int_{x'}^{x''} L_3^{-1}(x', x)\,\phi(x)\,dx. \tag{11b}$$

The last formula for T is obtained with the aid of the recurrence relation (8) for the matrix L_4. After replacing $\phi(x)$ with $V(x)\,L_2^{-1}(x', x)\,L_2(x', x'')$ in both formulas, (11a) and (11b), one gets the expressions for the Q^- and T^--matrices,

$$Q^-(x', x'') = -L_2(x', x'') \int_{x'}^{x''} L_2^{-1}(x, x'')\, V(x)\, L_2^{-1}(x', x)\, dx\, L_2(x', x''), \quad (12a)$$

$$T^-(x', x'') = L_3(x', x'') \int_{x'}^{x''} L_3^{-1}(x', x)\, V(x)\, L_2^{-1}(x', x)\, dx\, L_2(x', x''). \quad (12b)$$

By proper exploiting of the recurrence relations (8) for the matrices L_2, L_3 and their inverses, one can derive from (12a), (12b) the following recurrence relations for Q^- and T^-,

$$\begin{pmatrix} Q^-(x', x'') \\ T^-(x', x'') \end{pmatrix} = \begin{pmatrix} 0 \\ T^-(y, x'') \end{pmatrix} + \begin{pmatrix} Q^-(x', y) \\ T^+(y, x'') \end{pmatrix} l(x', y, x'')\, L_2(y, x'') \quad (13)$$

$$+ \begin{pmatrix} L_2(x', y) \\ L_3(y, x'') \end{pmatrix} l(x', y, x'')\, Q^-(y, x'') - \begin{pmatrix} L_2(x', y) \\ L_3(y, x'') \end{pmatrix}$$

$$\times l(x', y, x'')[T^-(x', y) - Q^+(y, x'')]\, l(x', y, x'')\, L_2(y, x''),$$

where T^+ and Q^+ are defined by the formulas

$$T^+(x', x'') = L_3(x', x'') \int_{x'}^{x''} L_3^{-1}(x', x)\, V(x)\, L_3^{-1}(x, x'')\, dx\, L_3(x', x''),$$

$$Q^+(x', x'') = -L_2(x', x'') \int_{x'}^{x''} L_2^{-1}(x, x'')\, V(x)\, L_3^{-1}(x, x'')\, dx\, L_3(x', x'').$$

All recurrence relations should be supplied with values of the corresponding quantities for zero-length intervals. Obviously, the quantities Q, T, Q^-, and T^- vanish for such intervals. The propagator L for a zero-length interval $[x', x']$ should be determined from the definition (4) and from the normalization of the Cauchy matrix; $\Omega(x', x') = 1$. It is evident that $L(x', x')$ does not exist. For computational purposes, however, one can set

$$L(x', x') = \begin{pmatrix} -1 & 1 \\ -1 & 1 \end{pmatrix} c,$$

where c is a large positive constant: $c \gg 1$.

To connect the above considerations with the description of the two-potential scattering problems, one has to apply the relation (3) to the solutions of the boundary value problems specified in the Introduction. One derives in that way the formulas relating the matrix $\mathscr{T}$ for the processes of interest to the propagator L and to the matrices T or T^- for Eq. (1). In the latter case, the formula obtained will con-

tain the matrix $\mathscr{T}_0$ occurring in the boundary condition (1c) for the function $\psi_0(x)$. This matrix, however, can be expressed also in terms of the propagator L. The formulas for the matrices $\mathscr{T}$ occurring in the problems (1)–(1b) do not depend, in fact, on any Q-quantity. This is because of the boundary condition (1a) which arises usually in this form in 3-dim. description of a physical system. Quite often, however, 1-dim. description must suffice. In such cases both boundary conditions for the solutions of the appropriate coupled equations are nonzero and the matrix $\mathscr{T}$ is involved in both. So, the final formulas for this matrix become essentially dependent on the Q-quantities.

Finally, one should mention some symmetry relations which take place in the case of Eq. (1), where the matrices B and V are real and symmetric [27]. Namely, in this case the following relations hold for the blocks of the propagator L [19],

$$L_1^{\mathrm{T}} = L_1, \qquad L_4^{\mathrm{T}} = L_4, \qquad L_2^{\mathrm{T}} = -L_3,$$

and on their basis the following can be proved for the matrices $T^{\pm}$, $Q^{\pm}$

$$(T^-)^{\mathrm{T}} = T^-, \qquad T^+ = -(Q^-)^{\mathrm{T}}, \qquad (Q^+)^{\mathrm{T}} = Q^+.$$

The present formulation of the two-potential scattering problems in terms of the propagator L and the associated quantities for inhomogeneous equations is only one of several possible invariant imbedding formulations. All formulations must be, of course, equivalent. So, from purely analytical point of view there is no major reason for distinguishing them. Quite important differences may arise, however, when computational aspects are taken into account. In this context it seems interesting to consider the connection between the present formulation of the scattering problems and the widely used formulation based on the matrix R. These considerations are postponed to the Appendix.

3. Algorithms

The object of primary interest in this section will be the derivation of approximate expressions for quantities L, Q, T, $Q^{\pm}$, and $T^{\pm}$ in small intervals. After insertion of these expressions in the appropriate recurrence relations we will get an algorithm for evaluating these quantities over intervals of desired length.

Determination of any invariant imbedding-type propagator for system of linear differential equations requires solving definite boundary value problems for these equations. The boundary value problems related to the propagator $L(x', x'')$ for the system (1) take the form [18]

$$\left[\frac{d^2}{dx^2} + B(x)\right] \psi^{\pm}(x) = 0, \tag{14a}$$

$$\psi^{\pm}(x') = \begin{cases} 1, \\ 0, \end{cases} \qquad \psi^{\pm}(x'') = \begin{cases} 0, \\ 1. \end{cases} \tag{14b}$$

The additional problem related to the quantities $Q(x', x'')$ and $T(x', x'')$ for inhomogeneous equations is

$$\left[\frac{d^2}{dx^2} + B(x)\right] \psi_I(x) = \phi(x), \tag{15a}$$

$$\psi_I(x') = 0, \qquad \psi_I(x'') = 0. \tag{15b}$$

In terms of solutions of these problems one gets

$$L(x', x'') = \begin{pmatrix} \dot{\psi}^+(x') & \dot{\psi}^-(x') \\ \dot{\psi}^+(x'') & \dot{\psi}^-(x'') \end{pmatrix}$$

and

$$\begin{pmatrix} Q(x', x'') \\ T(x', x'') \end{pmatrix} = \begin{pmatrix} \dot{\psi}_I(x') \\ \dot{\psi}_I(x'') \end{pmatrix}.$$

The solutions of the problem (15a), (15b) with inhomogeneities $V(x)\psi^{\pm}(x)$, denoted correspondingly by $\psi_I^{\pm}(x)$, give the matrices $Q^+(x', x'')$ and $T^{\pm}(x', x'')$,

$$\begin{pmatrix} Q^+(x', x'') & Q^-(x', x'') \\ T^+(x', x'') & T^-(x', x'') \end{pmatrix} = \begin{pmatrix} \dot{\psi}_I^+(x') & \dot{\psi}_I^-(x') \\ \dot{\psi}_I^+(x'') & \dot{\psi}_I^-(x'') \end{pmatrix}.$$

In a previous paper [18] a discretization procedure of the problem (14a), (14b) was presented which has led to the extended version of the log-derivative method for calculating the matrix L. An analogous procedure will be applied here to the problem (15a), (15b).

Before the discretization is performed the problem must be converted to an integral equation form. This is done by means of the Green's function,

$$G(x, y) = W^{-1}\varphi^-(x_<)\,\varphi^+(x_>) \tag{16}$$

which is built from solutions of the equations

$$\frac{d^2}{dx^2}\,\varphi^{\pm}(x) = 0 \tag{17a}$$

satisfying the boundary conditions appropriate for the L-matrix formulation, i.e.,

$$\varphi^{\pm}(x') = \begin{cases} 1, \\ 0, \end{cases} \qquad \varphi^{\pm}(x'') = \begin{cases} 0, \\ 1. \end{cases} \tag{17b}$$

W denotes the Wronskian of these solutions: $W = \varphi - \dot{\varphi}^+ - \dot{\varphi}^-\varphi^+$, and $x_<$ ($x_>$) is

the usual notation for the smaller (bigger) from x, y values. As they can be easily found the explicit formulas for the $\varphi^{\pm}$- and W matrices are

$$\varphi^{-}(x)=\frac{x-x'}{x''-x'}1, \qquad \varphi^{+}(x)=\frac{x-x''}{x'-x''}1, \qquad W=-\frac{1}{x''-x'}1. \tag{18}$$

The integral equation form of (15a), (15b) is

$$\psi_I(x)=-\int_{x'}^{x''} G(x, y)[B(y)\,\psi_I(y)-\phi(y)]\,dy. \tag{19}$$

For its discretization the modified Simpson formula [24] is chosen which for an integrand $g(x)$ with a discontinuous first derivative at the midpoint of an integration range $[x_0-h, x_0+h]$ gives

$$\int_{x_0-h}^{x_0+h} g(x)\,dx \sim \frac{h}{3}[g(x_0-h)+4g(x_0)+g(x_0+h)] + \frac{h^2}{6}\lim_{\varepsilon\to 0^+}[\dot{g}(x+\varepsilon)-\dot{g}(x-\varepsilon)]. \tag{20}$$

Thus arise the algebraic equations

$$\psi_I(x_i)=-\sum_{k=0}^{M}\omega_k G(x_i, x_k)[B(x_k)\,\psi_I(x_k)-\phi(x_k)] - \alpha_i[B(x_i)\,\psi_I(x_i)-\phi(x_i)] \qquad \text{for } i=0, 1, 2,..., M. \tag{21}$$

x_k, ω_k, for $k=0,..., M$, are points and their weights in the ordinary Simpson formula, i.e., $x_{k+1}=x_k+h$, $x_0=x'$, $x_M=x''$, $\omega_0=\omega_M=h/3$, $\omega_k=2h/3$ for even k and $\omega_k=4h/3$ for odd k. The second term in (21) occurs only at unevenly numbered points x_i, where $\alpha_i=h^2/6$. For even i $\alpha_i=0$. The above equations can be conveniently rewritten in the form

$$f(x_i)=-\sum_{k=0}^{M}\omega_k G(x_i, x_k)[1+\alpha_k B(x_k)]^{-1}[B(x_k)\,f(x_k)-\phi(x_k)], \tag{22}$$

where the new functions, $f(x_k)$ for $k=0,..., M$, are defined as

$$f(x_k)=[1+\alpha_k B(x_k)]\,\psi_I(x_k)-\alpha_k\phi(x_k).$$

To proceed with the derivation, let us introduce the functions $f_{l,l+1}(x_i)$ for $l=0, 1,..., M-1$, defined at two points, x_l and x_{l+1}, by the following equations analogous in form to Eq. (22) for f,

$$f_{l,l+1}(x_i)=-\sum_{k=l}^{l+1}\tilde{\omega}_k G_{l,l+1}(x_i, x_k)[1+\alpha_k B(x_k)]^{-1} \times [B(x_k)\,f_{l,l+1}(x_k)-\phi(x_k)]. \tag{23}$$

$G_{l,l+1}$ means the Green's function (16) built from the solutions $\varphi^{\pm}_{l,l+1}(x)$ of the problem (17a), (17b) in the interval $[x'=x_l,\ x''=x_{l+1}]$. $\tilde{\omega}_k=\omega_k$ for $k=0, M$ and $\tilde{\omega}_k=\frac{1}{2}\omega_k$ for $k=1, 2,..., M-1$. By solving Eqs. (23), one can find the formulas

$$\tilde{Q}_{l,l+1}=-q_l\tilde{\omega}_l\phi(x_l), \qquad \tilde{T}_{l,l+1}=q_{l+1}\tilde{\omega}_{l+1}\phi(x_{l+1}), \tag{24}$$

where $q_k=[1+\alpha_k B(x_k)]^{-1}$ for $k=l,\ l+1$; for the quantities $\tilde{Q}_{l,l+1}$ and $\tilde{T}_{l,l+1}$ defined as

$$\tilde{Q}_{l,l+1}=\dot{f}_{l,l+1}(x_l), \qquad \tilde{T}_{l,l+1}=\dot{f}_{l,l+1}(x_{l+1}). \tag{25}$$

These quantities arising from inhomogeneous equations correspond to the auxiliary propagators

$$\tilde{L}_{l,l+1}=\begin{pmatrix}\tilde{L}^{(1)}_{l,l+1} & \tilde{L}^{(2)}_{l,l+1}\\ \tilde{L}^{(3)}_{l,l+1} & \tilde{L}^{(4)}_{l,l+1}\end{pmatrix}$$

used in the derivation of the log-derivative algorithm for homogeneous equations [18]. They are not direct approximations to the quantities Q and T in any sector $[x_1, x_{l+1}]$ but when assembled together with L-propagators according to the recurrence relations (8) and (9) over p subsequent sectors $[x_k, x_{k+1}]$, for $k=l$, $l+1,..., l+p-1$ and l, p even, they give approximate values of these quantities in the interval $[x_l, x_{l+p}]$. Thus, in addition to the formulas for $\tilde{L}_{l,l+1}$ found in [18],

$$\tilde{L}_{l,l+1}=\begin{pmatrix}-\frac{1}{h}(1-hS_l) & \frac{1}{h}\\ -\frac{1}{h} & \frac{1}{h}(1-hS_{l+1})\end{pmatrix}, \tag{26}$$

where $S_k=[1+\alpha_k B(x_k)]^{-1}\tilde{\omega}_k B(x_k)$, $k=l, l+1$, the formulas (25) for $\tilde{Q}_{l,l+1}$ and $\tilde{T}_{l,l+1}$ are just what is needed for extending the log-derivative algorithm to inhomogeneous equations.

The necessary formulas for the quantities $\tilde{Q}^{\pm}_{l,l+1}$ and $\tilde{T}^{\pm}_{l,l+1}$ corresponding to the equations with inhomogeneous terms $V(x)\psi^{\pm}(x)$ are

$$\begin{aligned}\tilde{Q}^{+}_{l,l+1}&=-q_l\tilde{\omega}_l V(x_l)\,q_l, \qquad \tilde{Q}^{-}_{l,l+1}=0,\\ \tilde{T}^{+}_{l,l+1}&=0, \qquad \tilde{T}^{-}_{l,l+1}=q_{l+1}\tilde{\omega}_{l+1}V(x_{l+1})\,q_{l+1}.\end{aligned} \tag{27}$$

These formulas are obtained from (24) by inserting for $\phi(x_i)$ at $x_i=x_l,\ x_{l+1}$ the expressions $V(x_i)\psi^{\pm}_{l,l+1}(x_i)$ with functions $\psi^{\pm}_{l,l+1}(x_i)$ given by the equations

$$\begin{aligned}\psi^{\pm}_{l,l+1}(x_i)=\varphi^{\pm}_{l,l+1}(x_i)&-\sum_{k=l}^{l+1}\tilde{\omega}_k G(x_i, x_k)\,B(x_k)\,\psi^{\pm}_{l,l+1}(x_k)\\ &-\alpha_i B(x_i)\,\psi^{\pm}_{l,l+1}(x_i).\end{aligned} \tag{28}$$

Equations of this form arise from the discretization of the homogeneous problems (14a), (14b) with the aid of the formula (20) [18]. Their solutions are

$$\psi^{\pm}_{l,l+1}(x_l)=\begin{cases}q_l,\\0,\end{cases}\qquad \psi^{\pm}_{l,l+1}(x_{l+1})=\begin{cases}0,\\q_{l+1}.\end{cases} \tag{29}$$

For writing the final result of this section, some technical preparations remain to be made. First, the following notation is introduced for the approximate values of the L, T, Q, and T^- quantities in the interval $[x_0, x_l]$;

$$L_{0,l}=\begin{pmatrix}L^{(1)}_{0,l} & L^{(2)}_{0,l}\\ L^{(3)}_{0,l} & L^{(4)}_{0,l}\end{pmatrix},\qquad \begin{pmatrix}Q_{0,l}\\ T_{0,l}\end{pmatrix},\qquad \begin{pmatrix}Q^-_{0,l}\\ T^-_{0,l}\end{pmatrix}.$$

The same notation with an additional tilde will be used for the quantities accumulated according to the appropriate recurrence relations from the quantities defined for one sector by Eqs. (24) and (27). As was mentioned before, the quantities with and without tildes, coincide for l even.

Furthermore, the following working quantities are introduced with the purpose of simplifying the formulas to be given,

$$\begin{aligned}z_l&=h\tilde{L}^{(4)}_{0,l}+1-hS_l,\\ t_l&=h[\tilde{T}_{0,l}+q_l\tilde{\omega}_l\phi(x_l)],\\ t^-_l&=h[\tilde{T}^-_{0,l}+q_l\tilde{\omega}_l V(x_l)\,q_l].\end{aligned}$$

The final formulas, derived on the basis of the recurrence relations of the previous section, are

$$\begin{aligned}\tilde{Q}_{0,l}&=\tilde{Q}_{0,l-1}-\tilde{L}^2_{0,l-1}z^{-1}_{l-1}t_{l-1},\\ t_l&=2hq_l\tilde{\omega}_l\phi(x_l)+z^{-1}_{l-1}t_{l-1},\\ t^-_l&=2hq_l\tilde{\omega}_l V(x_l)\,q_l+z^{-1}_{l-1}t_{l-1}z^{-1}_{l-1}.\end{aligned}$$

Adding to them the recurrence formula for $\tilde{L}^{(2)}$ found in [18] and the formula for z_l from the original log-derivative method, one gets the following two versions of this method applicable, respectively, to the two cases of the two-potential problems specified in the Introduction:

(I) The "half-collision" version—the quantities required: $T_{0,M}$, $Q_{0,M}$,

$$z^{-1}_0=0,$$

$$\tilde{L}^{(2)}_{0,1}=\frac{1}{h},$$

$$\tilde{Q}_{0,1}=-\frac{h}{3}\phi_0,$$

$$t_0 = \frac{h^2}{3}\phi_0,$$

$$z_l = \begin{cases} -6 + g_l - z_{l-1}^{-1} & \text{for } l = 1, 3, 5, \ldots, M-1, \\ 2 - \frac{2h^2}{3} B_l - z_{l-1}^{-1} & \text{for } l = 2, 4, 6, \ldots, M, \end{cases}$$

$$t_l = \begin{cases} \frac{h^2}{6} g_l \phi_l + z_{l-1}^{-1} t_{l-1} & \text{for } l = 1, 3, 5, \ldots, M-1, \\ \frac{2h^2}{3} \phi_l + z_{l-1}^{-1} t_{l-1} & \text{for } l = 2, 4, 6, \ldots, M, \end{cases}$$

$$\left.\begin{aligned} \tilde{L}_{0,l}^{(2)} &= \tilde{L}_{0,l-1}^{(2)} z_{l-1}^{-1} \\ \tilde{Q}_{0,l} &= \tilde{Q}_{0,l-1} - \tilde{L}_{0,l}^{(2)} t_{l-1} \end{aligned}\right\} \quad \text{for } l = 2, 3, 4, 5, \ldots, M,$$

$$T_{0,M} = \tilde{T}_{0,M} = \frac{1}{h}\left(t_M - \frac{h^2}{3}\phi_M\right),$$

$$Q_{0,M} = \tilde{Q}_{0,M},$$

where

$$g_l = \left[0.125 + \frac{h^2}{48} B_l\right]^{-1}$$

$$B_l = B(x_l), \qquad \phi_l = \phi(x_l)$$

(II) the version for inelastic scattering problems formulated in a manner related to the distorted wave approximation—the matrix $T_{0,M}^{-}$ required

$$t_0^{-} = \frac{h^2}{3} V_0,$$

$$t_l^{-} = \begin{cases} \frac{4h^2}{3} g_l V_l g_l + z_{l-1}^{-1} t_{l-1}^{-} z_{l-1}^{-1} & \text{for } l = 1, 3, 5, \ldots, M-1, \\ \frac{2h^2}{3} V_l + z_{l-1}^{-1} t_{l-1}^{-} z_{l-1}^{-1} & \text{for } l = 2, 4, 6, \ldots, M, \end{cases}$$

$$T_{0,M}^{-} = \tilde{T}_{0,M}^{-} = \frac{1}{h}\left(t_M^{-} - \frac{h^2}{3} V_M\right),$$

where $V_l = V(x_l)$.

4. Numerical Tests and Discussion

The "half-collision" version of the log-derivative algorithm was tested on a simple one channel problem related to the photoionization of atomic hydrogen

$$\left[\frac{d^2}{dr^2}+\frac{2}{r}-\frac{2}{r^2}+k^2\right]\chi(r)=-4r^2e^{-2r}, \tag{30}$$

$$\chi(0)=0, \tag{30a}$$

$$\chi(r)\xrightarrow[r\to\infty]{}\frac{4}{k}e^{i[kr-(\pi/2)+(1/k)\ln(2kr)]}M. \tag{30b}$$

More details on this problem are given in [5] where it was specified with an analogous purpose of checking a new computational method. In this case a version of the R-matrix propagation method was tested.

As a check of correctness of our algorithm the values of the transition matrix element M, obtained in this work, are compared in Table I with the results reported in [5]. The question of interest is: What is the performance of the new algorithm in regions of rapidly varying potentials, such as the interval $[0, 3]$ for the potential $V(r)=(2/r^2)-(2/r)$ in Eq. (30). The original log-derivative algorithm is known as more appropriate for such regions than the approximate potential procedures and the tests for the above problem suggest that this feature is maintained in the present generalized version.

As an illustration to this point Figs. 1–3 are given. They show errors of the (1-dim.) matrices $L_4(0, r)$ and $T(0, r)$ for Eq. (30) with $k^2=1$ calculated by the log-derivative algorithm, by the approximate potential procedures with constant approximating potentials, and with constant or variable step sizes. The errors are referred to the results of the approximate solution calculations with the step size $h=0.0025$.

TABLE I

Test of Correctness of the Log-Derivative Method (Version I) on Problem (30)–(30b)[a]

k	M	$M(R)$
0.4472	0.64684	0.6483
0.6325	0.57729	0.5777
0.7746	0.49673	0.4971
0.8944	0.42667	0.4267
1.0	0.36865	0.3690
1.0954	0.32109	0.3211
1.1832	0.28190	0.2819
1.2649	0.24940	0.2495

[a] (R)-results by the R-matrix propagation method of [5].

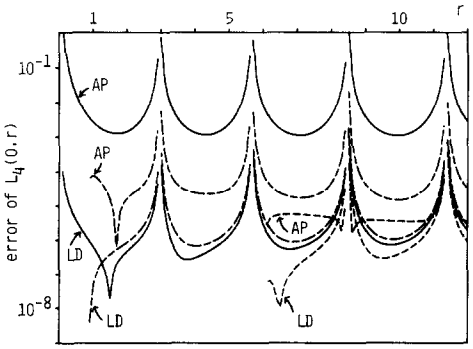

FIG. 1. Error of $L_4(0, r)$ calculated by the log-derivative method (LD) and by the approximate potential procedure (AP) with the same as in (LD) constant step size $h = 0.05$. Calculations started from exact values of $L_4(0, r_B)$ at different points r_B; $r_B = 0$ (—); $r_B = 0.8$ (·—·); $r_B = 6$ (---).

Figures 1 and 2 are in fact one more exemplification of the well-known difference between the approximate solution and approximate potential approaches. While the error propagation in the new algorithm is only slightly affected by starting the calculations from various points of the interaction range the differences in error level between the analogous calculations in the approximate potential approach are quite remarkable. The decisive factor is here clearly the shape of the potential in the region included.

Besides the difference in error sources Figs. 1 and 2 show also a similarity between the tested methods resulting from their common invariant imbedding origin. Namely, the quantities propagated by both methods become singular at some points in the classically allowed region. These points correspond to the maxima of error encountered in all tests. The local character of these maxima should be considered as a manifestation of numerical stability of the invariant imbedding recurrence relations.

For a comparison of the new algorithm to the approximate potential procedures

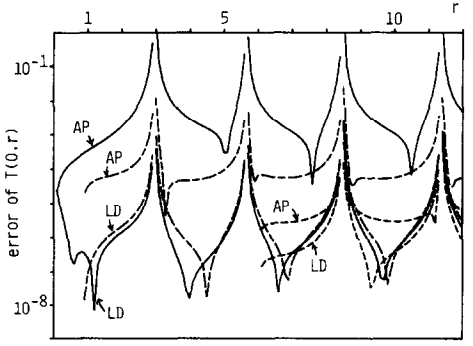

FIG. 2. Same as in Fig. 1 for $T(0, r)$.

in respect of accuracy, one should note that both Figs. 1 and 2 concern calculations with the same constant step size $h = 0.05$. The better accuracy of the approximate solution method in treating the regions of rapidly varying potential is evident from these figures.

The method was found to be more accurate also than the variable step version of the approximate potential procedure used. This is shown in Fig. 3. The slopes of the solid lines in this figure give $O(h^4)$ convergence of the quantities calculated by the approximate solution method. The convergence in the constant step approximate potential method is of $O(h^2)$ type, and in the variable step case it is not uniform. The criterion applied for changing step sizes was that of Stechel *et al.* [12]. The quantitative picture of the relative accuracy of the tested methods as given in Fig. 3 will change, of course, for other problems. For many channel problems, it may be even more favourable for the log-derivative method because additional errors, caused by rotations of the bases between sectors, arise in the approximate potential procedures.

The final question to ask is: How would a comparison look if we compared the present "half-collision" version of the log-derivative method with the R-matrix propagation method in respect of computational effort per sector. Obviously, the test on a one-channel model cannot serve here as a reliable basis for any quantitative estimates. Still, in view of the well-known findings of Thomas *et al.* [17] concerning the performance of the original versions of these methods in solving coupled homogeneous equations one may be interested in getting at least an idea of what effect have the additional operations required for inhomogeneous equations on the relative efficiency of both methods. It is easy to count these operations in the log-derivative method. To calculate the quantities T and Q for a system of N coupled equations (15a) with an inhomogeneity vector ϕ, one has to perform two multiplications of $N \times N$ matrices by vectors at each evenly numbered sector and three such multiplications at each odd sector. Evidently, this is not much additional

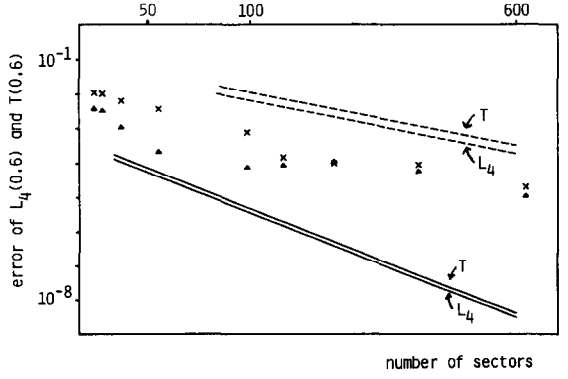

FIG. 3. Error of $L_4(0, 6)$ and $T(0, 6)$ versus number of sectors in the log-derivative method (—) and in the approximate potential procedures with constant (---) and variable [(Δ), L_4; (×), T] step sizes.

work as compared to the work needed for the basic matrix operations involved in the evaluation of the propagator L (see also [18; Eqs. 70–72]): multiplication of $N \times N$ matrices—two at each sector and inversions (of symmetric $N \times N$ matrices)—two at odd and one at even sectors.

In the R-matrix propagation method, extra work is required to calculate the quantities A_R and B_R (Eqs. (A6), (A7)) which carry the information equivalent to that contained in the quantities T and Q (see Appendix). To get A_R and B_R, one needs three multiplications of $N \times N$ matrices by vectors at each sector (see Eqs. (29), (30) in [4]). Moreover, the integrals occurring in Eqs. (A8), (A9) must be evaluated (see the procedure for the quantities "sos" and "soc" in [4]). Even though this is not a very detailed analysis, it indicates that the additional operations in the R-matrix propagation method outnumber the corresponding operations in the log-derivative method. Taking into account the fact that the number of matrix operations per sector needed for the evaluation of the propagator R in the approximate potential approach is significantly higher than the number of the operations listed above for the propagator L [11–13, 17], one can expect that the new version of the log-derivative method, like the original version, is superior in regions of rapidly varying potentials.

This suggests that a combination of the new algorithm with an appropriately extended version of the variable interval–variable step method [25] should give a very efficient procedure which would be a generalization of the hybrid log-derivative-VIVAS method [17] for inhomogeneous equations problems.

While the confrontation of the approximate solution and approximate potential approaches was the main point of testing the "half-collision" version of the log-derivative algorithm other aspects become important in the case of the second version designed for two-potential inelastic scattering problems. As was mentioned, this algorithm is the first attempt toward applying the invariant imbedding approach to such problems. Thus, the aspect to emphasize is the numerical stability. In this respect, the proposed algorithm should be superior to solution following methods [13]. Obviously, this stability can be best appreciated when many open channels and some closed are coupled in a problem. We did not perform any tests on such problems knowing that stability of our algorithm is guaranteed by its invariant imbedding origin. An open question remains, of course, how profitable this feature can be in cases of interest.

The performed tests were concentrated only on showing the type of convergence according to the formula of Jackson and Mott [26]. A sample of this comparison is given in Table II. One can see from the table that the error of the numerical results reveal a tendency to be proportional to fourth power of the step size.

Obviously, our estimation of both of the algorithms has only a preliminary character as being based on a rather limited computational material. It is believed, however, that the features of these algorithms, like their stability and convergence

TABLE II

Convergence Tests of the Log-Derivative Method (Version II) on the Secrest–Johnson Problem[a]

h	$P_{0\to1}$	Error $\times h^{-4}$	$P_{0\to2}$	Error $\times h^{-4}$	$P_{1\to2}$	Error $\times h^{-4}$	$P_{1\to3}$	Error $\times h^{-4}$	$P_{2\to3}$	Error $\times h^{-4}$
0.4	0.356012	0.209	0.597205(−5)	1.53	0.139720	0.331	0.687687(−7)	0.447	0.429503(−2)	0.146
0.2	0.354150	0.058	0.575723(−5)	1.16	0.140869	0.203	0.695333(−7)	0.288	0.427991(−2)	0.123
0.1	0.354118	0.016	0.574716(−5)	1.09	0.140912	0.188	0.695634(−7)	0.268	0.427912(−2)	0.119
0.05	0.354118	0.010	0.574657(−5)	1.08	0.140914	0.186	0.695652(−7)	0.265	0.427908(−2)	0.119
0.025	0.354117	0.009	0.574653(−5)	1.08	0.140914	0.185	0.695653(−7)	0.291	0.427907(−2)	0.119
Exact	0.354117		0.574653(−5)		0.140914		0.695653(−7)		0.427907(−2)	

[a] Distorted wave results for $E=8$ and $m=\frac{2}{3}$.

properties, support the opinion that they may be useful in solving inhomogeneous equations problems of scattering theory. Recalling the role of the original log-derivative method in the inelastic collision investigations, one can hope that the present extended versions of this method will find equally successful applications to two-potential problems of physical interest.

APPENDIX: Connection between the L-Matrix and R-Matrix Formulations of Scattering Problems

The R-matrix formulation of the problem of solving a system of second order linear differential equations starts from the relation

$$\begin{pmatrix} \psi(x') \\ \psi(x'') \end{pmatrix} = R(x', x'') \begin{pmatrix} \dot{\psi}(x') \\ \dot{\psi}(x'') \end{pmatrix} + \begin{pmatrix} Q_R(x', x'') \\ T_R(x', x'') \end{pmatrix}, \tag{A1}$$

which originates also in the standard relation (2) for this problem. Only a slightly different sign convention is applied here in comparison to the papers [11, 12]. Thus, the quantities involved in the L- and R-matrix formulations are connected as follows:

$$R = L^{-1}, \tag{A2}$$

$$\begin{pmatrix} Q_R \\ T_R \end{pmatrix} = -L^{-1} \begin{pmatrix} Q \\ T \end{pmatrix}. \tag{A3}$$

The most interesting point, however, lies in comparing the recurrence relations appropriate for both formulations. The structural identity of the recurrence relations for the corresponding blocks of the propagators L and R has been stated in [18]. The same correspondence also takes place between the pairs of quantities (Q, T) and (Q_R, T_R) introduced for inhomogeneous equations. The proof of that remains a matter of deriving the relations for Q_R and T_R. Essential for this derivation are the recurrence relations for the matrices R_i, $i = 1, 2, 3, 4$ (i.e., the relations (8)) which should be applied to the following expressions:

$$Q_R(x', x'') = R_2(x', x'') \int_{x'}^{x''} R_2^{-1}(x, x'')\, R_1(x, x'')\, \phi(x)\, dx, \tag{A4}$$

$$T_R(x', x'') = -R_3(x', x'') \int_{x'}^{x''} R_3^{-1}(x', x)\, R_4(x', x)\, \phi(x)\, dx. \tag{A5}$$

These expressions are obtained from Eqs. (2) and (A1) after some algebraic manipulations involving also the relations (8) for the R_i-matrices. Thus, the structures of the recurrence relations from the L- and R-matrix approaches to systems of

inhomogeneous equations are the same; the corresponding relations can be converted one into the other by the simple replacements:

$$Q \to Q_R, \qquad T \to T_R, \qquad L_i \to R_i \qquad \text{for} \quad i = 1, 2, 3, 4 \text{ or vice versa.}$$

This implies in practice a possibility of using all existing approximate potential procedures for the matrix R almost directly to the matrix L. The required adaptation is really slight and consists mainly in exploiting the relation (A2) in all sectors of integration range. It should be remainded here that in the approximate potential procedures the propagators for small sectors are determined as diagonal matrices. Similar practical suggestions can be made concerning evaluation of the Q and T quantities with the help of approximate potential procedures for the quantities Q_R and T_R. As was mentioned in the Introduction, there are two papers where such procedures were proposed.

In the paper by Schneider and Taylor [5], the recurrence relation for T_R is derived (in a different way) and implemented into the program for solving systems of homogeneous differential equations by the R-matrix propagation method. Kulander and Light [4] refered to the same method. They evaluated the overlap integrals $O(x', x'')$,

$$O(x', x'') = \int_{x'}^{x''} \phi^T(x)\, \psi_0(x)\, dx, \tag{A6}$$

between the inhomogeneity vector $\phi(x)$ and the solution of the system of homogeneous equations $\psi_0(x)$ by means of propagating the quantities A_R and B_R occurring in the formula

$$O(x', x'') = -A_R(x', x'')\, \dot{\psi}_0(x') + B_R(x', x'')\, \dot{\psi}_0(x''). \tag{A7}$$

This formula results from applying the relations (2) and (A1) to the function $\psi_0(x)$ in (A6). Simultaneously one gets the expressions

$$A_R(x', x'') = -\int_{x'}^{x''} \phi^T(x)[\Omega_1(x, x')\, R_1(x', x'') + \Omega_2(x, x')]\, dx, \tag{A8}$$

$$B_R(x', x'') = \int_{x'}^{x''} \phi^T(x)\, \Omega_1(x, x')\, R_2(x', x'')\, dx. \tag{A9}$$

With the aid of appropriate relations given in this paper one can transform these expressions to a form that demonstrates the following simple connection:

$$A_R = -Q_R^T, \qquad B_R = -T_R^T.$$

This connection confirms the opinion of Schneider and Taylor [5] about the possibility of computing the quantity T_R (and Q_R) by directly exploiting the elaborated in details procedure of Kulander and Light for the overlap integrals.

After a modification not affecting the speed of this procedure, it will give also the quantities T and Q. To realize this point, one should express the integral (A6) in the form

$$O(x', x'') = -A_L(x', x'')\,\psi_0(x') + B_L(x', x'')\,\psi_0(x''),$$

and prove that the quantities A_L and B_L are in fact the transposed quantities Q and T, i.e.,

$$A_L = Q^{\mathrm{T}}, \qquad B_L = T^{\mathrm{T}}.$$

The formulas for A_L and B_L,

$$A_L(x', x'') = -\int_{x'}^{x''} \phi^T(x)[\Omega_1(x, x') + \Omega_2(x, x')\,L_1(x', x'')]\,dx,$$

$$B_L(x', x'') = \int_{x'}^{x''} \phi^T(x)\,\Omega_2(x, x')\,L_2(x', x'')\,dx,$$

involve the same integrals as the formulas (A8) and (A9) for A_R and B_R.

The above remarks can be concluded with the statement that the analytically equivalent L-matrix and R-matrix formulations are equivalent also in some practical sense. Namely, they seem to be equally suitale for constructing approximate potential algorithms for solving homogeneous or inhomogeneous coupled equations. The same statement, however, is rather not expected to be true when the approximate solution approach to differential equations comes into consideration. A specific choice of the discretization procedure within this approach may favour one or another formulation of a problem as leading to simpler and more efficient algorithm for its solution.

The procedure described in Section 3 can serve as an example of a procedure which is better suited for the L-matrix formulation. The important element of this procedure is the conversion of the boundary value problems for the matrix L to the integral equation form. It should be noted that the extremely simple form of the Green's function used to this end was very essential for the final shape of the derived algorithms. There would be no possibility of using a simple Green's function if the derivation were started from the R-matrix formulation. In this case, one has to consider the boundary value problems for the matrix R,

$$\left[\frac{d^2}{dx^2} + B(x)\right]\psi_R^{\pm}(x) = 0,$$

$$\dot{\psi}_R^{\pm}(x') = \begin{cases} 1, \\ 0, \end{cases} \qquad \dot{\psi}_R^{\pm}(x'') = \begin{cases} 0, \\ 1; \end{cases}$$

$$R(x', x'') = \begin{pmatrix} \psi_R^{+}(x') & \psi_R^{-}(x') \\ \psi_R^{+}(x'') & \psi_R^{-}(x'') \end{pmatrix}.$$

The simplest Green's function for converting these problems to an integral equation form is built from the sine and cosine functions.

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