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Combined Variable-Phase- R -Matrix Approach to Scattering Problems*

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A procedure which combines the methods of variable-phase and R -matrix theory is formulated for multichannel scattering processes. R -matrix theory is used to obtain the logarithmic derivative of the scattering functions at a radius a , beyond which all exchange potentials are negligible. Variable-phase theory is used to construct a radially dependent reaction matrix which is integrated from a to infinity. The method is applied to a two-channel model which has some of the features of the low-energy electron-hydrogen problem. Essentially exact results are obtained with as few as 40 R -matrix states (20 per channel).

I. INTRODUCTION

In recent publications,¹⁻³ several computational procedures have been suggested for studying low-energy electron-atom scattering which do not require the direct solution of the coupled integrodifferential equations describing the scattering pro-

cess. In general, such procedures yield only approximate solutions to the coupled equations. However, the computational ease of these procedures is such as to allow for the coupling of more channels than might be attempted in a direct solution, and therefore it is hoped that any numerical inaccuracies introduced will be more than compensated

for by corrections arising from the additional channels.

In these methods, the scattering functions in the "near" region are obtained by an expansion in a finite basis set and a subsequent diagonalization of a Hamiltonian matrix. In the asymptotic region they can be obtained variationally as in the Harris-Nesbet method^{1,2} or by matching to numerical solution in the "far" region as in the method proposed by Burke *et al.*³ The ability of such techniques to give accurate results for a physical multichannel problem has been demonstrated by Seiler *et al.*⁴ who have investigated electron-hydrogen scattering.

In the present work we suggest an alternative procedure which combines variable-phase theory⁵ and *R*-matrix theory.⁶ 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

A. Variable-Phase Theory

In this section we present a review of variable-phase theory as applied to a multichannel problem.^{5,7} The scattering problem under investigation is described by the coupled equations

$$(\underline{H} - E)\underline{\Psi} = 0, \quad (1)$$

where

$$\underline{H} = \frac{-d^2}{dr^2} + \underline{L} + \underline{V} - \underline{W} + \underline{\epsilon}. \quad (2)$$

\underline{L} is the diagonal angular momentum matrix with elements $\delta_{ij}l_i(l_i+1)/r^2$, \underline{V} and \underline{W} are direct and exchange potential matrices, and $\underline{\epsilon}$ is the diagonal level-spacing matrix with elements $\delta_{ij}\epsilon_i$. $\underline{\Psi}$ is a square matrix with elements ψ_{ij} where j denotes the incident channel and i the outgoing channel. We allow for the possibility of both open and closed channels.

We define the real diagonal matrices \underline{J} and \underline{N} by

$$\begin{aligned} J_{ij} &= \delta_{ij}J_j, \quad N_{ij} = \delta_{ij}N_j, \\ J_j(k_j r) &= \begin{cases} k_j^{1/2} r j_{l_j}(k_j r), & j \text{ open} \\ (-1)^{l_j+2} (\frac{1}{2} k_j)^{1/2} r h_{l_j}^{(2)}(ik_j r), & j \text{ closed} \end{cases} \\ N_j(k_j r) &= \begin{cases} k_j^{1/2} r n_{l_j}(k_j r), & j \text{ open} \\ i^{l_j+2} (\frac{1}{2} k_j)^{1/2} r h_{l_j}^{(1)}(ik_j r), & j \text{ closed} \end{cases} \end{aligned} \quad (3)$$

where

$$k_j = + |E - \epsilon_j|^{1/2},$$

and $j_l(x)$ and $n_l(x)$ are spherical Bessel and Neumann functions, and $h_l^{(1)}(x)$ and $h_l^{(2)}(x)$ are Hankel functions.⁸ Auxiliary matrices $\underline{\delta}$, $\underline{\alpha}$ are defined by the

equations

$$\underline{\Psi} = \underline{J}\underline{\delta} - \underline{N}\underline{\alpha}, \quad (4a)$$

$$\underline{\Psi}' = \underline{J}'\underline{\delta} - \underline{N}'\underline{\alpha}, \quad (4b)$$

where prime means differentiations with respect to r . If the potentials fall off faster than r^{-1} for large r , the asymptotic properties of ψ_{ij} are

$$\begin{aligned} \psi_{ij}(r) \xrightarrow{r \rightarrow \infty} k_i^{-1/2} [\sin(k_i r - l_i \pi/2) \delta_{ij} \\ + \cos(k_i r - l_i \pi/2) K_{ij}], \quad i, j \text{ open.} \end{aligned} \quad (5)$$

We consider the matrix of functions

$$\underline{K}(r) = \underline{\alpha}(r)\underline{\delta}^{-1}(r),$$

with

$$K_{ij}(0) = \begin{cases} (-1)^{l_i+1} \delta_{ij}, & i \text{ closed} \\ 0, & \text{otherwise} \end{cases} \quad (6)$$

such that $K_{ij} \equiv K_{ij}(\infty)$, i and j open, are the elements of the reaction matrix. Using the properties of the functions \underline{J} and \underline{N} , we obtain the differential equations

$$\underline{\delta}'(r) = -\underline{N}(\underline{V} - \underline{W})\underline{\Psi}, \quad (7a)$$

$$\underline{\alpha}'(r) = -\underline{J}(\underline{V} - \underline{W})\underline{\Psi}, \quad (7b)$$

or

$$\underline{K}'(r) = -(\underline{J} - \underline{KN})(\underline{V} - \underline{W})\underline{\Psi}\underline{\delta}^{-1}, \quad (7c)$$

where the square brackets indicate that the integral operator \underline{W} acts only on $\underline{\Psi}$. These equations are of little practical use because of the difficulties inherent in solving coupled nonlinear integrodifferential equations.

However, if there exists a radius $r = a$ such that

$$W(r > a) \approx 0, \quad (8)$$

then Eq. (7) reduces to

$$\underline{K}'(r) = -(\underline{J} - \underline{KN})\underline{V}(\underline{J} - \underline{NK}), \quad r > a. \quad (9)$$

This is a particularly simple equation to solve since in general the direct potential matrix \underline{V} can be expressed analytically when Eq. (8) is a suitable approximation. Therefore we need only determine $\underline{K}(a)$ in order to begin the integration of Eq. (9). Using Eqs. (4a), (4b), and (6), we obtain

$$\underline{K}(a) = [(\underline{J}' - \underline{J}\underline{\Psi}'\underline{\Psi}^{-1})(\underline{N}' - \underline{N}\underline{\Psi}'\underline{\Psi}^{-1})^{-1}]_a. \quad (10)$$

Since the matrices \underline{J} , \underline{N} , and their derivatives are known, the problem then reduces to finding the logarithmic-derivative matrix

$$[\underline{\Psi}'\underline{\Psi}^{-1}]_a.$$

This may be obtained from *R*-matrix theory⁶ which we now discuss.

B. *R*-Matrix Theory

We wish to expand a column vector of $\underline{\Psi}$, defined by $\underline{\Psi}_j$ where j is the incident channel, into a complete set of states. If $f(r)$ is a function with the property

$$f(r) \underset{r \rightarrow 0}{\sim} r^{l+1}$$

and if η_{lm} is a complete set of orthonormal eigenstates of the operator

$$\frac{d^2}{dr^2} - \frac{l(l+1)}{r^2} + V(r)$$

satisfying the boundary conditions

$$\eta_{lm} \underset{r \rightarrow 0}{\sim} r^{l+1}, \quad (11a)$$

$$\left(\frac{r}{\eta_{lm}} \frac{d\eta_{lm}}{dr} \right)_a = b_l, \quad (11b)$$

then the functions η_{lm} , $m = 1, \dots, \infty$, form a complete basis set for $f(r)$ spanning the region 0 to a . Here $V(r)$ is an arbitrary potential and b_l is an arbitrary constant. For example, we choose $V(r) = 0$ and thus

$$\eta_{lm} \propto r j_l(\alpha_{lm} r/a), \quad (12)$$

where α_{lm} is the m th root of Eq. (11b), which can be reduced using standard recurrence relations to the form

$$\alpha_{lm} j_{l+1}(\alpha_{lm}) = (l+1 - b_l) j_l(\alpha_{lm}). \quad (13)$$

Then we construct the eigenvectors

$$\underline{X}_\lambda = \sum_m \begin{pmatrix} C_{1m}^\lambda & \eta_{1m} \\ \vdots & \vdots \\ C_{Nm}^\lambda & \eta_{Nm} \end{pmatrix}, \quad (14)$$

where N is the total number of channels and the coefficients C diagonalize the Hamiltonian matrix

$$\sum_{ij, mn} C_{im}^\lambda H_{im, jn} C_{jn}^\lambda = E_\lambda, \quad (15)$$

with

$$H_{im, jn} = (\eta_{1m} | H_{ij} | \eta_{1n}), \quad (16)$$

where the limits of integration are 0 to a . Thus the vectors \underline{X}_λ satisfy the boundary conditions

$$a \underline{X}'_\lambda(a) = \underline{B} \underline{X}_\lambda(a), \quad (17)$$

where \underline{B} is the diagonal matrix with elements $\delta_{ij} b_i$ ($b_i \equiv b_{l_i}$), and serve as a complete basis set for the vectors $\underline{\Psi}_j$,

$$\underline{\Psi}_j = \sum_\lambda A_{j\lambda} \underline{X}_\lambda. \quad (18)$$

The coefficient $A_{j\lambda}$ is given by Lane and Thomas⁶:

$$A_{j\lambda} = \underline{\tilde{X}}_\lambda(a) \frac{[\underline{\Psi}'_j - a^{-1} \underline{B} \underline{\Psi}_j]_a}{(E_\lambda - E)}. \quad (19)$$

By defining the *R* matrix with elements

$$R_{ki} = \sum_\lambda \frac{1}{a} \frac{[X_{k\lambda} X_{i\lambda}]_a}{(E_\lambda - E)} \quad (20)$$

and collecting the column vectors $\underline{\Psi}_j$ into the square matrix $\underline{\Psi}$, we obtain

$$a[\underline{\Psi}' \underline{\Psi}^{-1}]_a = \underline{R}^{-1}(1 + \underline{R} \underline{B}), \quad (21)$$

which can be inserted into Eq. (10) to yield

$$\underline{K}(a) = \{ [\underline{J}(1 + \underline{B} \underline{R}) - a \underline{J}' \underline{R}] [\underline{N}(1 + \underline{B} \underline{R}) - a \underline{N}' \underline{R}]^{-1} \}_a. \quad (22)$$

A practical problem is the rate of convergence of the *R*-matrix sum, Eq. (20). Buttler⁹ has considered this problem and has suggested a procedure to correct the *R* matrix when a finite basis set is used. The assumptions are as follows: The omitted states λ contribute predominantly to the diagonal elements of the *R* matrix since the off-diagonal coupling is small for these states. Therefore, the contribution from these states to the *R* matrix is the same as their contribution for the uncoupled problem. Further, it is assumed that the eigenvalues and eigenvectors for the included states λ are changed only slightly by the omission of higher states. The correction given by Buttler is then obtained as follows: The exact *R*-matrix element in channel i for the uncoupled problem is given by⁶

$$R_{ii}^{(0)} = \left[\left(\frac{a}{u_i} \frac{du_i}{dr} \right)_a - b_i \right]^{-1}, \quad (23)$$

where

$$H_{ii} u_i(r) = E u_i(r). \quad (24)$$

The contribution to $R_{ii}^{(0)}$ from included states λ is

$$R_{ii}^{(0)inc} = \sum_\lambda \frac{1}{a} \frac{[X_{i\lambda}^{(0)} X_{i\lambda}^{(0)}]_a}{(E_{i\lambda}^{(0)} - E)}, \quad (25)$$

where

$$(X_{i\lambda}^{(0)} | H_{ii} | X_{i\lambda}^{(0)}) = E_{i\lambda}^{(0)}. \quad (26)$$

Therefore the contribution from the omitted states λ to the diagonal *R*-matrix elements is

$$R_{ii}^{(0)omit} \approx R_{ii}^{(0)omit} = R_{ii}^{(0)} - R_{ii}^{(0)inc}. \quad (27)$$

The *R* matrix used in Eq. (22) is then the *R* matrix obtained from Eq. (20) with diagonal elements corrected using Eq. (27).

III. APPLICATION TO A MODEL PROBLEM

The formalism discussed in Sec. II is applied to a model two-channel problem with

$$\begin{aligned} W_{ij} &= 0, \\ V_{11} &= V_{22} = -\alpha/(r^2 + d^2)^2, \\ V_{12} &= V_{21} = -\beta(1 - e^{-r})^3/r^2, \\ l_1 &= 0, \quad l_2 = 1. \end{aligned} \quad (28)$$

TABLE I. Partial-wave cross sections Q_{ij} for a non-degenerate case. Column A: $n=20$, uncorrected; column B: $n=10$, corrected; column C: $n=20$, corrected; column D: numerical.

E (Ry)		A	B	C	D
0.1	Q_{11}	18.6520	18.6592	18.6307	18.6309
0.2	Q_{11}	12.5895	12.2819	12.2941	12.2941
0.5	Q_{11}	7.9999	7.9977	7.9975	7.9975
0.7	Q_{11}	5.5814	5.5861	5.5881	5.5881
0.749	Q_{11}	5.1441	5.1669	5.1686	5.1686
0.751	Q_{11}	5.1270	5.1508	5.1525	5.1525
	Q_{12}	0.0000	0.0000	0.0000	0.0000
	Q_{22}	0.0479	0.0452	0.0453	0.0453
0.8	Q_{11}	4.7172	4.7783	4.7701	4.7703
	Q_{12}	0.0072	0.0087	0.0082	0.0081
	Q_{22}	4.3126	3.7306	3.7292	3.7294
1.0	Q_{11}	3.3439	3.5162	3.5226	3.5226
	Q_{12}	0.0575	0.0642	0.0647	0.0647
	Q_{22}	4.1018	4.0455	4.0455	4.0456
1.5	Q_{11}	1.7632	1.7913	1.7921	1.7921
	Q_{12}	0.1863	0.1794	0.1793	0.1793
	Q_{22}	1.9205	1.8858	1.8848	1.8849

No essential simplification is made by neglecting the exchange potential since its sole effect in the present formalism is to give rise to an additional term in the matrix element H_{i_m, j_n} of Eq. (16). In the present application we choose $\alpha = 4.5$, $d^4 = \alpha$, $\beta = 6$.

The dependence of the cross sections

$$Q_{ij} = (4\pi/k_i^2) |[\underline{K}/(1 - i\underline{K})]_{ij}|^2 \quad (29)$$

on the logarithmic boundary-condition parameters b_i is investigated. We find that provided the values chosen for b_i are not too large, they do not have any significant effect on the results. We choose $b_i = -l_i$ since in this case the roots α_{im} can be obtained analytically from Eq. (13), and they are well spaced at intervals of π .

An increase in the matching radius a enlarges the space to be spanned by the basis set and more bases are needed to ensure comparable accuracy of the results. For example, we find that doubling the value of a requires approximately a doubling of the number of basis functions in order to retain the same degree of precision. Hence, a is chosen to be the smallest value of r such that Eq. (8) is a suitable approximation. In this paper, we choose $a = 8$.

We first consider the nondegenerate case $\epsilon_1 = 0$, $\epsilon_2 = 0.75$. Below the threshold for excitation only one element of the K matrix, K_{11} , is physically meaningful. The occurrence of nonphysical K -matrix elements and, in particular, their divergent behavior for large r , has been discussed by Zemach.⁷ Since

$$\underline{\Psi} \xrightarrow{r \rightarrow \infty} \underline{J} - \underline{N}\underline{K} \quad (30)$$

is well behaved while

$$J_i \underset{r \rightarrow \infty}{\sim} e^{k_j r}, \quad N_j \underset{r \rightarrow \infty}{\sim} e^{-k_j r} \quad (31)$$

for closed channels j , the closed-channel elements of K must diverge to cancel the divergent terms J_j . In principle, this behavior has no effect on the physically meaningful K -matrix elements. However, due to the cancellation of large numbers, loss of significant figures can result when solving Eq. (9). For this reason, we find it convenient, when closed channels are present, to eliminate explicitly the exponential behavior of J_j and N_j for closed channels j by transforming Eq. (9).¹⁰

In Table I we give cross sections both below and above threshold for the nondegenerate case. The numerical results, column D, which are obtained by solving Eq. (9) from zero to infinity, are compared with three calculations made using the present formalism. In column A, we use 20 basis functions in each channel [associated with the 20 lowest roots of Eq. (13)] but omit the Buttle corrections to the R matrix. Additional calculations are made with 10 and 20 bases; columns B and C, respectively, including these corrections. We observe the substantial improvement obtained by correcting the R -matrix elements according to Eq. (27). Essentially exact answers are obtained in a corrected 20 bases calculation. However, as few as 10 bases yield entirely satisfactory results when the Buttle correction is utilized. We note that no anomalies occur near the threshold.

Similar calculations are performed for the case of degenerate channels, $\epsilon_1 = \epsilon_2 = 0$, and results are presented in Table II, where the columns are as described for Table I. We note that, as in the non-degenerate case, it is important to include the Buttle correction and that as few as 10 bases then give results of acceptable quality.

TABLE II. Partial-wave cross sections Q_{ij} for the degenerate case. Column A: $n=20$, uncorrected; column B: $n=10$, corrected; column C: $n=20$, corrected; column D: numerical.

E (Ry)		A	B	C	D
0.1	Q_{11}	9.7781	10.0224	10.0370	10.0364
	Q_{12}	9.2239	9.2674	9.2767	9.2766
	Q_{22}	16.3390	16.1334	16.0897	16.0899
0.2	Q_{11}	0.2376	0.3320	0.3390	0.3393
	Q_{12}	1.4917	1.6483	1.6610	1.6615
	Q_{22}	16.7936	16.4998	16.4739	16.4727
0.4	Q_{11}	0.7655	0.6821	0.6732	0.6731
	Q_{12}	0.0304	0.0323	0.0312	0.0312
	Q_{22}	8.8579	8.9679	8.9662	8.9661
0.6	Q_{11}	1.1398	0.9879	0.9829	0.9828
	Q_{12}	0.3964	0.4683	0.4652	0.4652
	Q_{22}	4.5350	4.5591	4.5544	4.5542

The degenerate dipole coupling considered here is typical of the $2s$ - $2p$ coupling in e^- -H scattering and is of interest because of its extremely long range.¹¹ One of the advantages of the present formalism is that Eq. (9) can be numerically integrated from a to $r=r_0$, where the oscillations of the open-channel K -matrix elements have become small, and then a generalization of the Levy and Keller¹² technique can be used to extend these elements to a practical infinity. The effects of closed channels for large r can be given in terms of polarization potentials in the open channels.¹³

IV. SUMMARY AND DISCUSSION

We have presented a computational procedure for obtaining approximate solutions to the coupled integrodifferential equations which describe scattering processes. This procedure combines the methods of variable-phase theory and R -matrix theory. In the R -matrix calculation, a series of eigenvalue problems is solved and the results are used for all energies. Additions to the basis set

can be made in a systematic manner. Variable-phase theory is used to extend the reaction matrix from a matching radius to infinity. One of the advantages of this approach is the ability to monitor directly the convergence of the elements of the reaction matrix.

The method detailed here can be readily extended to scattering problems where the dominant asymptotic potentials are Coulombic, by replacing the functions \underline{J} and \underline{N} of Eq. (3) with Coulomb functions.¹⁴

If the scattering functions need to be orthogonalized to atomic states, this can be accomplished by a Schmidt orthogonalization of the basis states to these atomic states. The boundary conditions for these orthogonalized Bessel functions, Eq. (11), give rise to the same roots as the nonorthogonalized Bessel functions, since the atomic states are assumed to have vanished for $r \geq a$. In this case, an additional change, which must be made in the formalism presented here, is the modification of the Hamiltonian and overlap matrices of the eigenvalue problem.

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