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Reduced matrix equations for many-particle scattering. I. Electron-atom scattering at low energies

Yukap Hahn and J. F. Dirks*
Department of Physics, University of Connecticut, Storrs, Connecticut 06268

Augustine C. Chen
Department of Physics, St. John's University, Jamaica, New York 11439

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The reduction method developed previously for many-particle scattering is applied here to derive new sets of coupled equations for electron scattering from atomic targets at low energies, fully taking into account the exchange effect and target distortions. The reduced matrix equations have simpler structure than the Faddeev-Watson equations, with the iteration kernels connected only in those channels which are explicitly taken into account. Scatterings by atomic hydrogen, helium, and lithium targets are considered, and the resulting formalism is compared with the earlier work of Faddeev and others. Various approximation procedures are described, and their applicability is tested on the electron-hydrogen scattering system.

I. INTRODUCTION

It is well known[1] that the usual formulation of the rearrangement processes in terms of the Lippmann-Schwinger[2] equation does not always give a unique solution, mainly because the arrangement scattering functions are not mutually orthogonal[3] and the scattering kernels are not completely connected.[4] These, in turn, complicate the channel projections in the unified reaction theory.[5] The mathematically more rigorous formulations of the many-particle scattering problem, which avoid the difficulties mentioned above, have been developed by many people.[6-10] However, because of the inherent complexity of these theories, their applications beyond the simplest approximation have been difficult to carry out. Most of the accurate theoretical calculations which are presently available were obtained by conventional approaches without the explicit use of the rigorous formulations.

Evidently, the requirement that the iteration kernels of the theory should be completely connected may be too stringent from a practical point of view. Thus, we have considered[11,12] a reduction procedure by which the hierarchy of scattering equations may be simplified at the expense of slightly relaxing the rigor of the original theories. The reduced matrix equations (RME) obtained in this way retain the connectedness property only in the direct channels, while all the other indirect channels are to be treated by a noniterative method. The formalism has been rediscovered recently[13-15] starting from a different point of view. Kouri and Levin[13] introduce the channel coupling operator W in the equations for the scattering operator, in such a way that the iteration kernels for all the open rearrangement channels are connected. In its differential form, this new formulation has been shown[15] to be equivalent to the RME,[11,12] for the three-particle case.

It is the purpose of this paper to explore the potentiality of the RME by explicitly applying them to the electron-atom scattering systems. The RME contain two useful features which may be exploited in actual applications. Firstly, the equations allow one to introduce the distortion potentials in a nontrivial way. Thus, a judicious (self-consistent) choice of these potentials in the beginning of a given calculation could improve the result in the lowest order. Secondly, a simple set of channel projection operators can be introduced into the RME, such that the inelastic channels which are not explicitly included can be treated noniteratively in order to meet the mathematical requirement of connectedness. Such projection operators are not easy to construct for the other[1,5] formulations when rearrangement and exchange channels are present.[11] The availability of the projection operators will also facilitate the resonance state calculation for the electron-atom system.

The formal construction of the coupled equations using the reduction method[11] is carried out in Sec. II, explicitly for e^-H, e^-He, and e^-Li systems. Since the reduced sets are not unique in general, their properties are analyzed in some detail and compared with the previous result of Faddeev and others. Section III contains discussions on approximations which are applicable to the new sets of equations, and some of them are applied to the e^-H system in Sec. IV. The main purpose here is not so much in getting accurate phase shifts, but rather in bringing out some of the salient properties of the new coupled equations we have derived. The formalism presented here should also be useful in the study of positron scattering, with positronium formation, as $e^+ + A \to (e^+ + e^-) + A^+$.

II. REDUCED MATRIX EQUATIONS

The general reduction method developed previously[11] will be applied to specific atomic systems. For definiteness, we consider electron-hydrogen scattering in detail, and later extend the study to e^-He and e^-Li systems. At low energies, we have the two-channel process

$$\underset{\text{channel 1}}{e_1^- + (e_2^- + p^+)_0} \leftrightarrow \underset{\text{channel 2}}{e_2^- + (e_1^- + p^+)_0}. \tag{2.1}$$

The asymptotic channel Hamiltonians are given by

$$H_c = H - V_c, \quad c = 1, 2, \tag{2.2}$$

where

$$\begin{aligned} &H = T_1 + T_2 + V_{10} + V_{20} + V_{12} \equiv T + V, \\ &V_1 = V_{10} + V_{12}, \quad V_2 = V_{20} + V_{21}. \end{aligned} \tag{2.3}$$

If we write the total scattering function Ψ as

$$\Psi = \sum_{c=1}^{I} \Psi_c \quad (I = 2 \text{ here}), \tag{2.4}$$

then, the reduced matrix equations for (2.1) are given by[11]

$$\underline{D}\,\underline{\Psi} = \begin{bmatrix} H_1 + Y_1 - E & V_2 - Y_2 \\ V_1 - Y_1 & H_2 + Y_2 - E \end{bmatrix} \begin{bmatrix} \Psi_1 \\ \Psi_2 \end{bmatrix} = \begin{bmatrix} 0 \\ 0 \end{bmatrix} \equiv \underline{O}, \tag{2.5}$$

where Y_c are distortion potentials which are yet to be specified. Of course, (2.5) is valid for any Y_c. Forms other than (2.5) are also possible,[11,12] but we limit our discussion to this symmetric case. We note that channel 2 in (2.1) is the exchange channel, which is being regarded here as a rearrangement channel, and thus (2.5) will simplify in practice. That is, the two coupled equations reduce to a single integrodifferential equation.

The boundary conditions on Ψ_c may be specified now; for the total energy E below the first excitation threshold, we will have only two channels open, as indicated by (2.1), and, as $r_c \to \infty$,

$$\Psi_c \to \psi_0^{(c)} [A_c \mathcal{S}_c + B_c \mathcal{C}_c], \quad c = 1, 2, \tag{2.6}$$

where $\mathcal{S}_c$ and $\mathcal{C}_c$ are the scattering functions which behave like sine and cosine functions at large r_c, and $\psi_0^{(c)}$ are the target ground-state functions generated by

$$h_c \psi_n^{(c)} = e_n^{(c)} \psi_n^{(c)}, \quad h_c \equiv T_{c'} + V_{c'0} \quad (c' \neq c). \tag{2.7}$$

The channel projection operators can now be constructed in a very simple way,[16,11] as

$$\underline{P} = \begin{bmatrix} P_1 & 0 \\ 0 & P_2 \end{bmatrix} \quad \text{and} \quad \underline{Q} = \underline{1} - \underline{P} = \begin{bmatrix} Q_1 & 0 \\ 0 & Q_2 \end{bmatrix}, \tag{2.8}$$

where

$$P_c = |\psi_0^{(c)}\rangle\langle\psi_0^{(c)}|, \quad Q_c = 1_c - P_c,$$

with the obvious property that

$$P_c Q_c = Q_c P_c = 0, \quad P_1 P_2 \neq 0, \quad P_1 Q_2 \neq 0 \tag{2.9}$$

and

$$\underline{P}\,\underline{Q} = 0, \quad \underline{P} = \underline{P}^\dagger.$$

In order to have the correct connectedness property of the system, we demand that the potentials Y_c, which are yet to be specified, satisfy

$$[P_c, Y_c] = 0; \tag{2.10}$$

that is, the Y_c are functions of r_c only.

We now consider briefly Eqs. (2.5), together with (2.8). The projected equations are

$$\begin{aligned} &\underline{P}\,\underline{D}\,\underline{P}\,\underline{\Psi} = -\underline{P}\,\underline{D}_I\,\underline{Q}\,\underline{\Psi}, \\ &\underline{Q}\,\underline{D}\,\underline{Q}\,\underline{\Psi} = -\underline{Q}\,\underline{D}_I\,\underline{P}\,\underline{\Psi}, \end{aligned} \tag{2.11}$$

where

$$\underline{D}_I \equiv \begin{bmatrix} 0 & V_2 - Y_2 \\ V_1 - Y_1 & 0 \end{bmatrix} \tag{2.12}$$

and, for later use, we also define

$$\underline{D}_0 \equiv \underline{D} - \underline{D}_I = \begin{bmatrix} H_1 + Y_1 - E & 0 \\ 0 & H_2 + Y_2 - E \end{bmatrix}. \tag{2.13}$$

(a) First of all, the homogeneous $\underline{P}$ equations are the simple set

$$\underline{P}\,\underline{D}\,\underline{P}\,\underline{\Psi}^P = 0, \tag{2.14}$$

which is, explicitly,

$$\begin{aligned} &P_1[H_1 + Y_1 - E]P_1\Psi_1^P = -P_1(V_2 - Y_2)P_2\Psi_2^P \\ &P_2[H_2 + Y_2 - E]P_2\Psi^P = -P_2(V_1 - Y_1)P_1\Psi_1^P. \end{aligned} \tag{2.15}$$

If we choose

$$Y_c = \langle P_c V_c P_c \rangle_c \equiv \int d\vec{\mathrm{r}}_{c'}\, \psi_0^{(c)*}(\vec{\mathrm{r}}_{c'}) V_c \psi_0^{(c)}(\vec{\mathrm{r}}_{c'}), \tag{2.16}$$

then, (2.15) reduces to the form

$$P_c[H - E]P_c\Psi_c^P = -P_c[H - E]P_{c'}\Psi_{c'}^P, \quad c' \neq c, \tag{2.17}$$

which is the usual set of equations one obtains in the static exchange approximation.

We also note that the choice (2.16) allows the coupling in the right-hand side of (2.11) and (2.15) only to states which are orthogonal to the channel on the left-hand side; that is, with (2.16) for Y_c,

$$P_c(V_{c'} - Y_{c'})P_{c'} = P_c Q_{c'} V_{c'} P_{c'}, \quad c' \neq c, \tag{2.18}$$

where the explicit appearance of $Q_{c'}$ automatically orthogonalizes functions to its left. The properties (2.17) and (2.18) are valid only for the e^-H system, in which $[P_1, P_2] = 0$.

(b) Next, consider the homogeneous $\underline{Q}$ equations in (2.11), which are given explicitly as $(c' \neq c)$,

$$Q_c[H_c + Y_c - \mathcal{E}_n]Q_c \Phi_{cn} = -Q_c(V_{c'} - Y_{c'})Q_{c'} \Phi_{c'n}, \tag{2.19}$$

where we have modified the energy value E to $\mathcal{E}_n$, as the Q space defined in this way is closed. Equation (2.19) would be useful in the study of resonances.

(c) The coupling between the $\underline{P}$ and $\underline{Q}$ components in (2.11) can be formally dissolved by the use of the Green's functions; thus, we define

$$\underline{G}^P \equiv -[\underline{P}\,\underline{D}\,\underline{P}]^{-1}, \tag{2.20}$$

$$\underline{G}^Q \equiv -[\underline{Q}\,\underline{D}\,\underline{Q}]^{-1}, \tag{2.21}$$

and write the solution of (2.11) as

$$\begin{aligned} \underline{P}\,\underline{\Psi} &= \underline{P}\,\underline{\Psi}^P + \underline{G}^P \underline{P}\,\underline{D}_I \underline{Q}\,\underline{\Psi}, \\ \underline{Q}\,\underline{\Psi} &= \underline{G}^Q \underline{Q}\,\underline{D}_I \underline{P}\,\underline{\Psi}. \end{aligned} \tag{2.22}$$

The uncoupled equations are then

$$[\underline{P}\,\underline{D}\,\underline{P} + \underline{P}\,\underline{D}_I \underline{G}^Q \underline{D}_I \underline{P}]\underline{P}\,\underline{\Psi} = \underline{O} \tag{2.23}$$

and

$$[\underline{Q}\,\underline{D}\,\underline{Q} + \underline{Q}\,\underline{D}_I \underline{G}^P \underline{D}_I \underline{Q}]\underline{Q}\,\underline{\Psi} = -\underline{Q}\,\underline{D}_I \underline{P}\,\underline{\Psi}^P. \tag{2.24}$$

(d) Consider in a little more detail the structure of $\underline{G}^Q$; it is given by[11]

$$\underline{G}^Q = \begin{bmatrix} G^Q_{11} & G^Q_{12} \\ G^Q_{21} & G^Q_{22} \end{bmatrix}, \tag{2.25}$$

where

$$\begin{aligned} G^Q_{11} &= \{Q_1[E - H_1 - Y_1 - (V_2 - Y_2)g^Q_2(V_1 - Y_1)]Q_1\}^{-1}, \\ G^Q_{12} &= G^Q_{11}(V_2 - Y_2)g^Q_2, \quad \text{etc.}, \end{aligned} \tag{2.26}$$

with

$$g^Q_c = [Q_c(E - H_c - Y_c)Q_c]^{-1}, \quad c = 1 \text{ and } 2. \tag{2.27}$$

Therefore, the entire $\underline{G}^Q$ can be generated from the simple Green's functions g^Q_c of (2.27). This point will be useful in developing an approximation scheme, to be described in detail in Sec. III.

The result presented above for the e^-H system can immediately be extended to the e^-He and e^-Li systems. Once we define the appropriate operators $\underline{D}_0$ and $\underline{D}_I$ corresponding to the new wave function $\underline{\Psi}$, then the formal discussion given by (2.11), (2.14), and (2.20)–(2.24) will go through unchanged.

The difficulties with heavier targets are twofold; firstly, the target wave functions $\psi^{(c)}_0$ are not readily available in any simple forms. Secondly, even if the exact $\psi^{(c)}_0$ are given, the projection operator P which projects onto the elastic and the exchange channel is not easy to construct. On the other hand, a simple matrix form of $\underline{P}$ such as (2.8) can be constructed immediately for a proper set of matrix equations. This will greatly facilitate the resonance state and amplitude calculations for these complex systems.

For the e^-He system, we have, for $c = 1$, 2, and 3,

$$\begin{aligned} H_c &= T_1 + T_2 + T_3 + V_{c'0} + V_{c''0} + V_{c'c''}, \\ V_c &= V_{c0} + V_{cc'} + V_{cc''}, \end{aligned} \tag{2.28}$$

with c, c', c'' in cyclic order. The RME assume the following three different forms, however; either

$$\begin{bmatrix} H_1 + Y_1 - E & 0 & V_3 - Y_3 \\ V_1 - Y_1 & H_2 + Y_2 - E & 0 \\ 0 & V_2 - Y_2 & H_3 + Y_3 - E \end{bmatrix} \begin{bmatrix} \Psi_1 \\ \Psi_2 \\ \Psi_3 \end{bmatrix} = \underline{O} \tag{2.29}$$

or

$$\begin{bmatrix} H_1 + Y_1 - E & V_2 - Y_2 & 0 \\ 0 & H_2 + Y_2 - E & V_3 - Y_3 \\ V_1 - Y_1 & 0 & H_3 + Y_3 - E \end{bmatrix} \begin{bmatrix} \Psi_1 \\ \Psi_2 \\ \Psi_3 \end{bmatrix} = \underline{O}; \tag{2.30}$$

or, in a more symmetric form,

$$\begin{bmatrix} H_1 + Y^{(2)}_1 + Y^{(3)}_1 - E & V_{23} + \tfrac{1}{2}V_{20} - Y^{(1)}_2 & V_{23} + \tfrac{1}{2}V_{30} - Y^{(1)}_3 \\ V_{13} + \tfrac{1}{2}V_{10} - Y^{(2)}_1 & H_2 + Y^{(1)}_2 + Y^{(3)}_2 - E & V_{13} + \tfrac{1}{2}V_{30} - Y^{(2)}_3 \\ V_{12} + \tfrac{1}{2}V_{10} - Y^{(3)}_1 & V_{12} + \tfrac{1}{2}V_{20} - Y^{(3)}_2 & H_3 + Y^{(1)}_3 + Y^{(2)}_3 - E \end{bmatrix} \underline{\Psi} = \underline{O}, \tag{2.31}$$

where

$$Y^{(c')}_c + Y^{(c'')}_c = Y_c \quad (c', c'' \neq c).$$

It is interesting to note that (2.31), with all $Y_c = 0$, reduces[11] to the three-particle Faddeev equations[6] in the external field generated by the proton.

The equations analogous to (2.31) for the e^{-}Li system are given by

$$\begin{bmatrix} H_1+Y_1-E & \frac{1}{2}(V_{23}+V_{24})+\frac{1}{3}V_{20}-Y_2^{(1)} & \cdots \\ \frac{1}{2}(V_{13}+V_{14})+\frac{1}{3}V_{10}-Y_1^{(2)} & H_2+Y_2-E & \cdots \\ \frac{1}{2}(V_{12}+V_{14})+\frac{1}{3}V_{10}-Y_1^{(3)} & \frac{1}{2}(V_{12}+V_{24})+\frac{1}{3}V_{20}-Y_2^{(3)} & \cdots \\ \frac{1}{2}(V_{12}+V_{13})+\frac{1}{3}V_{10}-Y_1^{(4)} & \frac{1}{2}(V_{12}+V_{23})+\frac{1}{3}V_{20}-Y_2^{(4)} & \cdots \end{bmatrix} \begin{bmatrix} \Psi_1 \\ \Psi_2 \\ \Psi_3 \\ \Psi_4 \end{bmatrix} = \underline{O} \,. \tag{2.32}$$

Other sets similar to (2.29) and (2.30) for the present case can be obtained without difficulty. In all cases considered above, the potentials are completely screened in all channels.

The form (2.30), with $Y_c=0$, is precisely the transpose of the set derived by Kouri and Levin.[13] But, it is difficult at this stage of the development to determine their relative usefulness. It seems that the form (2.31) may contain more convenient features as all three channels are coupled to each other symmetrically. Obviously, this is not the case with (2.29), for example, where the Ψ_1 equation is coupled directly to Ψ_3 but not to Ψ_2; the effect of Ψ_2 is transmitted on Ψ_1 only through Ψ_3. This may not always be the case in actual situations; that is, in some cases, channel 1 may couple more strongly to channel 2, or may couple to both channels as in exchange scattering involving identical particles.

Two additional features of the equations we have derived above should be noted. Firstly, if we collect all the open channels at a given E in the P space, then g_c^Q will describe the propagation of the scattering system in the closed channel space Q_c. Therefore, we have immediately the important inequality

$$Q_c/(E-e_1^{(c)}) \leq g_c^Q < 0, \tag{2.33}$$

as long as Y_c do not introduce new discrete states below the Q_c space thresholds. Secondly, the distortion potentials Y_c may not necessarily be similar to the optical potential which occurs in the usual formulation[5] of the elastic scattering, because these potentials now play a different role in the new set of coupled equations in which the coupling between the rearrangement channels is emphasized.

The formalism presented above can immediately be extended to inelastic scattering by simply enlarging the $\underline{P}$ space. That is, for the case with $N+1$ open channels, we replace P_c by

$$P_c=\sum_{n=0}^{N} P_{cn} \quad (Q_c=1-P_c),$$

where

$$P_{cn}=|\psi_n^{(c)}\rangle\langle\psi_n^{(c)}|, \quad P_{cn}P_{cm}=P_{cn}\delta_{nm}.$$

III. APPROXIMATIONS

Since the structure of the coupled equations derived in Sec. II is quite distinct from the usual Schrödinger formulation, it may be of interest to consider several approximation schemes which may be used to solve the set of equations (2.11), often exploiting the unusual features of these equations.

(i) The static approximation; the simplest form of the approximation is to neglect the $Q_c\Psi_c$ components altogether in (2.11), and obtain (2.14). The solution of (2.14) *differs* from the usual static approximation in that V_c do not appear in the diagonal elements of $\underline{D}_0$. The potentials Y_c are still left undetermined. Due to the nonorthogonality $P_cP_{c'} \neq 0$ for $c' \neq c$, Ψ_c^P may still contain some excited state effects in this approximation.

(ii) Close-coupling approximation; rather than completely neglecting the $Q_c\Psi_c$ components, we may replace

$$\underline{Q} \to \underline{Q}^c = \begin{bmatrix} Q_1' & 0 \\ 0 & Q_2' \end{bmatrix}, \tag{3.1}$$

where Q_c' is composed of a *finite* number of states $\psi_n^{(c)}$. Obviously, this will give rise to a set of additional coupled equations, just as in the ordinary case.

(iii) Pseudostate method; in (ii) above, Q_c' is constructed using the eigenstates $\psi_n^{(c)}$ of the cluster in the channel c. However, this is not necessary and one can construct a set of pseudostates for the cluster with the internal Hamiltonian h_c, such as (2.7). It is often convenient to form a set of trial functions which are orthogonal to the $\psi_0^{(c)}$ state, and then diagonalize the energy matrix formed with these functions and the operator h_c.

(iv) As noted in Sec. II, the Q-space information is contained in the Green's function $\underline{G}^Q$ of (2.21). This, in turn, is determined by g_c^Q of (2.27), as is clear from (2.26). Therefore, a simple approximation on g_c^Q will generate $G_{cc'}^Q$ and thus determine $\underline{\Psi}$ from (2.22) and (2.23). The simplest approximation on g_c^Q is of course the closure approximation

$$g_c^Q \approx Q_c/(E-\overline{E}_c), \tag{3.2}$$

or a slightly improved form which approximates only the h_c part, as

$$g_c^Q \approx Q_c/(E-\bar{e}_c-T_c-Y_c). \tag{3.3}$$

(v) In place of (3.2) and (3.3), we can also introduce a separable approximation

$$g_c^Q \approx \frac{|Q_c\chi_t\rangle\langle Q_c\chi_t|}{\langle Q_c\chi_t,[E-H_c]Q_c\chi_t\rangle}, \tag{3.4}$$

or its generalized form involving more than one term.

The form (3.4) can be used to immediately reduce $G_{cc'}^Q$ to separable forms. [See Eq. (4.5).]

(vi) Still another approximation procedure is to determine the potentials Y_c, which are so far left undefined. Noting that the Q-space effect is coupled to the P_c components through the form

$$g_{c'}^Q(V_c-Y_c)P_c, \quad c'\neq c, \tag{3.5}$$

it is reasonable to require that Y_c be chosen such that the quantity

$$\tau' = |(P_c\Psi_t,[V_{c'}-Y_{c'}]g_{c'}^Q[V_c-Y_c]P_c\Psi_t)|, \tag{3.6}$$

or, a more symmetric form

$$\tau = (P_c\Psi_t,[V_c-Y_c]g_{c'}^Q[V_c-Y_c]P_c\Psi_t) \tag{3.7}$$

be a minimum for all possible forms of $P_c\Psi_t$. In fact, (3.7) has been used[17] to determine the Y_c potentials in the proton-hydrogen charge-exchange collisions at high energies, with moderate success. Further simplifications of (3.7) with (3.2) and (3.3) are also possible.

One of the major simplifying features of the Y_c's which satisfy τ = minimum is that the scattering equations (2.11) then uncouple, and we will have essentially the set (2.15), with the Y_c's already determined.

Some of the approximation procedures discussed above will be tested in the next section, specifically on the electron-hydrogen scattering system. In particular, we will explicitly consider the approximations (i) and (v), while the procedure (vi) will be applied in detail to the proton-hydrogen charge-exchange scattering at high energies.

IV. AN EXAMPLE: ELECTRON-HYDROGEN SCATTERING

In order to avoid unnecessary complications in the numerical solution of the coupled equations due to the presence of the redundant solution in the triplet state, we consider simply the $(L=0)$-wave singlet scattering. The units used are $m=\hbar=e^2=c=1$, and the length in units of a_0 and the energy in the Rydberg units.

(i) We first consider the equations in the "static" approximation (2.15). Explicitly,

$$\left(-\frac{d^2}{dr_1^2}+Y_1(r_1)-k^2\right)u_0^P(r_1) + 4r_1e^{-r_1}\int_0^\infty dr_2\, r_2\, e^{-r_2}\left(\frac{2}{r_>}-\frac{2}{r_2}-Y_2\right)u_0^P(r_2)=0, \tag{4.1}$$

where we have set

$$P_1\Psi_1^P \equiv \psi_0(r_2)u_0^P(r_1)/r_1, \quad P_2\Psi_2^P = P_1\Psi_1^P(1\leftrightarrow 2),$$

and

$$2E = e_0+k^2 = -1+k^2. \tag{4.2}$$

Equation (4.1) should be compared with the usual static equation

$$\left(-\frac{d^2}{dr_1^2}+V_{00}(r_1)-k^2\right)\bar{u}_0^P(r_1) + 4r_1e^{-r_1}\int_0^\infty dr_2\, r_2e^{-r_2}\left(-1-k^2+\frac{2}{r_>}\right)\bar{u}_0^P=0. \tag{4.1$'$}$$

Equation (4.1′) gives rise to the phase shift $\bar{\eta}^P$, which is well known.[18] We have solved (4.1), with and without the Y potentials, where of course, $Y_1(r_1)=Y_2(r_1)$ by symmetry. The result is given in Table I. η^P is obtained from (4.1) with $Y_c=0$. This result agrees with the values obtained by Baer and Kouri[13] from their transposed equations.

We note that, when $Y_1(r_1)=V_{00}(r_1)$ is taken in (4.1), η^P reduces to $\bar{\eta}^P$, as expected from the discussion in Sec. II.

(ii) It is of some interest to study the Q-space component of the equations (2.11), the homogeneous Q equations. The Q-space trial functions are constructed simply as

$$\bar{\varphi}(1)=\varphi(1)-b\bar{\psi}_0(1), \quad (\bar{\varphi},\bar{\psi}_0)=0, \tag{4.3}$$

where

TABLE I. Phase shifts calculated in different approximations. $\bar{\eta}^P$ is the ordinary static value. $\bar{\eta}_s$ is for all s states included in Q space, while $\bar{\eta}_{s+p}$ includes both s and p states. $\bar{\eta}$ denotes the exact $L=0$, $S=0$ phase shift as given by Schwartz. The unbarred phase shifts are obtained from the reduced matrix equations. η^P is obtained in the static approximation, while η_{st} includes all the s states in Q space by a one-term approximation on g_c^Q.

ka_0	0.2	0.4	0.6	0.8
$\bar{\eta}^P$	1.871	1.240	0.869	0.651
$\bar{\eta}_s$	1.960	1.270	0.911	0.726
$\bar{\eta}_{s+p}$	2.051	1.403	1.028	0.873
$\bar{\eta}$	2.067	1.415	1.041	0.887
η^P	2.041	1.334	0.870	0.552
η_{st}	2.064	1.387	0.922	0.564

$$\varphi(1) = e^{-ar_1}, \quad (\varphi, \bar{\psi}_0) = \tfrac{1}{4}b,$$
$$\bar{\psi}_0(1) = e^{-r_1}, \quad \psi_0 \equiv (4\pi)^{-1/2}\, 2\bar{\psi}_0,$$

and

$$b = 8(1 + a)^{-3}.$$

$\bar{\varphi}(1)$ contains one nonlinear parameter a, which we vary to study the various properties. The functions φ and $\bar{\varphi}$ are used to define

$$\begin{aligned} Q_1\Phi_{1t} &\equiv \bar{\varphi}(2)\varphi(1) \equiv |1), \\ Q_2\Phi_{2t} &\equiv \bar{\varphi}(1)\varphi(2) \equiv |2), \\ Q\Phi_t &\equiv \bar{\varphi}(1)\bar{\varphi}(2) \equiv |12). \end{aligned} \tag{4.4}$$

The various energy integrals of interest are then defined by

$$\begin{aligned} E_A &= \frac{(12|H|12)}{(12|12)}, \quad E_B = \frac{(1|H|1) + (1|H|2)}{(1|1) + (1|2)}, \\ E_C &= \frac{(1|H_1|1) + (1|V_2|2)}{(1|1)}, \quad E_D = \frac{(1|H_1|1)}{(1|1)}, \\ E_F &= \left((1|H_1|1) - (1|V_2|2)\frac{1}{(2|H_2|2) - E(2|2)}(2|V_1|1)\right) \\ &\quad \times (1|1)^{-1}, \end{aligned} \tag{4.5}$$

and

$$E_{A'} = \frac{(1|H|1)}{(1|1)}, \quad E_{B'} = \frac{(1|H_1|1) + (1|H|2)}{(1|1) + (1|2)}.$$

All these quantities are dependent on the parameter a. The variations of the E's with respect to a are demonstrated in Table II.

As expected, E_A is *bounded from below* by the first excitation threshold $e_1 = -0.25$ Ry, i.e., $E_A \geqslant e_1$ for the crude form of the trial function (4.4) we have chosen. On the other hand, E_B dips down *below* e_1. This is a fairly important result, because the generalized variational bound formulation[19] corrects this E_B by adding the effect of the shift operator, which effectively converts $|1)$ into $|12)$.

E_c is the most relevant quantity here, insofar as the Q space is concerned; it corresponds to the operator $\underline{Q}(\underline{D}+\underline{E})\underline{Q}$, and Table II shows that it is most likely bounded from below by e_1. (Since we have used only one term in the minimization, it is not possible to rigorously prove by this method that the operator is in fact bounded from below. Therefore, our result only provides a strong indication for such a bound property.)

The quantities E_D and E_F are directly related to the g_c^Q and G_{cc}^Q as we defined in (2.26) and (2.27), where the approximation (3.4) is introduced in (4.5). Both of them seem to be bounded by e_1, indicating strongly that $\underline{G}^Q$ may indeed be negative for $E < e_1$. As will be discussed below, however, such a bound property does not necessarily imply a bound on the phase shift, simply because the asymmetry in the optical potential $\underline{P}\,\underline{D}_I\,\underline{G}^Q\,\underline{D}_I\,\underline{P}$ does not allow the monotonicity theorem to be operative.

(iii) As a first crude improvement on η^P obtained from the static equation, (4.1), we have included the $\underline{G}^Q$-dependent optical potential term in (2.23), in the approximation (3.4) with $Q_c\chi_t = Q_c\Phi_{ct}$ of (4.4). Of course, the resulting phase shift, denoted by η_{st}, depends on the parameter a. Since we have only one term in g_c^Q, η_{st} is fairly sensitive to this parameter (although we expect that, as g_c^Q is improved by adding more terms, η_{st} should become less and less sensitive). The variation of η_{st} on the parameter a is shown in

TABLE II. Variation of the E's defined by (4) on the parameter a. The underlined values are the minima. All values are given in the rydberg units. Note that the first excitation threshold is -0.250 Ry.

a	E_A	E_B	E_C	E_D	E_F	$E_{A'}$	$E_{B'}$
0.05	−0.122	−0.125	−0.122	−0.090	−0.092	−0.127	−0.106
0.10	−0.199	−0.213	−0.194	−0.150	−0.155	−0.227	−0.174
0.15	−0.232	−0.268	$\underline{-0.217}$	−0.181	−0.185	−0.299	−0.205
0.20	$\underline{-0.234}$	−0.298	−0.201	$\underline{-0.188}$	$\underline{-0.188}$	−0.348	$\underline{-0.206}$
0.25	−0.211	$\underline{-0.308}$	−0.157	−0.175	−0.176	−0.376	−0.183
0.30	−0.169	−0.301	−0.092	−0.147	−0.155	$\underline{-0.380}$	−0.137
0.35	−0.111	−0.275	−0.012	−0.105	−0.127	−0.358	−0.066
0.40	−0.040	−0.225	+0.080	−0.051	−0.088	−0.304	−0.035
0.45	+0.042	−0.141	0.179	+0.015	−0.038	−0.208	+0.175
0.50	0.135	−0.008	0.286	0.090	+0.025	−0.058	0.368
0.60	0.350	+0.500	0.513	0.269	0.191	+0.494	1.008
0.70	0.600	1.656	0.757	0.484	0.408	1.680	2.301
0.80	0.873	4.487	1.016	0.734	0.669	4.496	5.264
0.90	1.239	14.012	1.290	1.017	0.967	13.935	14.909

TABLE III. Variation of the phase shift η_{st} as a function of the parameter a, at $ka_0 = 0.4$.

a	$\eta_{st}\,(Y=0)$	$\eta_{st}\,(Y\neq 0)$	E_C
0.05	1.334	1.240	−0.122
0.10	1.338	1.246	−0.194
0.15	1.355	1.275	−0.217
0.20	1.388	1.333	−0.201
0.25	1.429	1.412	−0.157
0.30	1.467	1.495	−0.092
0.35	1.497	1.570	−0.012
0.40	1.514	1.627	+0.080

Table III, at $ka_0 = 0.4$. Both cases with and without the Y_c potentials are considered.

Apparently, there is no extremum value assumed by η_{st} as the parameter a is varied; although $\underline{G}^Q$ seems to be bounded from above, $\underline{D}_J$ is not symmetric and this destroys the negative definiteness of the optical potential which appears in the $\underline{P}$ equation. The values for η_{st} quoted in Table I are determined with the choice $a \approx 0.20$, which gives both E_C and E_D near their minima.

As is clear from the result in Table I, the goodness of η^P at small ka_0 is unexpected and probably accidental. On the other hand, it could be interpreted that the coupling to the exchange channel, as given in (4.1), provides enough short-range distortions to the elastic wave function. However, we do not yet fully understand the reason why η^P should be poorer at higher values of ka_0. With the addition of the Q-space distortions, η_{st} improved, with apparent bound on the true phase shift η when the parameter a is chosen in the way described above. Again, there is no appreciable improvement in η_{st} at larger ka_0; this may be caused by the lack of the p-state contribution of the target to the distortion. Thus, an improved calculation which includes $1s$, $2s$, and $2p$ states explicitly (in addition to one or more pseudostates) would clarify the present situation.

V. DISCUSSION

In this paper, we have reformulated the electron-atom scattering problem using the result of the reduction procedure. The relevant set of equations for each system may be written down quite simply, as shown in Sec. II. The solution is much more difficult to obtain, and requires approximations. Several useful techniques were described in Sec. III, and only the approximations (i) and (v) of Sec. III were tested; we did not make the optimum use of the potentials Y_c, for example. Since the presence of Y_c is a nontrivial feature of the theory, the procedure for the determination of Y_c, such as that suggested in (vi) of Sec. III, should be carefully examined. This will be the subject of a report on proton-hydrogen charge-exchange scattering.[17]

The numerical study of the e^-H system has revealed many interesting properties of the reduced matrix equations. In particular, the boundedness of g_c^Q would be of great importance as the separable approximation (3.4) is to be improved by adding more terms, using the diagonalization procedure. A monotonically converging approximation on the g_c^Q does not necessarily give a bounded approximation on $\bar{\eta}$. Nevertheless, we can optimize the g_c^Q part of the calculation very effectively; once an approximate g_c^Q is determined, the rest of the calculation requires no further approximations.

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*Present address: S. B. Sutpin Research Center, Plastic Coating Corp., Div. of Scott Paper Co., South Hadley, Mass. 01075.

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