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Generalized Variational Bounds on the Positron-Hydrogen Reaction Matrix.
I. The Coupled-Static Approximation

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The theory of generalized variational bounds is applied to two-channel collisions of positrons on hydrogen leading to positronium formation. The formalism is developed in detail for this problem, and the zero partial-wave solution is obtained in the coupled-static approximation. The nonlocal coupling kernels and the behavior of the wave functions are exhibited in detail. Eigenphase shifts and coupling parameters, and the stripping and pickup cross sections, as well as the elastic amplitudes for positron-hydrogen and positronium-proton collisions, are studied as functions of scattering energies. The unitarity limits are exhibited, one of which is nearly saturated in the Ps-p channel. A useful iteration procedure for solving the coupled equations with large coupling kernels is developed.

I. INTRODUCTION

The three-particle problem in quantum-mechanical collision theory has been studied for many years.[1,2] In particular, a formally consistent mathematical procedure has been given by Faddeev[3] and others,[4] but its application to specific physical systems is a much more formidable task.[5,6] When only a few two-body channels are open, however, a theoretically more tractable procedure is available in the form of the generalized variational bounds[7] (GVB). It correctly treats the nonorthogonality problem of the rearrangement channels, and the effect of distortions due to coupling to other closed channels is estimated variationally with the strong *bound* property. The theory is essentially of the same degree of applicability for the low-energy scattering problem as the Ritz variational principle is for the bound-state problems. Its earlier version[8] has been applied to the elastic positron-hydrogen scattering[9] and elastic electron-hydrogen scattering,[10] where the simple channel projection operators are explicitly available.[11] The result gave a valuable insight into the effect of distortions on the scattering parameters and also on the resonance structures.[12]

This is the first of a series of reports on the detailed theoretical analysis of the positron-hydrogen scattering system, using the formalism of GVB. By restricting the scattering energies to the region below the first excitation threshold in the positron-hydrogen channel (channel 1) but above the positronium-proton elastic threshold (channel 2), we have probably the simplest two-channel scattering problem in which rearrangement of the electron takes place as

$$\underset{\text{channel 1}}{e^+ + (e^- + p^+)} \rightarrow \underset{\text{channel 2}}{(e^+ + e^-) + p^+} \quad . \qquad (1.1)$$

The effect of the coupling to the electromagnetic field may be neglected, and the ability to distinguish between the two light particles and the very heavy proton core simplifies the analysis to a manageable level with the computers available at present. Because of complicated nonorthogonality between the two open-channel wave functions, no simple channel projection operators of the Feshbach type[13] are available, and GVB, which explicitly avoid such a requirement, can thus be effectively applied to this problem.

The reaction (1.1) has been studied many times in the past in various approximations.[14–17] In particular, Bransden and Jundi[14] have solved the problem in the coupled-static approximation (CSA); they also include certain polarization potentials phenomenologically in order to estimate the effect of distortions due to other channels. Their work constitutes the first important step of a more complete treatment of the problem within the framework of GVB; we will discuss in detail in the present paper its relevance to our calculation.

Desirability of a solution to such reactions as (1. 1) can hardly be overemphasized. Aside from the possible interest in the e^+H system itself, (1. 1) also provides an important model problem with which various other simpler approximation procedures may be tested, such as the plane-wave Born approximation, the distorted-wave Born approximation,[18,19] the effective polarization approximation, the polarized orbital method and its variations,[16,20] and so on. In particular, the nonorthogonality problem[2,4,21] and the nonlocality[19] of the effective interactions and its effect on the wave functions may be readily studied using the model reaction (1. 1). For this purpose we have tried to supply here as much information from our analysis as may be relevant to such studies.

In Sec. II, we summarize and further analyze the theory of GVB relevant to the reaction (1. 1) and define the notations. The formalism necessary to evaluate the reaction matrix K, eigenphases and coupling parameters, amplitudes and cross sections for $1\rightarrow 1$, $1\rightarrow 2$, $2\rightarrow 1$, and $2\rightarrow 2$ are defined. Section III contains a brief summary of the derivation of the coupled equations in the CSA. The structure of the nonlocal coupling kernels is discussed. The details of the method used to solve the problem in the CSA and the results are given in Sec. IV.

Throughout the paper, we restrict ourselves to the scattering with the zero total partial wave, $L=0$. Contribution of the higher partial waves, $L>0$, to the cross sections is known to be important,[14] and such a study is being planned. In the second paper, we will present a detailed variational estimate of the correction to the amplitudes in the CSA, also for $L=0$. The solution of the reduced matrix equations,[22] which are derived essentially from the Faddeev equations,[3] will be presented elsewhere.[23]

II. GVB THEORY

The formalism of GVB[7] used in our study will be summarized in this section, explicitly for the reactions (1. 1), and we will also define notations. The Hamiltonian in the Schrödinger scattering equation

$$(H-E)\Psi=0 \tag{2. 1}$$

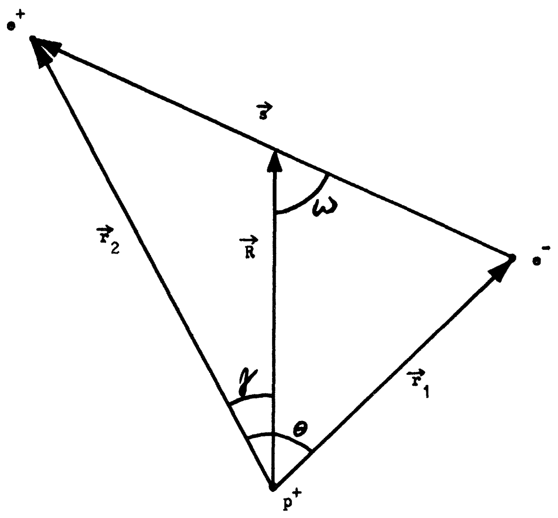

FIG. 1. Coordinates and angles used in the calculation.

may be written as

$$H=H_1+V_1=H_2+V_2\ , \tag{2. 2}$$

where

$$H_1=-\tfrac{1}{2}\nabla^2_{\vec{r}_2}+(-\tfrac{1}{2}\nabla^2_{\vec{r}_1}-r_1^{-1})\ ,\quad V_1=r_2^{-1}-s^{-1}\ , \tag{2. 3}$$

$$H_2=-\tfrac{1}{4}\nabla^2_{\vec{R}}+(-\nabla^2_{\vec{s}}-s^{-1})\ ,\quad V_2=r_2^{-1}-r_1^{-1}\ . \tag{2. 4}$$

In (2. 3) and (2. 4), we have taken $m=\hbar=e^2=1$. $\vec{r}_1$ and $\vec{r}_2$ are the electron and positron coordinates, respectively (Fig. 1), and $\vec{s}$ is the electron-positron relative coordinates, while $\vec{R}$ denotes the (e^+e^-) center of mass from the proton.

The scattering problem is then completely defined by (2. 1) and the boundary conditions on Ψ as

$$\Psi\rightarrow P_1\Psi_1 \quad \text{as} \quad r_2\rightarrow\infty\ , \tag{2. 5a}$$

$$\Psi\rightarrow P_2\Psi_2 \quad \text{as} \quad R\rightarrow\infty\ , \tag{2. 5b}$$

and the regularity requirements at $r_2=r_1=0$ or $s=R=0$. In (2. 5), we have introduced the projection operators P_i, $i=1$ and 2, defined by

$$\begin{aligned} P_1&=\psi_0(\vec{r}_1))(\psi_0(\vec{r}_1{}')\ ,\\ P_2&=\varphi_0(\vec{s}))(\varphi_0(\vec{s}\,')\ , \end{aligned} \tag{2. 6}$$

and where

$$\begin{aligned} [-\tfrac{1}{2}\nabla^2_{\vec{r}_1}-r_1^{-1}]\,\psi_m(\vec{r}_1)&=E_m{}^{(1)}\,\psi_m(\vec{r}_1)\ ,\\ [-\nabla_{\vec{s}}{}^2-s^{-1}]\,\varphi_n(\vec{s})&=E_n{}^{(2)}\,\varphi_n(\vec{s})\ . \end{aligned} \tag{2. 7}$$

In order to have only two channels open, we limit the energy E to the region (in a. u.)

$$-\tfrac{1}{4}=E_0^{(2)}\leqslant E<E_1^{(1)}=-\tfrac{1}{8}\ . \tag{2. 8}$$

Defining the energies as

$$E=E_0^{(1)}+\tfrac{1}{2}k^2=E_0^{(2)}+\tfrac{1}{4}p^2\ , \tag{2. 9}$$

(2. 8) gives

$$\tfrac{1}{2} \leqslant k^2 < \tfrac{3}{4} \ , \qquad 0 \leqslant p^2 < \tfrac{1}{2} \ . \tag{2.10}$$

In general, it is very difficult, if not impossible, to evaluate explicitly the projection operator P which projects onto the two open channels of (1.1), and the formalism of GVB *does not* require such an operator. However, for the convenience of formal discussion, we simply assume that the operator P and its complement $Q = 1 - P$ are given (implicitly in a formal sense only). In fact, such an operator is written down by Mittleman[24] using the procedure developed by Feshbach.[13] The operator P has, *by definition*, the property that

$$P\Psi = P_1\Psi_1 + P_2\Psi_2 \ , \tag{2.11}$$

$$P^2 = P = P^\dagger \ , \tag{2.12a}$$

$$P_i P = P_i = P P_i \ , \tag{2.12b}$$

$$QP = PQ = 0 \ , \tag{2.12c}$$

$$P_i Q = Q P_i = 0 \ ; \tag{2.12d}$$

but

$$[P_1, P_2] \neq 0 \ . \tag{2.13}$$

It is important to note that P of (2.11) with (2.12) is *not* a simple linear combination of P_1 and P_2, due to (2.13). The boundary conditions (2.5) then become explicitly

$$P_1\Psi_1 \to (\mu_1/k)^{1/2}\psi_0(\vec{r}_1)[a_1\sin(kr_2) + b_1\cos(kr_2)]/r_2, \quad r_2 \to \infty \tag{2.14a}$$

$$P_2\Psi_2 \to (\mu_2/p)^{1/2}\varphi_0(\vec{s})[a_2\sin(pR) + b_2\cos(pR)]/R, \quad R \to \infty \ , \tag{2.14b}$$

where $\mu_1 = 1$, $\mu_2 = 2$ in our units; and as either r_2 or R or both $\to \infty$,

$$Q\Psi \to 0 \ \text{ faster than } \ r_2^{-1} \text{ and } R^{-1} \ , \tag{2.15}$$

as we limit our discussion throughout for $L = 0$ partial wave.

The difficulty with the rearrangement collision such as (1.1) is essentially that the asymptotic boundary conditions (2.14) and (2.15) cannot readily be imposed. Quantities which appear in the intermediate stages of the calculation often involve nonunique operations.[25] As will be shown below, such ambiguity does not arise in GVB.

A. GVB

The GVB follow essentially from the important orthogonality property of the operator M and the function N defined below. The original Schrödinger equation (2.11) separates as

$$P(H-E)P\Psi = -P(H-E)Q\Psi \ , \tag{2.16}$$

$$Q(H-E)Q\Psi = -Q(H-E)P\Psi \ . \tag{2.17}$$

(2.16) is a set of coupled equations for $P_1\Psi_1$ and $P_2\Psi_2$ for given $Q\Psi$. We define the homogeneous part of (2.16) as

$$P(H-E)P\Psi^P = 0 \tag{2.18}$$

$$P(H-E)PG^P P = -P \ . \tag{2.19}$$

The boundary conditions on $P\Psi^P$ are the same as (2.14), with b_i replaced by $b_i{}^P$. Furthermore, we define G^P such that for a square-integrable function f,

$$P_1 G^P P_f \to (\text{const})\,\psi_0(\vec{r}_1)\cos(kr_2)/r_2, \quad r_2 \to \infty, \tag{2.20a}$$

$$P_2 G^P P_f \to (\text{const})\,\varphi_0(\vec{s})\cos(pR)/R, \quad R \to \infty. \tag{2.20b}$$

Then, (2.16) may be solved formally as

$$P\Psi = P\Psi^P + PG^P P(H-E)Q\Psi \ , \tag{2.21}$$

and, thus (2.17) becomes

$$(QMQ)Q\Psi = -QN \ , \tag{2.22}$$

where

$$\begin{aligned} M &\equiv H - E + (H-E)G^P(H-E) \\ &= H - E + S \ , \end{aligned} \tag{2.23}$$

$$N = (H-E)\Psi^P \ . \tag{2.24}$$

Note that M and N are defined here *without* Q, although they appear in (2.22) with Q. We also dropped P in PG^PP and $P\Psi^P$ to stress the fact that these functions *can be obtained without the explicit use of P*. Similarly, we have for (2.16),

$$P\{H - E + (H-E)[Q(E-H)Q]^{-1}(H-E)\}P\Psi = 0 \ , \tag{2.25}$$

or

$$P(H-E)P\Psi = P(H-E)Q(QMQ)^{-1}QN \ , \tag{2.26}$$

which is a set of coupled inhomogeneous equations with a given right-hand side. Any of Eqs. (2.22), (2.25), or (2.26) are completely equivalent to (2.16) and (2.17); we use in our discussion (2.25) and (2.26) interchangeably.

The theory of GVB follows from the observation that the Q space is closed, so that

$$-(QG^QQ)^{-1} = Q(H-E)Q > 0 \tag{2.27}$$

for E below the lowest possible "resonance" energy. This can, of course, be relaxed as more variational parameters are included in the estimate of $[Q(E-H)Q]^{-1}$. Thus, for a set of square-integrable trial functions $Q\chi_n$, we can write an inequality

$$QG^QQ \leqslant QG_t^QQ = \sum_{n,m} Q\chi_n)(D^{-1})_{nm}(Q\chi_m \leqslant 0 \ , \tag{2.28}$$

where D^{-1} is the inverse of a matrix with elements

$(Q\chi_i, [E-H]Q\chi_j)$. When the asymptotic boundary conditions (2.14), (2.15), and (2.20) are used in (2.25), we obtain the scattering parameters

$$\lambda - \lambda^P \equiv \Delta = (P\Psi^P,\ P(H-E)\,G^Q(H-E)\,P\Psi\ ) \ , \tag{2.29}$$

where

$$\begin{aligned} \lambda &= -\ 2\pi\vec{a}\cdot\vec{b} = -\ 2\pi(a_1 b_1 + a_2 b_2) \ , \\ \lambda^P &= -\ 2\pi\vec{a}\cdot\vec{b}^P = -\ 2\pi(a_1 b_1{}^P + a_2 b_2{}^P) \ . \end{aligned} \tag{2.30}$$

Equation (2.29) may also be written as

$$\Delta = (P\Psi^P,\ P(H-E)\,\mathcal{G}^Q\,(H-E)\,P\Psi^P) \ , \tag{2.31a}$$

$$\Delta = (P\Psi^P,\ P(H-E)\,Q\Psi) = (QN, Q\Psi) \ , \tag{2.31b}$$

$$\Delta = -\ (Q\Psi, MQ\Psi) \ , \tag{2.31c}$$

where

$$\mathcal{G}^Q = -\ (QMQ)^{-1} \ .$$

So far, the results (2.29)–(2.31) are *exact*. However, the complexity of $\mathcal{G}^Q$ makes it impossible to evaluate Δ, and we make here a variational estimate of this operator.

Since the shift operator $QSQ = Q(H-E)G^P(H-E)Q$ in QMQ vanishes asymptotically, we expect the continuum spectrum of QMQ to be similar to that of QHQ. Thus, we can write

$$\mathcal{G}^Q \leqslant \mathcal{G}^Q{}_t = -\ \sum_{n,m} Q\chi_n)\,[(QMQ)^{-1}]_{nm}\,(Q\chi_m \leqslant 0 , \tag{2.32}$$

and from (2.31a) and (2.32) we immediately have

$$\Delta \leqslant \Delta_t = (QN, \mathcal{G}^Q{}_t\, QN) < 0 \ \ , \tag{2.33}$$

where possible subtraction terms are neglected. This is the basic relation of the variational bounds.[8]

The form (2.33) is still not quite satisfactory, since it *cannot* be used unless the Q operator is explicitly known, and we have stated earlier that such operator is not available for the reactions (1.1). The crucial step in the derivation of GVB is the observation that[7]

$$M = QMQ \ \ , \tag{2.34}$$

$$N = QN \ \ . \tag{2.35}$$

The proof that

$$PM = MP = 0 \ \ , \qquad PN = 0 \tag{2.36}$$

follows directly from the definitions of G^P and $P\Psi^P$ as given by (2.18) and (2.19). That is, the properties (2.34) and (2.35) depend critically on (2.18) and (2.19), so that, in order to preserve the orthogonality properties (2.34) and (2.35), we have to solve for $P\Psi^P$ and G^P *exactly*. In general, we expect then a critical cancellation between the terms, e.g.,

$$(\chi_n, [H-E]\,\chi_n) \ \ ,$$

$$(\chi_n,\ S\chi_n) \ \ .$$

This will be discussed in detail in paper II. Thus, we finally write (2.33) as

$$\Delta \leqslant \Delta_t = (\Psi^P,\ [H-E]\,\mathcal{G}^Q{}_t[H-E]\,\Psi^P) \ \ , \tag{2.37}$$

$$\lambda \leqslant \lambda_t \ \ , \tag{2.38}$$

with

$$\lambda_t = \lambda^P + \Delta_t \ \ , \tag{2.39}$$

$$\mathcal{G}^Q{}_t = -\ \sum_{n,m} \chi_n)\,([M]^{-1})_{nm}(\chi_m \ . \tag{2.40}$$

In (2.37), the Q operator has completely disappeared, and we simply dropped P, because (2.18) and (2.19) *can* be rewritten completely in terms of P_i alone using the property (2.12b). (2.37) or (2.38) are the desired GVB. A trivial result of (2.37) is simply

$$\Delta_t = 0 \ \ ,$$

with

$$\lambda \leqslant \lambda_t = \lambda^P \ \ . \tag{2.41}$$

This relation (2.41) is the coupled-static approximation and will be evaluated explicitly in this paper, and the estimate of Δ_t will be described later. The complication in (2.39) due to the appearance of the G^P can be avoided by the sum-rule technique[7]; this will be discussed further in Sec. III.

B. Resonances

In many of the earlier applications,[12] the resonance energies of e^-H and e^-He$^+$ systems were variationally estimated using the operator QHQ, where Q is known explicitly as $Q = Q_1Q_2 = Q_2Q_1$. The calculation involved is then essentially identical to the Ritz method for the true bound-state problem, except for the orthogonalization of the trial functions to both P_1 and P_2. The shift effect due to the coupling to the P space is then estimated by the perturbation theory.

When the operator Q is not explicitly available, the above procedure is not applicable, and we have to use the operator M of (2.23), where, as we have seen in (2.34), the shift operator S plays a major role in keeping M in the Q space. It is also noted that the energy E in M can be arbitrary, in so far as the resonance-energy calculation is concerned, but should be used consistently throughout M; otherwise the orthogonality (2.36) is destroyed. Unless E is chosen to be equal to a particular resonance energy, the resulting shift on that energy value may be only approximate. However, for cases in which the shift is small and insensitive to E, this problem is not critical, and one can always improve the situation to arbitrary accuracy by adjusting the value E. Thus, by diagonalizing the energy matrix as

$$AMA^{-1} = \mathcal{E}_D \ ,$$

we have the resonance energies

$$\mathcal{E}^Q_{nt} = \mathcal{E}_{Dn} + E \ . \tag{2.42}$$

Actually, this diagonalization also makes the expression of $\mathcal{G}^Q_t$ simple, as

$$\mathcal{G}^Q_t = \textstyle\sum_n X_n)\,(E - \mathcal{E}_{nt}{}^Q)^{-1}\,(X_n \ , \tag{2.43}$$

where

$$X_n = \textstyle\sum_m A^T_{nm}\chi_m \ .$$

Unlike in the earlier calculation of the similar type,[26] $\mathcal{G}^Q_t$ will not have singularities at $E = \mathcal{E}^Q_{nt}$ as long as E is taken below the lowest $\mathcal{E}^Q_{nt}$, because, although X_n are not entirely in the Q space, M is. We then have

$$\Delta_t = \textstyle\sum_n (N, X_n)\,(E - \mathcal{E}^Q_n)^{-1}\,(X_n, N) \ . \tag{2.44}$$

C. Amplitudes and Cross Sections

The parameters b_i in (2.14) and (2.30) are related to the reaction matrix K as

$$b_i = \sum_{j=1}^{2} K_{ij} a_j \ . \tag{2.45}$$

[This form is slightly different from the one given by Bransden and Jundi, because of different asymptotic behavior assumed in (2.14).] Similarly, we have

$$b^P_i = \sum_{j=1}^{2} K^P_{ij} a_j \ . \tag{2.46}$$

Thus, from (2.30) and (2.29) we have

$$-2\pi\sum_{ij} a_i K_{ij} a_j \leq -2\pi\sum_{ij} a_i K^P_{ij} a_j + \Delta_t \ . \tag{2.47}$$

A special case is

$$-K_{11} \leq -K^P_{11}, \quad -K_{22} \leq -K^P_{22} \ . \tag{2.48}$$

If we define an orthogonal matrix U with the coupling parameter ϵ as

$$U = \begin{pmatrix} \cos\epsilon & \sin\epsilon \\ -\sin\epsilon & \cos\epsilon \end{pmatrix}, \tag{2.49}$$

then

$$K = UK_D U^{-1} \ , \tag{2.50}$$

where

$$K_D = \begin{pmatrix} \tan\delta_1 & 0 \\ 0 & \tan\delta_2 \end{pmatrix} . \tag{2.51}$$

δ_i are the eigenphase shifts. It follows from (2.48) that

$$\delta_i > \delta_i{}^P \ , \tag{2.52}$$

but no direct bound on ϵ is possible except in some special cases. Explicitly,

$$K = \begin{pmatrix} \cos^2\epsilon\tan\delta_1 + \sin^2\epsilon\tan\delta_2 & \cos\epsilon\sin\epsilon\,(\tan\delta_1 - \tan\delta_2) \\ \cos\epsilon\sin\epsilon\,(\tan\delta_1 - \tan\delta_2) & \sin^2\epsilon\tan\delta_1 + \cos^2\epsilon\tan\delta_2 \end{pmatrix} . \tag{2.53}$$

We define the amplitudes for $i \rightarrow f$ reactions as

$$T_{fi} = [K(1 - iK)^{-1}]_{fi}/k_i \, , \quad i, f = 1, 2 \tag{2.54}$$

with $k_1 \equiv k$ and $k_2 \equiv p$. The cross sections for $i \rightarrow f$ for $L = 0$ are then given by σ_{fi} with

$$\sigma_{fi} = 4\pi\,|\,T_{fi}\,|^2 \ . \tag{2.55}$$

We have constructed the amplitudes in (2.54) from the Hermitian K matrix, and thus they satisfy the unitarity constraints automatically:

$$\sigma^U_{ii} = 4\pi/k^2_i \, , \quad i = 1, 2 \ . \tag{2.56}$$

Contrary to what one might expect, (2.56) do not give useful checks on the goodness of T_{ii} in the present calculation, simply because we evaluate these amplitudes from the Hermitian K matrix. Only when the asymmetric K matrix from the actual calculation is kept, we expect (2.56) to be useful near the maximum of σ_{ii}.

So far, possible subtraction terms in (2.37) have been neglected completely. If there are a finite number of eigenstates of the operator M below E, then we have to include enough terms in the trial functions[8] such that the *same* number of $\mathcal{E}^Q_{nt}$ lie below E. This requirement is essential in maintaining the inequality (2.38), and thus places a stringent condition on the trial function. Obviously, (2.41) is immediately violated whenever this condition is not satisfied and it will be of major importance as we add the Q-space component in Δ_t (paper II). It is especially important to note that $\mathcal{E}^Q_{nt}$ *depend* on E, so that the number of required subtractions may change as a function of E. The states generated by the operator M manifest themselves as resonances only when any one state *coincides* with E, while the rest of the states may or may not be resonances. These points will be discussed in more detail later.

III. COUPLED-STATIC APPROXIMATION

A. Coupled Equations and Kernels

In this section, we analyze the scattering equations (2. 18) in the coupled-static approximation (CSA). This part of the problem is essential in carrying out the GVB calculation. Using the property (2. 12b) and Eq. (2. 11), (2. 18) can be written as

$$P_1(H-E)P_1\Psi_1^P=-P_1(H-E)P_2\Psi_2^P \;, \qquad (3.1)$$

$$P_2(H-E)P_2\Psi_2^P=-P_2(H-E)P_1\Psi_1^P \;. \qquad (3.2)$$

For the total angular momentum $L=0$, we neglect the Euler angles for the center of mass and take the variable sets (r_1, r_2, θ) for the channel 1 and take (s, R, W) for the channel 2 in analyzing (3. 1) and (3. 2). For the Q-space effect, the set (r_1, r_2, s) may be more convenient, but one can also conveniently switch among the different sets during the various integrations.

The coupled equations above have been studied by Cody and Smith,[15] by Cody *et al.*,[15] and by Bransden and Jundi,[14] so that we only sketch the analysis in so far as it concerns our numerical calculation. We write

$$P_1\Psi_1^P=\psi_0(r_1)F_1^P(r_2)/r_2 \;, \qquad (3.3a)$$

$$P_2\Psi_2^P=\varphi_0(s)F_2^P(R)/R \;, \qquad (3.3b)$$

with

$$\psi_0(r_1)=\sqrt{2}\,e^{-r_1}\;, \quad \varphi_0(s)=2^{-1}e^{-s/2}\;,$$

$$P_0(\cos\theta)=P_0(\cos\omega)=1 \;.$$

The projection operators are explicitly given by

$$P_1=\psi_0(r_1)\int_0^\infty r_1'^2dr_1'\int_{-1}^1 d(\cos\theta')\,\psi_0(r_1')$$

$$=\sqrt{2}\,e^{-r_1}\int_0^\infty\sqrt{2}\,e^{-r_1'}r_1'dr_1'\int_{|r_2-r_1'|}^{r_2+r_2'} s\,ds/r_2 \;, \qquad (3.4a)$$

$$P_2=\varphi_0(s)\int_0^\infty s'^2ds'\int_{-1}^1 d(\cos\omega')\,\varphi_0(s')$$

$$=(\tfrac{1}{2}e^{-s/2})\int_0^\infty \tfrac{1}{2}e^{-s'/2}s'ds'\int_{|R-s'/2|}^{R+s'/2} 2(r_1/R)\,dr_1 \;, \qquad (3.4b)$$

which satisfy the properties $P_i^2=P_i=P_i^\dagger$. [This volume element makes 2π in (2. 30) unnecessary.] When (3. 3) are put into (3. 1) and (3. 2), and relevant integrations are carried out (Appendix), we obtain the coupled equations for $F_1^P(r_2)$ and $F_2^P(R)$ as

$$\left[\frac{d^2}{dr_2^2}+k^2-2\left(\frac{1}{r_2}+1\right)e^{-2r_2}\right]F_1^P(r_2)$$

$$=r_2\int_0^\infty R\,dR\,K_{12}(r_2,R)F_2^P(R) \;, \qquad (3.5a)$$

$$\left[\frac{d^2}{dR^2}+p^2\right]F_2^P(R)=2R\int_0^\infty r_2dr_2K_{21}(R,r_2)F_1^P(r_2) \qquad (3.5b)$$

where

$$K_{12}(r_2,R)=K_{21}(R,r_2)=K(r_2,R) \;, \qquad (3.6)$$

$$K(r_2,R)$$

$$=8\int_{-1}^1 d(\cos\gamma)\left\{\left[-2-k^2+2\left(-\frac{1}{r_1}+\frac{1}{r_2}-\frac{1}{s}\right)\right]\psi_0\varphi_0\right.$$

$$\left.-4\frac{d\psi_0}{dr_1}\frac{d\varphi_0}{ds}\hat{r}_1\cdot\hat{s}\right\} \;. \qquad (3.7)$$

The ranges of k^2 and p^2 are given by (2. 10), with the definition (2. 9). As expected, K is a nonlocal energy-dependent coupling kernel expressing particle rearrangement and nonorthogonality of channels 1 and 2. Owing to various singularities of the integrand of K, care has to be exercised in evaluating the integral in $d(\cos\gamma)$. The resulting K has many points with discontinuous first derivatives in r_2 and R. By substitution of new variables,[27] K can be rewritten in the form convenient for numerical integration. After some algebra, (3. 7) reduces to the form

$$K(r_2,R)=4\sqrt{2}\int_{-1}^1 dx\,e^{-r_1}e^{-s/2}\left(-2-k^2+\frac{2}{r_1}+\frac{2}{r_2}+\frac{2}{s}\right.$$

$$\left.-\frac{4(2R^2+r_2^2-3Rr_2x)}{r_1s}\right) \;, \qquad (3.8)$$

where

$$r_1=(4R^2+r_2^2-4Rr_2x)^{1/2} \;,$$

$$s=2(R^2+r_2^2-2Rr_2x)^{1/2} \;,$$

$$x=\cos\gamma \;.$$

B. Iteration Procedure

The main part of the effort in solving (3. 5) went into the evaluation of K in the region $0\leqslant r_2, R \leqslant 32a_0$.

Once K is evaluated, we can solve (3. 5) for F_i^P and obtain b_i^P from the asymptotic behavior of scattering functions. Bransden and Jundi[14] solved this set of coupled equations by first converting them into a set of integral equations and then inverting matrices of the form $[1-g_{i0}^PK_{ij}g_{j0}^PK_{ji}]$, where g_{i0}^P are the Green's functions for the operators on the left-hand sides of (3. 5).

We decided to solve (3. 5) directly by an iteration method, mainly because the inversion procedure would limit the accuracy of solutions, especially when long-range forces are involved as we put in the Q-space functions. Unfortunately, the effects of K on F_i^P were very large, and the iteration series did not converge very well. A special procedure had to be devised, as explained next.

If we write an equation to be solved iteratively simply as

$$Df=Bf \;, \qquad (3.9)$$

then the function $f^{(n)}$ obtained after the nth iteration is given by the usual Born series, for $n>1$:

$$f^{(n)}=af^{(0)}+g_0Bf^{(n-1)}$$
$$=a(f^{(0)}+d_0f^{(0)}+d_0^2f^{(0)}+\cdots+d_0^nf^{(0)}) \ , \quad (3.10)$$

with

$$Df^{(0)}=0 \ , \quad Dg_0=1 \ , \quad d_0=g_0B \ ,$$

and a is a fixed normalization constant.

Now, when the effect of B is very large, (3.10) may not converge, and we have the convergence criterion[1,4]

$$\|g_0B\|<1 \quad (3.11)$$

for all the strength eigenvalues of the operator g_0B.

A much better convergent series is obtained if, instead of fixing the normalization at the origin $r=0$ (slope of f) or at infinity (the free-wave part), we require the *function to be unchanged* at $r=r_0$, where B is appreciable, or rather where g_0B is large. That is, we adjust $a^{(n)}$ such that

$$f^{(n)}=f^{(n-1)} \quad \text{at} \quad r=r_0 \ . \quad (3.12)$$

The resulting series is then given by

$$f^{(n)}=a^{(n)}f^{(0)}+g_0Bf^{(n-1)} \ , \quad (3.13)$$

with

$$a^{(n)}=[(f^{(n-1)}-g_0Bf^{(n-1)})/f^{(0)}]_{r=r_0} \ .$$

Since $f^{(n)}$ is not changed from $f^{(n-1)}$, but can change only in its slope in the region around r_0, we expect the over-all behavior of $f^{(n)}$ to be more stable. This is born out by actual calculation, and the procedure did converge well for (3.5) with r_0 over a substantial range.

Obviously, the above procedure is a generalization of the usual method in which $r_0=0$ or $r_0=\infty$ is used. Recently, Austern[28] discussed a modified procedure of the earlier theory by Sasakawa,[29] which seems to have an improved convergence in the case of *short-range* potentials. It is not clear whether such procedure may also be applied to the present case, where long-range interactions are critically involved.

As usual, two independent sets of solutions $P\Psi^P$ are needed to completely extract the K^P matrix. The above iteration procedure gives two sets which may not have the desired initial conditions a; proper combinations are made at the end to adjust these, but the essential point is, of course, to get sets of convergent solutions.

C. Green's Function G^P

The Green's function G^P in the CSA is defined by (2.19), which can be written explicitly as[7]

$$P_1(H-E)PG_1^PP_1=-P_1 \ , \quad (3.14a)$$
$$P_2(H-E)PG_2^PP_1=-P_2 \ , \quad (3.14b)$$

where

$$PG^PP=PG_1^PP_1+PG_2^PP_2 \ , \quad (3.15)$$

$$\left.\begin{aligned}PG_1^PP_1&=P_1G_{11}^PP_1+P_2G_{21}^PP_1 \ ,\\ PG_2^PP_2&=P_1G_{12}^PP_2+P_2G_{22}^PP_2 \ .\end{aligned}\right\} \quad (3.16)$$

It is obvious now that, as with $P\Psi^P$, G^P may be obtained without the explicit use of the unknown operator P. Of course, this point was essential in the derivation of GVB in Sec. II.

The structure of G_{ij}^P is extremely complicated, and we do not evaluate G^P explicitly. In fact, GVB does *not* require G^P in its full generality, but always in the specialized form

$$P\mathcal{Y}_n=G^P(H-E)\chi_n \ . \quad (3.17)$$

Therefore, instead of evaluating G^P directly, we solve for the functions $P\mathcal{Y}_n$ for each given χ_n, as

$$P_i(H-E)P\mathcal{Y}_n=-P_i(H-E)\chi_n \ , \quad (3.18)$$

where $P\mathcal{Y}_n$ satisfy the same boundary conditions as G^P does. Equation (3.18) is an inhomogeneous version of (3.5) and can be readily solved with the *same* iteration procedure. Of course, in principle, the right-hand side of (3.18) should not come in in the iteration convergence problem. However, if we start the iteration using $P\Psi^P$ as the zero-order solution, then the right-hand side disturbs the solution sufficiently strongly so that the series may not converge again. This problem can be handled, however, by readjusting the value r_0 and by scaling the right-hand side. These procedures will be discussed more fully in paper II.

IV. RESULT OF CALCULATIONS

We present in this section a summary of the result of the analysis. The coupling kernel $K(r_2,R)$ is described first, and for later applications, the wave functions F_i^P of $P\Psi^P$ are given. Evaluation of the reaction matrix K^P, eigenphases δ_i^P, and the coupling parameter ϵ^P, the amplitudes T_{fi}^P, and cross sections σ_{fi}^P is given for all four possible reactions $i\to f$, with i, $f=1, 2$.

A. Coupling Kernel $K(r_2,R)$.

The Coulomb singularities $1/r_1$ and $1/s$ in (3.8) persist in the x integration, resulting in the discontinuity in the first derivative at values $r_2=R$ and $r_2=2R$. For convenience of solution and because of limitation of the available storage space in the computer, we have taken the meshes in the r_2 and R variables as

$$n_1=40 \ , \quad h_1=0.1 \ , \quad 0.0\leqslant r_2, R\leqslant 4.0 \ ,$$

$$\begin{aligned} &n_2 = 20\,, \quad h_2 = 0.2\,, \quad 4.0 \leq r_2, R \leq 8.0\,, \\ &n_3 = 20\,, \quad h_3 = 0.4\,, \quad 8.0 \leq r_2, R \leq 16.0\,, \\ &n_4 = 20\,, \quad h_4 = 0.8\,, \quad 16.0 \leq r_2, R \leq 32.0\,, \end{aligned} \tag{4.1}$$

with the total number of mesh points $n = 101$. Equations (4.1) seem to be the optimum choice, with the expected accuracy in the final wave functions and the K^P elements of better than three parts in 10^4. Unfortunately, the discontinuity points in the region with h_1 do not always fall on the mesh points and had to be extrapolated (or interpolated), but for other regions, the above choice guarantees that all such anomalous points are on the mesh points.

The dx integration was complicated by the occurrence of these singularities. The problem was avoided completely by the clever transformations of coordinates devised by Bransden and Jundi,[27] as

$$z' = [s - |r_2 - R| - (r_2 + R)]/[(r_2 + R) - |r_2 - R|] \tag{4.2a}$$

in the region $r_2 < \frac{3}{2}R$, and

$$z'' = [2r_1 - |r_2 - 2R| - (2R + r_2)]/[(r_2 + 2R) - |2R - r_2|]\,, \tag{4.2b}$$

in the region $r_2 > \frac{3}{2}R$.

The resulting $K(r_2, R)$ are given in its numerical values in Fig. 2 and Table I. The integration is carried out using the seven-point Newton-Cotes formula.

Evaluation of K took roughly 10 min for each energy value E.

B. Wave Functions $P\Psi^P$.

The integrations involved in the right-hand sides of (3.5) were performed using either the three- or four-point Newton-Cotes formula, and the differential operators on the left-hand sides were treated by the Runge-Kutta fourth-order formula, which allows ready change of interval sizes h_i. Starting with the plane sine waves, the solution converged usually after 60–100 iterations, which required approximately 5 min of computer time for each energy value.

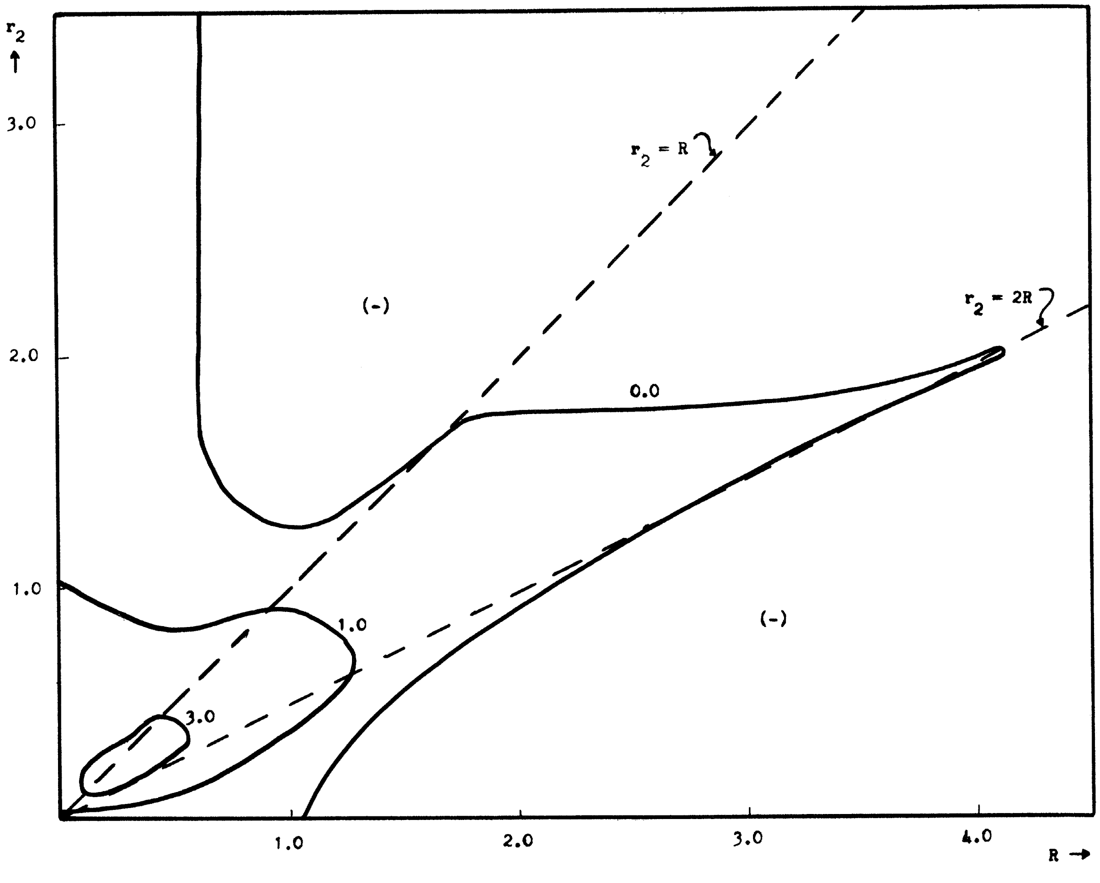

FIG. 2. Contour map of the coupling kernel $K(r_2, R)$ at $E = -0.18$ a.u. ($k = 0.8$). The lines $r_2 = R$ and $r_2 = 2R$ denote the discontinuities in the first derivative of the kernel.

TABLE I. Values of the coupling kernel $K(r_2, R)$ at several points of R for $E=-0.18$ a.u. ($k=0.8$).

r_2	$R=0.1$	$R=0.2$	$R=0.4$	$R=0.8$
0.0	1.676 28	2.483 64	2.726 10	1.692 17
0.2	3.104 49	3.844 15	2.838 60	1.304 86
0.4	1.628 66	3.476 37	3.367 70	1.047 44
0.6	0.778 02	1.703 15	2.849 96	0.989 09
0.8	0.308 85	0.710 24	2.352 86	1.401 94
1.0	0.063 81	0.182 35	0.895 13	1.208 97
1.2	−0.053 45	−0.076 33	0.143 42	1.023 60
1.4	−0.100 42	−0.184 93	−0.212 76	0.867 02
1.6	−0.110 65	−0.213 91	−0.351 34	0.745 03
1.8	−0.103 23	−0.203 81	−0.376 28	−0.036 02
2.0	−0.088 69	−0.177 18	−0.347 02	−0.372 05
2.2	−0.072 52	−0.145 99	−0.296 38	−0.480 13
2.4	−0.057 37	−0.116 12	−0.241 53	−0.476 08
2.6	−0.044 33	−0.090 08	−0.190 69	−0.422 38
2.8	−0.033 65	−0.068 60	−0.147 15	−0.352 44
3.0	−0.025 20	−0.051 49	−0.111 61	−0.282 76
3.2	−0.018 66	−0.038 21	−0.083 52	−0.220 77
3.4	−0.013 70	−0.028 09	−0.061 83	−0.168 95
3.6	−0.009 98	−0.020 49	−0.045 36	−0.127 32
3.8	−0.007 22	−0.014 85	−0.033 04	−0.094 79
4.0	−0.005 20	−0.010 70	−0.023 91	−0.069 87
4.4	−0.002 66	−0.005 48	−0.012 33	−0.037 10
4.8	−0.001 34	−0.002 76	−0.006 25	−0.019 24
5.2	−0.000 67	−0.001 38	−0.003 13	−0.009 80
5.6	−0.000 33	−0.000 68	−0.001 56	−0.004 92

The position r_0 at which the wave functions F_i^P are fixed throughout the iteration can be varied somewhat in the range $0.6a_0 < r_0 < 3.0a_0$, without affecting the convergence property, and a slightly different procedure has been used with $r_0 = 0.9$. The effect of K on F_i^P is very large, and we show the wave functions in Table II for $k = 0.8$, for the two independent sets of initial conditions

$$a^{\mathrm{I}} = \begin{pmatrix} 1 \\ 0 \end{pmatrix} \quad \text{and} \quad a^{\mathrm{II}} = \begin{pmatrix} 0 \\ 1 \end{pmatrix} . \tag{4.3}$$

The difference between these functions and $\sin(kr_2)$ or $\sin(pR)$ is striking. Moreover, since the calculation of K^P and $P\Psi^P$ was carried out at discrete values of k, it is important to examine whether sharp variations in a small k interval have been missed, such as those caused by resonance states. One direct way to study this is to check the variation of $P\Psi^P$ as k and p are increased and watch the change in the positions of nodes. For complicated nonlocal energy-dependent couplings such as what we have, it is not rigorously proven that an extra node in the wave function is a sign of the presence of a resonance. On the other hand, the theorem on the relation between the presence of bound states and the number of nodes obtained for the local interaction is plausible in most cases, and, in any case, a drastic change will show up in the wave function.

The explicit values of $K(r_2, R)$ at several sample points and the wave functions $P\Psi^P$ at $k = 0.8$ are supplied, since they may be of special interest in the study of properties in the distorted-wave Born approximation (DWBA).[19] It is well known, for example, that the nonlocal interaction drastically modifies the wave function in the interaction re-

TABLE II. Solutions of the coupled equations in the CSA listed for $E=-0.18$ a.u. The two sets are normalized according to (2.14) and satisfy the initial conditions (4.3).

R	$F_{1\mathrm{I}}^P$	$F_{2\mathrm{I}}^P$	$F_{1\mathrm{II}}^P$	$F_{2\mathrm{II}}^P$
0.2	0.0938	−0.0502	−0.1993	0.1674
0.4	0.2085	−0.0892	−0.4172	0.3143
0.6	0.3375	−0.1093	−0.6447	0.4324
0.8	0.4736	−0.1076	−0.8731	0.5269
1.0	0.6096	−0.0857	−1.0953	0.6138
1.2	0.7389	−0.0480	−1.3059	0.7145
1.4	0.8556	−0.0006	−1.5013	0.8511
1.6	0.9549	0.0503	−1.6794	1.0432
1.8	1.0329	0.0993	−1.8389	1.3052
2.0	1.0867	0.1423	−1.9797	1.6462
2.2	1.1142	0.1768	−2.1018	2.0687
2.4	1.1143	0.2014	−2.2058	2.5704
2.6	1.0864	0.2162	−2.2922	3.1448
2.8	1.0311	0.2219	−2.3619	3.7812
3.0	0.9495	0.2200	−2.4156	4.4665
3.2	0.8433	0.2120	−2.4540	5.1856
3.4	0.7150	0.1998	−2.4780	5.9222
3.6	0.5676	0.1849	−2.4884	6.6598
3.8	0.4047	0.1688	−2.4860	7.3820
4.0	0.2302	0.1526	−2.4717	8.0729
4.4	−0.1360	0.1231	−2.4108	9.3016
4.8	−0.4947	0.1001	−2.3133	10.2418
5.2	−0.8099	0.0844	−2.1867	10.8126
5.6	−1.0494	0.0743	−2.0386	10.9603
6.0	−1.1885	0.0677	−1.8758	10.6578
6.4	−1.2124	0.0624	−1.7046	9.9047
6.8	−1.1179	0.0567	−1.5303	8.7254
7.2	−0.9139	0.0496	−1.3570	7.1665
7.6	−0.6204	0.0405	−1.1885	5.2936
8.0	−0.2664	0.0295	−1.0272	3.1881
8.8	0.4785	0.0032	−0.7341	− 1.3443
9.6	1.0291	−0.0247	−0.4881	− 5.6364
10.4	1.1695	−0.0487	−0.2952	− 8.9325
11.2	0.8454	−0.0642	−0.1575	−10.6514
12.0	0.1857	−0.0684	−0.0724	−10.4899
12.8	−0.5481	−0.0605	−0.0318	− 8.4764
13.6	−1.0652	−0.0419	−0.0227	− 4.9665
14.4	−1.1609	−0.0159	−0.0292	− 0.5799
15.2	−0.7972	0.0129	−0.0365	3.9092
16.0	−0.1180	0.0395	−0.0344	7.7081
17.6	1.0936	0.0682	0.0038	10.7935
19.2	0.7450	0.0509	0.0422	6.5932
20.8	−0.6665	−0.0007	0.0263	− 2.0575
22.4	−1.1271	−0.0519	−0.0235	− 9.3195
24.0	0.0204	−0.0680	−0.0379	−10.2908
25.6	1.1389	−0.0382	0.0025	− 4.3157
27.2	0.6326	0.0174	0.0396	4.5725
28.8	−0.7763	0.0612	0.0203	10.3744
30.4	−1.0777	0.0638	−0.0280	9.1734
32.0	0.1585	0.0233	−0.0363	1.7803

TABLE III. Elements of the reactance matrix K_{ij}^{P} in the CSA as functions of the energy. The off-diagonal elements are given as they were determined numerically from the asymptotic forms of the solutions. The asymmetry indicates the degree of accuracy of the calculation.

k	K_{11}^{P}	K_{12}^{P}	K_{21}^{P}	K_{22}^{P}
0.725	−0.310	−0.002	−0.002	− 0.750
0.750	−0.322	−0.006	−0.005	− 1.485
0.775	−0.335	−0.014	−0.013	− 2.643
0.800	−0.346	−0.036	−0.035	− 5.475
0.825	−0.360	−0.270	−0.266	−32.434
0.835	−0.359	+0.402	+0.397	+44.314
0.850	−0.367	+0.106	+0.104	+10.290

gion. The anomalous behavior of $P_2\Psi_2^P$ in the first set, for example, indicates that it is not clear whether local effective potentials one often introduces to fit the elastic cross sections can also accurately reproduce $P\Psi^P$. It will be interesting also to clarify the role of the elastic wave functions in the T_{21} amplitude in DWBA.

C. Scattering Amplitudes and Cross Sections.

Two independent sets of solutions $P\Psi^P$ obtained with different initial conditions a give b_i^P's, which are diagonalized using (2.46) to obtain K_{ij}^P. Since K_{12}^P and K_{21}^P can be obtained independently, the procedure gives an excellent check on the numerical accuracy involved and also on any possible asymmetric errors. We give in Table III the values of K_{ij}^P without arbitrary symmetrization. The off-diagonal elements are small and their accuracy poor, especially for k near the threshold. As will be seen in paper II, this situation will change drastically as we include the effect of the Q space, so that the inaccuracy of K_{ij}^P at this point is not so serious.

Diagonalization of the K^P matrix gives the eigenphase shifts δ_i^P and the coupling parameter ϵ^P from (2.50) and (2.51). These are reported in Table IV. Using (2.54) and (2.55), corresponding amplitudes and cross sections are evaluated and given in Tables V and VI. Owing to δ_2^P going through $-\frac{1}{2}\pi$ at $k\approx 0.830$, σ_{22}^P nearly saturates the unitarity limit of $4\pi/p^2$ at that point. Contrary to what one may expect, a near saturation of this limit does *not* reflect the accuracy of the calculation, as we arbitrarily symmetrized the input K^P matrix. Rather, it simply shows that the unitarization of the amplitudes with (2.45) is done correctly for a Hermitian K^P. If we used the asymmetric K^P in the evaluation of σ_{22}^P, the limit may have been violated.

The variation of K^P around the value $k=0.830$ is violent, and K_{22}^P goes through infinities. However, the eigenphase shifts δ_i^P and T_{22}^P, as well as σ_{22}^P, are all very smooth in this region. Also, by examining the behavior of the wave functions, we have concluded that the point $k\approx 0.830$ does not show a compound resonance with the phase increasing rapidly by π, but merely an antiresonance with δ_2^P slowly decreasing past $-\frac{1}{2}\pi$, in accordance with the Wigner's theorem.[30]

TABLE IV. Eigenphase shifts and coupling parameter in the CSA. The symmetrized K_{ij}^P are used in the diagonalization.

k	δ_1^P	δ_2^P	ϵ^P
0.725	−0.301	−0.643	0.004
0.750	−0.312	−0.978	0.005
0.775	−0.324	−1.209	0.006
0.800	−0.333	−1.390	0.007
0.825	−0.344	−1.540	0.008
0.835	−0.347	−1.593	0.009
0.850	−0.353	−1.668	0.010

V. DISCUSSION

The solutions of (3.5) in the CSA provide the starting point for a more complete treatment of the reactions (1.1) by the GVB method. The result reported here agrees well with that obtained earlier by Bransden and Jundi,[14] with some improvements in accuracy. Although (3.5) is the simplest approximation possible for this complicated problem, K^P and $P\Psi^P$ obtained here are probably the first rigorous treatment by the GVB of the three-particle rearrangement collisions, with the full effect of nonlocality and energy dependence taken into account.

The calculation reported above falls short of a complete solution, obviously because we have neglected the effect of the Q space. Physically rich dynamics is contained in that part and the GVB would allow a consistent treatment of this distor-

TABLE V. Scattering amplitudes in the CSA for all four processes of the two-channel system. By construction, they are properly unitarized.

k	T_{11}^{P}	T_{21}^{P}	T_{12}^{P}	T_{22}^{P}
0.725	−0.390 $+i0.121$	−0.001 $+i0.001$	−0.003 $-i0.005$	−2.120 $+i1.590$
0.750	−0.380 $+i0.126$	−0.001 $+i0.004$	−0.002 $-i0.008$	−1.310 $+i1.946$
0.775	−0.389 $+i0.130$	−0.000 $+i0.006$	−0.000 $-i0.010$	−0.738 $+i1.950$
0.800	−0.386 $+i0.133$	+0.001 $+i0.007$	+0.002 $-i0.011$	−0.334 $+i1.829$
0.825	−0.385 $+i0.138$	0.003 $+i0.009$	0.004 $-i0.012$	−0.051 $+i1.662$
0.835	−0.383 $+i0.139$	0.004 $+i0.009$	0.005 $-i0.013$	+0.036 $+i1.591$
0.850	−0.381 $+i0.141$	0.005 $+i0.010$	0.006 $-i0.013$	0.144 $+i1.485$

TABLE VI. Scattering cross sections in the CSA at various E(or k) for the zero total angular momentum. The unitarity limits for the elastic scatterings are also given.

k	σ_{11}^P	σ_{21}^P	σ_{12}^P	σ_{22}^P	σ_{11}^U	σ_{22}^U
0.725	2.096	0.0000	0.0004	88.24	23.91	245.20
0.750	2.103	0.0002	0.0008	69.17	22.34	100.53
0.775	2.115	0.0004	0.0012	54.62	20.92	62.44
0.800	2.093	0.0007	0.0017	43.43	19.64	44.88
0.825	2.097	0.0011	0.0021	34.75	18.46	34.79
0.835	2.090	0.0013	0.0023	31.84	18.02	31.86
0.850	2.077	0.0016	0.0026	27.97	17.39	28.24

tion effect in a variational way, with the bound property (2.38). A variational estimate of the resonance energies which lie below the first excitation threshold of hydrogen may be made at the same time. From the earlier study made by Bransden and Jundi using phenomenological polarization potentials, we expect that the effect of the Q space will be very large, especially on the elastic cross sections σ_{11} and σ_{22}. This problem will be reported on in detail in paper II of this series, again for the zero total partial wave.

In addition to the Q-space effect, some further work is required to calculate the contributions from the higher partial waves. Few lower partial waves are known to contribute significantly to total cross sections.[14] This extension is in progress, again using GVB. It would also be of interest to solve the reactions (1.1) in the Faddeev formalism, and a convenient theory has been given[22] in the form of the reduced matrix equations with effective interactions Y_i. Here, the solutions in the direct-channel distortion approximation with local potentials Y_i are being obtained and compared with the solutions of the GVB approach.

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APPENDIX: COUPLED-STATIC EQUATIONS

The coupling terms in (3.1) and (3.2) are rather involved to evaluate because of the particle rearrangement. If we define

$$h_{r_1} = -\tfrac{1}{2}\nabla_{\vec{r}_1}^2 - 1/r_1 , \quad h_s = -\nabla_{\vec{s}}^2 - 1/s , \tag{A1}$$

and drop the common factor $2^{1/2}e^{-r_1}$, then $P_1 (H-E) P_2 \Psi_2^P$ becomes

$$J_1 = \int_0^\infty r_1^2 dr_1 \int_1^{-1} d(\cos\theta)\, \psi_0(r_1) \times \left(-\tfrac{1}{4}\nabla_{\vec{R}}^2 + V_2 + h_s - E\right) \varphi_0(s) F_2^P(R)/R \tag{A2}$$

Using the coordinate transformation

$$r_1^2 dr_1\, d(\cos\theta) = 8R^2 dR\, d(\cos\gamma) , \tag{A3}$$

with r_2 fixed, we obtain by partial integration

$$\begin{aligned} J_1 &= 8\int_0^\infty R^2 dR \int_{-1}^{1} d(\cos\gamma)\, \psi_0(r_1)\, \varphi_0(s) \\ &\quad \times \left(-\tfrac{1}{4}\nabla_{\vec{R}}^2 + V_2 + E_0^{(2)} - E\right) F_2^P(R)/R \\ &= 8\int_0^\infty R^2 dR \int_{-1}^{1} d(\cos\gamma)\, F_2^P(R)\, R^{-1} \\ &\quad \times \left(-\tfrac{1}{4}\nabla_{\vec{R}}^2 + V_2 + E_0^{(2)} - E\right) \psi_0(r_1)\, \varphi_0(s) \\ &\equiv \tfrac{1}{2}\int_0^\infty R\, dR\, F_2^P(R)\, K_{12}(r_2, R) , \end{aligned} \tag{A4}$$

where

$$K_{12}(r_2, R) = 16\int_{-1}^{1} d(\cos\gamma) \left(-\tfrac{1}{4}\nabla_{\vec{R}}^2 + V_2 + E_0^{(2)} - E\right) \times \psi_0(r_1)\, \varphi_0(s) . \tag{A5}$$

Now, the $\nabla_{\vec{R}}^2$ term can be written as

$$\begin{aligned} &\nabla_{\vec{R}}^2 [\psi_0(|2\vec{R} - \vec{r}_2|)\, \varphi_0(|2\vec{R} - 2\vec{r}_2|)] \\ &\quad = 4\psi_0(r_1)\, \nabla_{\vec{s}}^2 \varphi_0(s) + 4\varphi_0(s)\, \nabla_{\vec{r}_1}^2 \psi_0(r_1) \\ &\quad + 8\, \nabla_{\vec{r}_1} \psi_0(r_1) \cdot \nabla_{\vec{s}} \varphi_0(s) , \end{aligned} \tag{A6}$$

so that (A5) reduces to (3.7) when explicit forms for $\psi_0(r_1)$ and $\varphi_0(s)$ are used. For the coupling term in (3.2), we again drop the common factor $\tfrac{1}{2}\exp(\tfrac{1}{2}s)$ and obtain for $P_2(H-E)P_1\Psi_1^P$,

$$J_2 = \int_0^\infty s^2 ds \int_{-1}^{1} d(\cos\omega)\, \varphi_0(s)$$

$$\times \left(-\tfrac{1}{2}\nabla^2_{\vec{r}_2} + h_{r_1} + V_1 - E\right)\psi_0(r_1)\,F_1^P(r_2)/r_2 \ . \tag{A7}$$

Using the coordinate transformation

$$s^2 ds\, d(\cos\omega) = 8 r_2^2 dr_2 d(\cos\gamma) \ , \tag{A8}$$

with R fixed, we obtain by the partial integration

$$J_2 = 8\int_0^\infty r_2^2 dr_2 \int_{-1}^{1} d(\cos\gamma)\,\varphi_0(s)\,\psi_0(r_1)$$

$$\times \left(-\tfrac{1}{2}\nabla^2_{\vec{r}_2} + V_1 + E_0^{(1)} - E\right) F_1^P(r_2)/r_2$$

$$= 8\int_0^\infty r_2^2 dr_2 \int_{-1}^{1} d(\cos\gamma)\,F_1^P(r_2)\,r_2^{-1}$$

$$\times \left(-\tfrac{1}{2}\nabla^2_{\vec{r}_2} + E_0^{(1)} + V_1 - E\right)\psi_0(r_1)\,\varphi_0(s)$$

$$\equiv \tfrac{1}{2}\int_0^\infty r_2 dr_2 F_1^P(r_2)\,K_{21}(R, r_2) \ . \tag{A9}$$

where

$$K_{21}(R, r_2) = 16\int_{-1}^{1} d(\cos\gamma)\left(-\tfrac{1}{2}\nabla^2_{\vec{r}_2} + V_1 + E_0^{(1)} - E\right)$$

$$\times\, \psi_0(r_1)\,\varphi_0(s) \ . \tag{A10}$$

The $\nabla^2_{\vec{r}_2}$ term in (A10) may be written as

$$\nabla^2_{\vec{r}_2}\left[\psi_0(|2\vec{R} - \vec{r}_2|)\,\varphi_0(|2\vec{R} - 2\vec{r}_2|)\right]$$

$$= 4\psi_0(r_1)\,\nabla^2_{\vec{s}}\,\varphi_0(s) + \varphi_0(s)\,\nabla^2_{\vec{r}_1}\,\psi_0(r_1)$$

$$+ 4\,\nabla_{\vec{r}_1}\psi_0(r_1)\cdot\nabla_{\vec{s}}\,\varphi_0(s) \ , \tag{A11}$$

which again gives the exactly same forms (3. 7) and (A5). Thus, we have

$$K_{21}(R, r_2) = K_{12}(r_2, R) \equiv K(r_2, R) \ .$$

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