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Generalized Variational Bounds on the Positron-Hydrogen Reaction Matrix. II. Effective Distortions

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The problem of the two-channel positron-hydrogen rearrangement collision is studied with the formalism of the generalized variational bounds. For the zero total partial wave, a reasonably complete treatment of this scattering system is presented, including a detailed discussion of the energy spectrum of the closed-channel Hamiltonian M. The coupling of the open channels to the closed channels gives rise to the effective interaction potentials, and these distortion terms are estimated variationally using the bound property of M. The orthogonality of M to the open-channel space is maintained by the presence of the energy-shift operator S, and the role of S is demonstrated in detail numerically, which produces essential cancellation of various terms. Partly owing to the crudity of the trial functions used, we have not been able to find resonance states below the first excitation threshold. Bounds on the diagonal K matrix elements and eigenphase shifts are presented.

I. INTRODUCTION

This is the second part of a series of studies on the positron-hydrogen rearrangement collision. We have reported in I [1] the result of a calculation in the coupled-static approximation (CSA) in which the effect of distortions due to the coupling of the open channels to other closed channels is completely neglected. A rigorous treatment of this scattering system using the formalism of the generalized variational bounds[2] (GVB) requires the exact solution in the CSA, and we complete the program here by incorporating the effect of distortions to the result of I. It is well known[3] that the e^+H scattering system demands a careful treatment of the distortion effect before a meaningful result can be obtained. This system, which is probably the simplest three-particle scattering problem where the rearrangement process is possible, has been a very fertile ground for the development of theoretical methods even for the single-channel case, and, as will be seen below, this is certainly the case when two channels are open.

We are interested in the zero total partial-wave scattering of the form

$$e^+ + (e^- + p^+) \rightleftharpoons (e^+ + e^-) + p^+ \qquad (1.1)$$

with the scattering energies E in the range $E_L \leq E < E_U$, where $E_L = -0.250$ a.u. and $E_U = -0.125$ a.u. As discussed in I, the closed-channel projection operator Q is not readily available for (1.1), and thus the Q-space effect cannot easily be incorporated into the theory. The GVB formalism circumvents this difficulty and also allows one to evaluate directly the resonance energies variationally. Instead of the closed-channel Hamiltonian QHQ, we use the operator M which implicitly contains the effect of Q. Various orthogonality properties of the operator M and the function N are maintained through remarkable cancellations built into the theory, and this peculiarity of the GVB is demonstrated in the following.

The formalism of the GVB provides, in general, bounds on the diagonal elements of the K matrix and also on the eigenphase shifts. However, such bounds are only valid if the lowest value of the spectrum E_1^Q of M is above E. If any number of E_n^Q lie below E, then one has to improve the trial functions sufficiently to account for these states. Therefore, it is essential for the GVB to first estimate the approximate location of these states, which may give rise to resonances when coupled with the open-channel space.

We briefly summarize in Sec. II the formalisms which are needed for the present part of the calculation, with fuller discussion of several points of interest than was given in I. The evaluation of the Green's function G^P in the CSA is replaced by the calculation of the auxiliary function Y_{im}, and this is given in Sec. III. Sections IV and V give results of the calculation of the spectrum of M and evaluation of amplitudes using the functions Y_{im}.

II. EFFECTIVE POTENTIALS AND GVB

We have already given a general discussion of the GVB for the e^+H system in I and thus will collect here only those results which are relevant to the Q-space calculation, modified in the way used here, and also make several additional remarks on the orthogonality property of M and N.

The P part of the problem in the CSA, as reported in I, requires the exact numerical solution of the equations

$$P_i (H - E)\Psi^P = 0, \qquad (2.1)$$

which completely neglects the Q-space effect. On

the other hand, the original scattering problem can be written in terms of the effective potentials W as

$$P_t[H-E+W]P\Psi=0, \tag{2.2}$$

with

$$W=(H-E)G^Q(H-E), \quad G^Q=[Q(E-H)Q]^{-1}, \tag{2.3}$$

$$P\Psi\equiv P_1\Psi_1+P_2\Psi_2 .$$

Equation (2.2) can be modified to assume the form

$$P_t(H-E)P\Psi=P_t(H-E)M^{-1}N , \tag{2.4}$$

where M and N are given, as before, as

$$M=H-E+S(E), \quad S=(H-E)G^P(H-E) \tag{2.5}$$

and

$$N=(H-E)P\Psi^P, \quad P\Psi^P=P_1\Psi_1^P+P_2\Psi_2^P . \tag{2.6}$$

In (2.5), $G^P(E)$ satisfies the equations

$$P_t(H-E)G_t^P=-P_t . \tag{2.7}$$

The amplitudes are defined as

$$\lambda=\lambda^P+\Delta , \tag{2.8}$$

with

$$\lambda=-\vec{a}\circ\vec{K}\vec{a} , \quad \Delta=-(N,M^{-1}N)\equiv(N,\mathcal{G}^QN) , \tag{2.9}$$

where the factor 2π in λ disappeared because of the particular integration used in Δ. For the scattering energy E chosen below the lowest spectrum of M, we have

$$M>0, \tag{2.10}$$

and thus

$$\mathcal{G}^Q\leq\mathcal{G}_t^Q=-\sum_{m,n}\chi_m[(M)_t^{-1}]_{mn}\chi_n\leq 0 . \tag{2.11}$$

The inequality (2.10) is a result of the orthogonality property

$$M=QM=MQ, \quad PM=MP=0, \tag{2.12}$$

while (2.9) follows from the property

$$PN=0, \quad QN=N. \tag{2.13}$$

The properties (2.12), (2.13), and (2.10) have already been discussed in I. The GVB is then given by

$$\Delta\leq\Delta_t=(N,\ G_t^QN), \tag{2.14}$$

which does not require P or Q.

By definition of the Q space, and because of (2.12) and (2.13), the operator M has its continuum spectrum starting at the energy corresponding to the first excitation threshold $E_U=-0.125$ a.u. and may also possess a number of discrete spectra below this threshold. Now, if E is equal to any one of these discrete energies, then Δ becomes infinite and we usually have a resonance in the open channels. To study the discrete spectrum more explicitly, we may diagonalize the matrix M_{kl} defined by

$$M_{kl}=(\chi_k,M\chi_l) . \tag{2.15}$$

Here, the correct normalization of χ_l is not known, but, as will be discussed in Sec. IV, the resonance energies are independent of the normalization. The coordinates used and the energy integrals involved in (2.15) are given in Appendices A and B, respectively. Thus, we have

$$AMA^{-1}=E_D, \tag{2.16}$$

where E_D is the diagonal matrix with elements E_{nt}, and A is the orthogonal matrix composed of eigenfunctions

$$X_n=\sum_m A_{nm}^T\chi_m . \tag{2.17}$$

The correct "resonance" energies are then given by I (2.42),

$$E_{nt}^Q(E)=E_{nt}+E=E, \tag{2.18}$$

if E_{nt}^Q lie below E_U. In this diagonalization procedure, it is essential that we keep the same E throughout M until the last step (2.18); otherwise the orthogonality property (2.12) will be lost and we will have nonsensical results. The shift operator S, defined by (2.5), would of course be exact only when E in it is replaced by a particular E_{nt}^Q. However, in general the E dependence of S is not so drastic and one has reasonable values of E_{nt}^Q without finer adjustment, although this can be done easily. (This is not the case in the present problem, as will be seen in Sec. IV.)

Once the M_{kl} matrix is diagonalized, we can immediately write $\mathcal{G}_t^Q$ in the form I (2.43),

$$\mathcal{G}_t^Q=\sum_n|X_n)(E-E_{nt}^Q)^{-1}(X_n| , \tag{2.19}$$

and thus

$$\Delta_t=\sum_n\ (N,X_n)(E-E_{nt}^Q)^{-1}(X_n,N) . \tag{2.20}$$

In (2.14) with (2.20), it is assumed that $E_n^Q>E$ for all n. However, if there are a finite number N of E_n^Q which lie below given E, then (2.14) is not valid in general and (2.20) requires N subtractions.[4,5] This requirement may be met automatically if the trial functions X_n are good enough so that

$$E>E_{nt}^Q(E)>E_n^Q(E) \tag{2.21}$$

for *all* $n=1,\ldots,N$, where the last inequality in (2.21) follows from the Hylleraas-Undheim theorem.[6] With this additional constraint, (2.14) may be still valid. This can also be seen physically since

$$E_n^Q\leq E_{nt}^Q<E, \quad n=1,2,\ldots,N$$

$$E^Q_{nt} > E^Q_n > E, \quad n > N \tag{2.22}$$

gives

$$(E - E^Q_n)^{-1} \leq (E - E^Q_{nt})^{-1} \tag{2.23}$$

for all $n = 1, \ldots, N, \ldots$, irrespective of the signs of each term. Therefore, in order to make a definite statement of the bound property of Δ_t, it is necessary to know in advance the locations and the number of resonance levels which lie below E. In this respect, the availability of the operator M in the Q space is very important, so that one can judge whether (2.14) is valid or not.

Now, the evaluation of M_{mn} is rather involved for the present problem mainly owing to the presence of $S(E)$. However, for the purpose of evaluating only M_{mn}, we do not need G^P in its full generality but only as combined with $(H-E)\chi_n$. Therefore, if we solve instead[7]

$$P_i(H-E)(P_1 Y_{1n} + P_2 Y_{2n}) = -P_i(H-E)\chi_n \tag{2.24}$$

for each χ_n, then

$$(\chi_m, M\chi_n) \equiv H_{mn} - E_{mn} + S_{mn}, \tag{2.25}$$

where

$$S_{mn} = (\chi_m, [H-E][P_1 Y_{1n} + P_2 Y_{2n}]). \tag{2.26}$$

[We use $Y_{1n}(r_2)$ and $P_1 Y_{1n}(r_2, r_1) = \psi_0(r_1) Y_{1n}(r_2)$ interchangeably in the following.] PY_n satisfies the same boundary conditions as G^P, and (2.24) is very much like (2.1) for Ψ^P and the same technique as explained in I may be used to obtain PY_n. It is also obvious that PY_n are independent of choice of the initial boundary conditions a^{I} and a^{II}. Explicitly, we have, for $i \neq j$,

$$P_i(H-E)P_i Y_{in} + P_i(H-E)P_j Y_{jn} = -dP_i(H-E)\chi_n, \tag{2.27}$$

where d is an arbitrary constant. Since χ_n contains a large amount of the P component in general, the right-hand side can be abnormally large and disturb the convergence of the iteration series. A constant d can be included to improve the convergence and its effect divided out at the end (Sec. III).

From (2.25) it is clear that, for M to have the energy spectrum we have stated above, there should be subtle cancellations between H_{mn} and S_{mn}, since the full Hamiltonian H has the continuum starting at -0.50, and thus H_{mn} alone will dip down near this value. Details of this cancellation and the indication of the boundedness of M will be discussed in Sec. IV.

Similar cancellation should also appear in the matrix elements (X_n, N) in (2.20). If we write

$$N_n = (X_n, N) = N_{1n} + N_{2n}, \tag{2.28}$$

where

$$N_{in} = (X_n, [H-E]P_i \Psi^P_i), \tag{2.29}$$

then N_{1n} or N_{2n} alone may be large since X_n is not preorthogonalized to P, but the sum of the two should cancel in such a way that any part of X_n in the P space should disappear in N_n. This cancellation, combined with the one in M_{mn}, results in the bound (2.14). We will come back to this point more fully in Sec. V.

The cancellation as in (2.25) and (2.28) can also be seen in the complete wave function Ψ_t. If we define the function for a given χ_t,

$$P\tilde{\Psi}_t = P\Psi^P + G^P(H-E)\chi_t, \tag{2.30}$$

then the solution of the equation $P(H-E)\Psi_t = 0$ may be written in the form

$$\Psi_t = P\tilde{\Psi}_t + \chi_t = P\Psi^P + G^P(H-E)\chi_t + \chi_t. \tag{2.31}$$

If we let

$$\chi_t = P\chi_t + Q\chi_t, \tag{2.32}$$

then

$$\begin{aligned}\Psi_t &= [P\Psi^P + G^P(H-E)(P\chi_t + Q\chi_t)] + (P\chi_t + Q\chi_t) \\ &= [P\Psi^P - P\chi_t + G^P(H-E)Q\chi_t] + P\chi_t + Q\chi_t.\end{aligned} \tag{2.33}$$

Thus, $-P\chi_t$ in the square bracket cancels the $P\chi_t$ component of χ_t, giving

$$\Psi_t = P\Psi^P + G^P(H-E)Q\chi_t + Q\chi_t, \tag{2.34}$$

which is the correct form, and we could have used it if P and Q were explicitly known. Of course, throughout the calculation, we never see $Q\chi_t$ and we are not able to decompose χ_t as (2.32), but the use of M and N in (2.14) will do the same automatically.

For the calculation of Δ_t, one can do better by not using (2.20) as it is given, which requires the calculation of Y_n for each χ_n. One can first diagonalize the matrix[8]

$$D_{mn} = H_{mn} - E_{mn} \tag{2.35}$$

without S_{mn} of (2.25). This will give an approximation to W in the form

$$W \approx W_t = \sum_n (H-E)\,|\,\xi_n)(-\epsilon_n)^{-1}(\xi_n\,|\,(H-E), \tag{2.36}$$

where ϵ_n and ξ are the eigenvalues and eigenvectors of D_{mn}. With this in (2.2), we have to solve for $P\Psi_t$ just once. This will considerably improve the accuracy of the calculation, but the information on the resonance energies is then lost and we will not be able to make a definite statement on the bound property. Furthermore, D_{mn} has spurious zeros due to the continuum spectrum of H, although these singularities should cancel at the end and thus not affect the final result.

Finally, we should point out one important exception to the discussion on the resonance energies

given above, with the result (2.18). This has to do with the particular normalization of the wave functions $P\Psi^P$ and $P\Psi$ and the peculiarity of the trigonometric functions $\tan\delta_i$ involved in K_{ij}. The particular normalization of the wave function chosen in the present study, as given by I (2.14), corresponds to $\theta = \frac{1}{2}(2n+1)\pi$ of Ref. 5 for n an integer. Therefore, whenever the situation arises in which $\delta_i^P < \theta < \delta_i$ with the above θ, we expect to have one spurious state of M below E. This state has nothing to do with the true physical resonances, but nevertheless would affect the bound property of K_{iit} and δ_{it}. This indeed is the case with K_{22} and δ_2, as shown in Sec. IV.

III. ENERGY SHIFT OPERATOR $S(E)$

The function PY_n needed in M_{mn} is given by

$$PY_n \equiv P_1 Y_{1n} + P_2 Y_{2n} \tag{3.1}$$

and satisfies the coupled equations (2.27), with $d = 1$. An exactly identical form without the χ_n term was solved in I to obtain Ψ^P, and we have used the identical procedure for PY_n. Equation (2.27) again involves the complicated coupling kernel $P_i(H-E)P_j \to K_{12}(r_2, R)$, and thus the limit of accuracy of PY_n is placed by that of K_{12}. Eventually E_{nt}^Q and the amplitudes will be affected by the same limitation.

The trial functions χ_n are chosen to be of the form

$$\chi_n = C_n e^{-\alpha_n r_1 - \beta_n s}, \tag{3.2}$$

where $C_n = (2\alpha_n\beta_n)^{-3/2}$, and r_1 and s are the coordinates of the electron from the proton and the positron, respectively. This form is especially convenient not only because it contains all l contributions for the total angular momentum $L = 0$, but most of the integrations can also be done easily. We switch back and forth between different sets of variables (r_1, r_2, s), (s, R, r_1), (s, R, r_2), and $(r_1, R, \frac{1}{2}s)$, etc., as listed in Appendix A. The explicit form of equations for Y_{in} is given in Appendix C. The inhomogeneous terms

$$\Gamma_{in} = P_i(H-E)\chi_n \tag{3.3}$$

are given in Table I for a typical choice of $\alpha_n = 0.6$ and $\beta_n = 0.4$ for $k = 0.8a_0^{-1}$, and $P_i Y_{in}$ for this χ_n are also given there. $P_i Y_{in}$ satisfy the same asymptotic boundary conditions as G^P, and thus it is clear that they are independent of the initial conditions a^{I} and a^{II}. This is borne out by the calculation. They are first calculated by solving (2.27) with the usual boundary conditions

$$\begin{aligned} P_1 \bar{Y}_{1n}^{\mathrm{I}} &\to (a_1^{\mathrm{I}} \sin kr_2 + b_1^{\mathrm{I}} \cos kr_2)\psi_0(r_1)/r_2, \\ P_2 \bar{Y}_{2n}^{\mathrm{I}} &\to (a_2^{\mathrm{I}} \sin pR + b_2^{\mathrm{I}} \cos pR)\varphi(S)/R, \end{aligned} \tag{3.4}$$

and similarly for the second set a^{II}. By linear combinations with coefficients $(C_1^{\mathrm{I}}, C_2^{\mathrm{I}})$ and $(C_1^{\mathrm{II}}, C_2^{\mathrm{II}})$, we obtain the sets $P\bar{Y}_n^{\mathrm{I}}$ and $P\bar{Y}_n^{\mathrm{II}}$, with

TABLE I. Values of $\Gamma_{1n}(r_2)$, $\Gamma_{2n}(R)$ and $Y_{1n}(r_2)$, $Y_{2n}(R)$ at $k = 0.8a_0^{-1}$ for the parameters $\alpha_n = 0.6a_0^{-1}$ and $\beta_n = 0.4a_0^{-1}$.

r	Γ_1	Γ_2	Y_1	Y_2
0.20	0.18770	0.01378	−0.00564	−0.04261
0.40	0.14206	0.01416	−0.00911	−0.08322
0.60	0.09947	0.00627	−0.01110	−0.12111
0.80	0.06190	−0.00795	−0.01237	−0.15655
1.00	0.02849	−0.02373	−0.01357	−0.19065
1.20	0.00020	−0.03806	−0.01521	−0.22492
1.40	−0.02424	−0.05077	−0.01758	−0.26087
1.60	−0.04440	−0.05985	−0.02086	−0.29988
1.80	−0.06140	−0.06688	−0.02504	−0.34295
2.00	−0.07510	−0.07072	−0.03004	−0.39071
2.20	−0.08634	−0.07301	−0.03566	−0.44339
2.40	−0.09513	−0.07316	−0.04167	−0.50091
2.60	−0.10206	−0.07240	−0.04781	−0.56279
2.80	−0.10719	−0.07039	−0.05381	−0.62831
3.00	−0.11094	−0.06793	−0.05939	−0.69665
3.20	−0.11338	−0.06484	−0.06431	−0.76675
3.40	−0.11481	−0.06160	−0.06832	−0.83750
3.60	−0.11531	−0.05812	−0.07125	−0.90773
3.80	−0.11507	−0.05466	−0.07294	−0.97618
4.00	−0.11416	−0.05116	−0.07326	−1.04168
4.40	−0.11085	−0.04447	−0.06959	−1.15920
4.80	−0.10606	−0.03830	−0.06034	−1.25144
5.20	−0.10030	−0.03276	−0.04617	−1.31097
5.60	−0.09395	−0.02785	−0.02854	−1.33193
6.00	−0.08732	−0.02357	−0.00926	−1.31062
6.40	−0.08062	−0.01986	0.00956	−1.24538
6.80	−0.07402	−0.01668	0.02575	−1.13691
7.20	−0.06762	−0.01396	0.03746	−0.98806
7.60	−0.06150	−0.01165	0.04313	−0.80385
8.00	−0.05572	−0.00970	0.04191	−0.59105
8.80	−0.04530	−0.00668	0.01892	−0.11391
9.60	−0.03642	−0.00456	−0.02428	0.36660
10.40	−0.02901	−0.00308	−0.07169	0.77089
11.20	−0.02293	−0.00207	−0.10485	1.03129
12.00	−0.01801	−0.00139	−0.11023	1.10436
12.80	−0.01407	−0.00092	−0.08479	0.97890
13.60	−0.01093	−0.00061	−0.03730	0.67827
14.40	−0.00846	−0.00040	0.01489	0.25634
15.20	−0.00652	−0.00027	0.05261	−0.21188
16.00	−0.00501	−0.00017	0.06237	−0.64338
17.60	−0.00293	−0.00007	−0.00033	−1.11069
19.20	−0.00170	−0.00003	−0.07615	−0.82903
20.80	−0.00098	−0.00001	−0.05158	0.01191
22.40	−0.00056	−0.00001	0.04175	0.84467
24.00	−0.00032	−0.00000	0.07276	1.10723
25.60	−0.00018	−0.00000	−0.00158	0.62238
27.20	−0.00010	−0.00000	−0.07453	−0.28259
28.80	−0.00006	−0.00000	−0.04162	−0.99683
30.40	−0.00003	−0.00000	0.05041	−1.03822
32.00	−0.00002	−0.00000	0.07038	−0.37878

$$a^{\mathrm{I}} = \begin{pmatrix} 1 \\ 0 \end{pmatrix} \quad \text{and} \quad a^{\mathrm{II}} = \begin{pmatrix} 0 \\ 1 \end{pmatrix}. \tag{3.5}$$

The desired functions are then given by

$$P_i Y_{in} = (P_i \bar{Y}_{in}^{\mathrm{I}} - P_i \Psi_i^{P\mathrm{I}})/[d(C_1^{\mathrm{I}} + C_2^{\mathrm{I}})], \tag{3.6}$$

and similarly with the second set on the right-hand

side of (3.6). Two sets give identical $P_t Y_{tn}$ to better than one part in 10^4 at their maxima. While the coupling kernel $K_{12}(r_2, R)$ decays rapidly to be negligible beyond $32a_0$, Γ_{tn} with α or β small have long tails and we limited our calculation to a cutoff at $80a_0$, and $\alpha, \beta \geq 0.2a_0^{-1}$.

Since the rest of the calculation depends on the goodness of $P_t Y_{tn}$, much effort has gone into a proper evaluation of this function. Any further improvements of the present calculation require better evaluation of $K_{12}(r_2, R)$ and Y_{tn}.

The total wave function $P\Psi_t$ may now be expressed in terms of PY_n as follows: Since $P\Psi_t$ satisfies the equations

$$P(H-E)P\Psi_t + \sum_{nm} \Gamma_n [(E-H)_t^{-1}]_{nm} (\Gamma_m, P\Psi_t) = 0, \tag{3.7}$$

we have immediately

$$P\Psi_t = P\Psi^P + \sum_n C_n PY_n, \tag{3.8}$$

where

$$C_n = -\sum_m [(M)_t^{-1}]_{nm} (\Gamma_m, P\Psi^P), \tag{3.9}$$

$$M_{lk} = (\chi_l, [H-E]\chi_k) + (\Gamma_l, PY_k). \tag{3.10}$$

The solutions (3.8) are given formally, but can easily be written out in detail in terms of the P_1 and P_2 components of the various quantities. We could have solved (3.7) once for each E and predetermined Γ_n, but we are equally interested in the eigenvalues of M_{lk} in (3.10), and thus (3.7) was not used in our calculation.

IV. SPECTRUM OF OPERATOR M

Evaluation of M_{mn} and its diagonalization is now a simple matter using $P_t Y_{tn}$ obtained in Sec. III. In order to examine the cancellation between H_{mn} and S_{mn}, we have listed the one-term values in Table II at $k = 0.85a_0^{-1}$, where

$$S_{nn}^{(t)} = (\chi_n, [H-E]P_t Y_{tn}) = (\Gamma_{tn}, P_t Y_{tn}). \tag{4.1}$$

Since we do not have the explicit Q operator in the calculation of M_{mn}, H_{nn}, for example, are to scatter over the energy range down to -0.5 a.u. In each case, however, S_{nn} have the correct signs and magnitudes to bring the sums $H_{nn} + S_{nn}$ up to the values near $E_U = -0.125$ a.u. Of course, by definition, E_{nt}^Q depends on the value of E chosen. For $E = -0.1388$ a.u., e.g. (or $k = 0.85$), we have the minimum

$$E_1^Q \lesssim E_{1t}^Q = -0.1473 \tag{4.2}$$

for $\alpha = 0.4$ and $\beta = 0.4$. This already shows two important results: (i) The operator M is most likely bounded from below with the continuum spectrum starting at $E \approx E_U$. (ii) There exists at least one state of M below E with the upper bound on E_1^Q given by (4.2). The result (ii) is rigorous so long as we are only interested in the spectrum of M. Its connection to resonance states will be clarified later. The point (i) is not a rigorous proof but the values in Table II certainly provide a strong indication.

We can improve on the values of E_{1t}^Q given in Table II by including more than one terms in M_{mn} and diagonalizing it. In general, $S_{mn}^{(t)}$ are not symmetric, i.e.,

$$S_{mn}^{(t)} \neq S_{nm}^{(t)}, \tag{4.3}$$

since we have no way of separating the Q_t part in χ_n. However, we expect that

$$S_{mn} = S_{nm} = S_{nm}^{(1)} + S_{nm}^{(2)}. \tag{4.4}$$

This is borne out by the calculation. Owing to insufficient accuracy in our calculation of $P_t Y_{tn}$, Γ_{tn}, and subsequent integrations, and more importantly, owing to a simple choice of the trial functions χ_n introduced in (3.2), we have encountered a severe cancellation problem in the diagonalization procedure, and, as a result, it has not been possible to include more than two terms with consistent results. Table III shows the energy values E_{nt}^Q using the best two-term sets at different values of E. The accuracies of E_{1t}^Q and E_{2t}^Q are roughly ± 0.005 and ± 0.01, respectively.

Various checks on the accuracy of E_{nt}^Q come from the symmetry (4.4), improvement of E_{1t}^Q as another function is added, and the change in K_{ttt}, as de-

TABLE II. Components of M_{mn} and E_{1t}^Q for various sets of parameters (α_n, β_n) $E = -0.1388$ a.u. $(k = 0.85a_0^{-1})$.

Set	(α, β)	H_{nn}	$S_{nn}^{(1)}$	$S_{nn}^{(2)}$	E_{1t}^Q
1	(0.4, 0.2)	−0.3170	0.2161	−0.0255	−0.1265
2	(0.4, 0.4)	−0.3100	0.2459	−0.0832	−0.1473
3	(0.4, 0.5)	−0.2929	0.2306	−0.0789	−0.1412
4	(0.4, 0.6)	−0.2624	0.2044	−0.0597	−0.1177
5	(0.4, 0.7)	−0.2166	0.1746	−0.0345	−0.0765
6	(0.6, 0.2)	−0.4019	0.3625	−0.0949	−0.1343
7	(0.6, 0.4)	−0.3624	0.4135	−0.1969	−0.1458
8	(0.9, 0.9)	−0.0225	0.2144	0.0366	0.2285

TABLE III. Most reliable values of E_{1t}^Q and E_{2t}^Q obtained by the two-term diagonalization of the energy matrix M_{nn}. The parameters for E_{1t}^Q are (0.2, 0.6) and (0.4, 0.4) for (α_n, β_n).

E (a.u.)	ka_0^{-1}	E_{1t}^Q	E_{2t}^Q
−0.2372	0.725	−0.222	−0.20
−0.2188	0.750	−0.204	−0.17
−0.1997	0.775	−0.185	−0.15
−0.1800	0.800	−0.167	−0.12
−0.1597	0.825	...	...
−0.1388	0.850	−0.148	−0.12

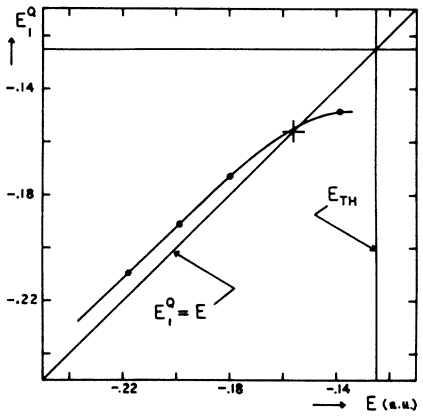

FIG. 1. Energy dependence of the energy $E_{1t}^Q(E)$ of the operator $M(E)$ at various E's. The point $E_{1t}^Q(E) = E$ should be above the exact value $E = -0.156$ a.u. according to the assumption that E_1^Q is a spurious state caused by the particular normalization used.

scribed in Sec. V. We have evaluated S_{mn} with Y_n and S_{nm} with Y_m; (4.3) is well satisfied to accuracy of a few parts in 10^4. The result with three-term diagonalizations, although unreliable in most cases, has provided further indications of the extent to which cancellations spoiled the diagonalization, and also the convergence of E_{nt}^Q as functions of the number of terms.

As we have stressed earlier, the eigenstates of $M(E)$ do not necessarily manifest themselves as resonances unless any one of E_n^Q equals E. We have also noted that the normalization of the wave function may sometimes give rise to one spurious state of M. Reserving this latter point for later discussion, we thus define the resonance state as the point spectrum of M with $E_n^Q = E$ in a self-consistent way. From the several values of E where E_{1t}^Q is estimated, we can interpolate to obtain $E_1^Q(E) = E$. This is shown in Fig. 1, with the result

$$E_1^Q \lesssim -0.153 \pm 0.005 \text{ a.u.}$$
or
$$E_1^Q \approx -0.160 \pm 0.010 \text{ a.u.}, \tag{4.5}$$

where the second value in (4.5) is an estimate of E_1^Q if an infinite number of terms were included in the diagonalization. The result with two- and three-term diagonalizations indicates also that there may be another state of M at higher energy, separated by approximately 0.03 a.u., but our calculation does not have enough accuracy to make a definite statement on E_2^Q. Further improvement of E_{nt}^Q by addition of more functions in M_{mn} would thus be most desirable. This requires first of all better evaluation of the static coupling kernel $K(r_2, R)$. The functions Γ_{in} are evaluated numerically and they have to be improved as well, giving a better set of Y_{in}. The cancellations in the diagonalization may be eased somewhat by a better choice of the trial functions, such as

$$\chi_n = C_n r_1 S\, e^{-\alpha_n r_1 - \beta_n S}. \tag{4.6}$$

The variation of $E_1^Q(E)$ as a function of E is the outstanding feature of this problem. The rapid E dependence seems to come from the fact that the second (e^+e^-) channel momentum $p = k_2$ changes rapidly in this region, while, as in the e^-H case,[9] $k = k_1$ varies rather slowly. The proximity of E_1^Q to the E line also makes it difficult to determine whether any E_n^Q may come down below E. Such a possibility is left open insofar as the present calculation is concerned, and definitely points to the desirability of obtaining a lower bound on E_n^Q.

We now come to the question of the spurious state. We recall that, in the CSA of I, the eigenphase shift δ_2^P of the second channel assumes the value $-\frac{1}{2}\pi$ at $k = 0.830$ giving $K_{22}^P = \infty$. This corresponds to $E = -0.156$ a.u., which is rather close to the estimate of E_1^Q given by (4.5). In fact, for δ_{2t} to increase from the value δ_2^P at all according to the bound statement, we expect that, for $E > -0.156$, K_{22t} will sooner or later assume the values $\pm\infty$. Taking into consideration the E dependence of δ_{2t} as obtained in Sec. V, we believe, therefore, that the lowest state of M, E_1^Q, observed in our calculation is not a resonance but the spurious state coming from the particular normalization chosen. Thus, we have $E_1^Q(E) = E \equiv -0.156$. Although we could have avoided this singularity from the beginning by choosing a different normalization, such as $\theta = \delta_2^P$, the fact that the estimate (4.5) is very close to the exact value gives a strong indication that the sets of trial functions used are reasonable and also that M is indeed bounded. The two-term functions contain essentially four nonlinear and two linear parameters which have been searched rather carefully, so that we feel the resulting K_{iit} are probably of comparable accuracy as E_{1t}^Q of (4.5).

V. BOUNDS ON K MATRIX AND SCATTERING AMPLITUDES

For the discussion in this section, we assume that the estimate on the position of E_1^Q given by (4.5) is correct. The change in its position would not alter the qualitative conclusions reached here. For $E < E_1^Q$, we then expect that

$$\lambda \leq \lambda^P, \quad E < E_1^Q, \tag{5.1}$$

$$\lambda \leq \lambda_t, \quad E < E_1^Q \tag{5.2}$$

for all possible forms of the trial functions. On the other hand, for E in the range $E_2^Q > E > E_1^Q$, we have

$$\lambda \not< \lambda^P, \quad E > E_1^Q, \tag{5.3}$$

but

$$\lambda \leq \lambda_t , \tag{5.4}$$

only for those cases in which $E_{1t}^Q < E$. A similar argument can be given when more than one state of M is below E.

Using the definitions of λ and λ_t as given by I (2.45) and I (2.38), we can rewrite (5.1) and (5.2) for the K-matrix elements as

$$\begin{aligned} K_{11} \geq K_{11t} &= K_{11}^P - 2\sum_n N_n^{\mathrm{I}}(E - E_{nt}^Q)^{-1}N_n^{\mathrm{I}} , \\ K_{22} \geq K_{22t} &= K_{22}^P - 2\sum_n N_n^{\mathrm{II}}(E - E_{nt}^Q)^{-1}N_n^{\mathrm{II}} \end{aligned} \tag{5.5}$$

and

$$\begin{aligned} K_{12} \approx K_{12t} &= K_{12}^P - 2\sum_n N_n^{\mathrm{I}}(E - E_{nt}^Q)^{-1}N_n^{\mathrm{II}} , \\ K_{21} \approx K_{21t} &= K_{21}^P - 2\sum_n N_n^{\mathrm{II}}(E - E_{nt}^Q)^{-1}N_n^{\mathrm{I}} . \end{aligned}$$

In (5.5) and (5.6), we have the initial conditions a^{I} and a^{II} given by (3.5), and we used the quantities

$$\begin{aligned} N_n^{\mathrm{I}} &= (P\Psi^{P\mathrm{I}}, [H - E]X_n) , \\ N_n^{\mathrm{II}} &= (P\Psi^{P\mathrm{II}}, [H - E]X_n) . \end{aligned} \tag{5.7}$$

(5.6) is obtained by the mixture of a^{I} and a^{II}. These are completely equivalent to those obtained directly from b_i^{I} and b_i^{II} by studying the asymptotic behavior of $P\Psi_t$. Note that the α- and β-dependent terms on the right-hand sides of (5.5) are positive definite, while the analogous terms in (5.6) are not.

We give in Table IV the result of the one-term calculation of K_{ijt} for $k = 0.85a_0^{-1}$, where $E_1^Q < E < E_2^Q$ is assumed. We immediately note that, for all those cases in which $E_{1t}^Q > E$, K_{iit} still increased from the values K_{ii}^P. However, this does not mean that K_{iit} and K_{ii}^P are the bounds on K_{ii}. On the other hand, for those cases in which $E_{1t}^Q < E$, K_{iit} usually decrease from K_{ii}^P, but, from (5.3), K_{ii}^P are not bounds so that nothing is violated. Instead, K_{iit} are now bounds, and we can correctly determine the best K_{iit} by choosing the highest value among the sets with $E_{1t}^Q < E$. The only complication here is that one function may be effective in improving K_{11} while another function is good only for K_{22}. Therefore, it seems to be necessary to have sets with at least two functions in order to obtain the best K_{11t} and K_{22t} simultaneously. Incidentally, it is clear from Tables II and IV that the set with best E_{1t}^Q is not necessarily the one with best K_{iit}.

TABLE IV. K-matrix elements K_{ijt} for $k = 0.85a_0^{-1}$ for various sets of (α_n, β_n). Only the sets 2, 3, and 7 give bounds on K_{ii}, while the set 0 is the static values K_{ij}^P.

Set	(α_1, β_1)	K_{11t}	$K_{12t} = K_{21t}$	K_{22t}
0	(∞, ∞)	−0.367	0.106	10.290
1	(0.4, 0.2)	−0.351	0.466	18.394
2	(0.4, 0.4)	−0.389	0.992	−25.612
3	(0.4, 0.5)	−0.967	8.912	$\sim \pm\infty$
4	(0.4, 0.6)	−0.160	−1.565	23.748
5	(0.4, 0.7)	−0.225	−0.606	13.835
6	(0.6, 0.2)	−0.363	0.487	45.482
7	(0.6, 0.4)	−0.572	3.608	−49.495
8	(0.9, 0.9)	−0.184	0.036	10.316

TABLE V. Search for the two-function sets for K_{ijt} at $E = -0.1388$ a.u. The bound property is determined from the $E_{1t}^Q < E$ by the various sets considered. The set with (0.4, 0.4) (0.9, 0.9) gives the most reliable values. If $E_2^Q < E$ and $E_{2t}^Q > E$, then the bound property will have to be modified.

Parameters	K_{11t}	$K_{12t} = K_{21t}$	K_{22t}	Bounds
(0.6, 0.2) (0.4, 0.4)	−0.366	0.957	−25.56	Yes
(0.6, 0.2) (0.9, 0.9)	−0.182	0.336	45.61	No
(0.6, 0.4) (0.9, 0.9)	−0.184	−0.018	−15.59	Yes
(0.4, 0.7) (0.9, 0.9)	−0.184	0.030	23.88	No
(0.4, 0.4) (0.9, 0.9)	−0.185	−0.105	−19.71	Yes
(0.4, 0.2) (0.9, 0.9)	−0.183	0.153	18.98	No
(0.2, 0.4) (0.4, 0.2)	−0.351	0.426	22.49	No
(0.2, 0.4) (0.4, 0.4)	−0.387	1.092	−19.13	Yes
(0.2, 0.6) (0.4, 0.4)	−0.367	1.028	−25.55	Yes

In Sec. IV, we have seen that the cancellation among the elements of M_{mn} produces the bound property which comes about by the orthogonality (2.12). It was also stressed in Sec. II that N, as defined by (2.6), also has the property (2.13). This is achieved in practice through the cancellation between the two components of N. For example, at $k = 0.85a_0^{-1}$, we have for the second set with a^{II}

$$N_1^{\mathrm{II}} = -1.100 \text{ and } N_2^{\mathrm{II}} = 1.277 \text{ for } \alpha = 0.6,\ \beta = 0.4,$$

$$N_1^{\mathrm{II}} = -0.813 \text{ and } N_2^{\mathrm{II}} = 0.958 \text{ for } \alpha = 0.4,\ \beta = 0.6$$

The cancellation is less severe with the first set (a^{I}), which indicates that $(H - E)\Psi_i^{P\mathrm{I}}$ contains very little of the P component, while most of $(H - E)\Psi_i^{P\mathrm{II}}$ are in the P space and irrelevant for the calculation.

The two-term sets give improved K_{iit} over those values with a one-term trial function and K_{ii}^P for $E < E_1^Q$. Both K_{11t} and K_{22t} increase simultaneously as new functions are added. Thus, the best one-function sets for K_{11t} and K_{22t} give, when combined, improved values on both. For $E > E_1^Q$, the improvement with two-function sets is possible, of course, only if $E_{1t}^Q < E$ as well. Therefore, we have many inequalities among K_{iit} with different numbers of functions, and these give extremely sensitive checks on the accuracy of the diagonalization procedure and final values. We have listed several sample cases in Table V for $k = 0.85a_0^{-1}$. Unfortunately, the bounds on the diagonal K-matrix elements (5.5) do not improve the values K_{12t} very much. The situation would improve as we add more functions, however. Table VI contains the best K_{ijt} obtained with two-function sets at different values of E. In all cases, we have chosen those sets with $E_{1t}^Q < E$ if $E_1^Q < E$ or $E < E_1^Q < E_{1t}^Q$, so that K_{iit} are the lower

bounds on K_{ii}. Since we do not have the bound property on the off-diagonal K_{12}, it is not possible to choose the best K_{12} separately. We simply assume, therefore, that K_{12t} obtained from the set with the best K_{iit} is probably better. (This would certainly be the case in the limit of a large number of trial functions.) Because of the smallness of K_{12} at all E, its value is not well settled with two functions. The eigenphase shifts δ_{it} and the coupling parameter ϵ_t are also listed in Table VI for the best two-function sets, and Table VII contains the cross sections for all four processes, $1 \rightarrow 1$, $1 \rightarrow 2$, $2 \rightarrow 2$. We should remark here that we can choose two trial functions, both of which improve only K_{11t}, for example, and not K_{22t}, thus obtaining slightly better values than those quoted in Table VI.

Finally, we compare our results with those obtained previously by various authors.[10,11] Since the distortion effect is usually included by introducing various phenomenological effective potentials, their results do not give bounds on K_{iit} and the resonance states were not found. However, the cross sections with different choices of parameters involved in the polarization potentials are given to indicate the possible ranges of values. Our result on the elastic cross sections σ_{11t} and σ_{22t} is expected to be reliable since K_{iit} are reasonably large and converged well. On the other hand, K_{12t} is small and still fluctuates even with two-function sets, and we have no way of judging whether it has converged. Thus, our values on σ_{12t} and σ_{21t} are not conclusive, except perhaps to indicate that they are probably small compared with σ_{iit}.

For example, at $E = -0.18$ a.u., we have the elastic cross section $\sigma_{11t} \approx 0.48 a_0^2$ which is probably an upper bound since K_{11t} is negative and increasing (i.e., decreasing in absolute magnitude). This value may be compared with $\sigma_{11} \approx 0.6 a_0^2$ of Fels and Mittleman which seems to be a little too high and $\sigma_{11} \approx 0.13 a_0^2$ of Bransden and Jundi which seems to be too low. The pickup cross section $\sigma_{21} \approx 10^{-3} a_0^2$ is more or less consistent with the estimate of Fels and Mittleman and much smaller than that given by Bransden and Jundi. However, our results on σ_{21t} and σ_{12t} are less conclusive owing to the inaccuracy in our trial functions used.

VI. DISCUSSION AND SUMMARY

In the Paper I and here, we have given a comprehensive treatment of the three-particle two-channel scattering system e^+H, and learned a great deal about its spectral structure and dynamical behavior as manifested in the amplitudes. As in the single-channel elastic scattering below the pickup threshold, the process (1.1) requires a careful treatment of the distortion effects, which not only modify the amplitude in a significant way, but may also produce resonances, although we were not able to find them here.[12]

Specifically, we have shown that the M operator is indeed in the Q space and bounded from below, with the continuum starting at E_U. The GVB formulation is capable of giving reliable amplitudes provided the numerical calculation is carried out with sufficient accuracy. The complication due to the presence of the shift operator S can be overcome and reliable resonance energies can be obtained if they exist below E.

The present study falls short of the complete solution, however. First of all, the calculation of Y_{in} is not accurate enough to further improve the energy spectrum of M. As pointed out earlier, the limitation here has to do with the capacity of computers available and the limited machine time. Some improvements may be possible with initially combining the functions with proper constants multiplication, as stated in Sec. III.

Secondly, we have restricted our discussion only to the zero total partial wave. In order to compare the theoretical values with possible future experiments, higher partial waves have to be estimated also. Preliminary study by Bransden and Jundi[10] indicates that their contributions are significant.

In addition to obtaining the estimate on the spectrum of M, obtaining bounds on the K-matrix elements, and demonstrating that GVB can be effectively applied to this problem, the result presented here may also be useful for other purposes:

(i) Various theoretical approaches such as the DWBA and the coupled-equations method with local optical potentials may be examined in detail as to their regions of validity. This may then facilitate

TABLE VI. K_{ijt} elements obtained by the two-function sets with (0.9, 0.9) (0.4, 0.4), and the eigenphase shifts and coupling parameter calculated from them. All the elements K_{iit} given satisfy the bound property $K_{iit} < K_{ii}$ (except at $k = 0.850$ if $E_2^Q < E$ and $E_{2t}^Q > E$).

k	E	K_{11t}	$K_{12t} = K_{21t}$	K_{22t}	δ_{1t}	δ_{2t}	ϵ_t
0.725	−0.2372	−0.119	−0.0012	−0.306	−0.118	−0.297	0.006
0.750	−0.2188	−0.133	−0.0027	−0.805	−0.132	−0.678	0.004
0.775	−0.1997	−0.146	−0.0063	−1.430	−0.145	−0.961	0.005
0.800	−0.1800	−0.159	−0.0087	−2.448	−0.158	−1.183	0.004
0.825	−0.1597	−0.172	···	···	−0.170	−1.37	···
0.850	−0.1388	−0.185	−0.1052	−19.713	−0.182	−1.520	0.005

TABLE VII. Cross sections calculated from K_{ijt} of Table VI, at various energies E, in the units a_0^2.

E	σ_{11t}	σ_{21t}	σ_{12t}	σ_{22t}	σ_{11}^U	σ_{22}^U
−0.2372	0.332	0.0000	0.0003	21.05	23.91	245.20
−0.2188	0.386	0.0001	0.0004	39.55	22.34	100.53
−0.1997	0.438	0.0003	0.0008	41.94	20.92	62.44
−0.1800	0.483	0.0002	0.0005	38.46	19.64	44.88
−0.1597	0.52	...	...	33.6	18.46	34.79
−0.1388	0.572	0.0005	0.0008	28.17	17.39	28.24

the theoretical analyses of experiments without carrying out extensive calculations. Especially, the nonlocality and the energy dependence of the effective potentials W and the nonorthogonality of rearrangement channels should be carefully examined.

(ii) Better understanding of the approximation methods reached by studying the present solution should help in formulating the e^+ He scattering case, where experimental results are already available. Similarly, nuclear (d,p) reactions may be analyzed better to give improved understanding of the forces and nuclear structures.

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APPENDIX A: COORDINATE SYSTEM AND TRANSFORMATIONS

We write the Hamiltonian H as

$$H = T + V = T_0 + T_x + V, \tag{A1}$$

where

$$T_0 = T_{0,12} + T_{0,23} + T_{0,31},$$

$$T_{0,ij} = -\frac{\hbar^2}{2m_{ij}}\frac{1}{r_{ij}}\frac{\partial}{\partial r_{ij}}\left(r_{ij}^2\frac{\partial}{\partial r_{ij}}\right), \tag{A2}$$

$$T_x = T_{x,12} + T_{x,23} + T_{x,31},$$

$$T_{x,ij} = -\frac{\hbar^2}{2m_k}\left(\frac{r_{jk}^2 + r_{ki}^2 - r_{ij}^2}{r_{jk}r_{ki}}\frac{\partial^2}{\partial r_{jk}\,\partial r_{ki}}\right), \tag{A3}$$

$$V = \frac{Z_1Z_2e^2}{r_{12}} + \frac{Z_2Z_3e^2}{r_{23}} + \frac{Z_3Z_1e^2}{r_{31}}, \tag{A4}$$

and

$$\frac{1}{m_{ij}} = \frac{1}{m_i} + \frac{1}{m_j}. \tag{A5}$$

The volume integral operators used are

$$\int d\tau_{r_1r_2} = \int_0^\infty r_1\,dr_1 \int_0^\infty r_2\,dr_2 \int_{s=|r_1-r_2|}^{s=r_1+r_2} s\,ds, \tag{A6}$$

and

$$\int d\tau_{Rs} = 2\int_0^\infty R\,dR \int_0^\infty s\,ds \int_{r_2=|R-s/2|}^{r_2=R+s/2} r_2\,dr_2$$

$$= \int d\tau_{r_1r_2}. \tag{A7}$$

Owing to their symmetry, r_1 and r_2 can be interchanged.

APPENDIX B: ENERGY INTEGRATION

In order to obtain the energy matrix value H_{mn}, we need the following formula:

$$I = \int_0^\infty r_1\,dr_1 \int_0^\infty s\,ds \int_{r_2=|r_1-s|}^{r_2=r_1+s} r_2\,dr_2 \times\left(\frac{A}{r_1} + \frac{B}{r_2} + \frac{C}{s} + D\right)e^{-ar_1}e^{-bs}$$

$$= \frac{4}{a^3b^3(a+b)^3}\left[(aA + bB + 2D)(a+b)^3 + (a^3b + 3a^2b^2 + ab^3)C\right]. \tag{B1}$$

Most of the integrals needed in the matrix elements M_{mn} are reduced to a form similar to this, and then coded on a computer.

APPENDIX C: COMPLETE GVB EQUATIONS FOR $P_i\Psi_{it}$ and P_iY_{it}

The integrodifferential equations which were solved with the computer are

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

$$= r_2\int_0^\infty R\,dR\,K_{12}(r_2,R)F_2(R) + 2d\int_0^\infty 2^{1/2}e^{-(\alpha+1)r_1}\,dr_1 \times\int_{s=|r_2-r_1|}^{s=r_2+r_1} e^{-\beta s}\,ds\,V(r_1,r_2,s,\alpha,\beta,k), \tag{C1}$$

$$\left(\frac{d^2}{dR^2}+p^2\right)F_2(R)$$
$$=2R\int_0^\infty r_2\,dr_2\,K_{21}(R,r_2)F_1(r_2)$$
$$+4d\int_0^\infty e^{-(\beta+1/2)s}\,ds$$
$$\times\int_{r_1=|R-S/2}^{r_1=R+S/2} e^{-\alpha r_1}dr_1\,V(r_1,r_2,s,\alpha,\beta,k), \tag{C2}$$

where

$$V(r_1,r_2,s,\alpha,\beta,s)=[(\alpha-1)s+r_1s/r_2+(2\beta-1)$$
$$-\tfrac{1}{2}(\alpha^2+2\beta^2+k^2-1)r_1s-\tfrac{1}{2}(r_1^2+s^2-r_2^2)\alpha\beta] \tag{C3}$$

and, as defined previously,

$$K_{12}(r_2,R)=K_{21}(R,r_2)=K(r_2,R)\,. \tag{C4}$$

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