Rigorous stationary bounds on e^--atom scattering lengths: Target ground-state wave functions imprecisely known

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In recent work, the existence of stationary bounds on bound-state matrix elements for rather broad classes of quantum-mechanical operators was used to obtain a stationary upper bound on the scattering length for the collision of positrons with atoms whose target wave functions are not precisely known. This was done by obtaining calculable stationary bounds on the unknown matrix elements which appear in the formal expression for the bound on the scattering length. This method is extended in the present paper to electron-atom scattering for which it is necessary to obtain—in addition to bounds of the previous type—stationary bounds on the various exchange integrals. These latter cannot be obtained by means of techniques previously described. New techniques are presented for deriving such bounds, which are then used to obtain rigorous stationary upper bounds on the scattering length for the collisions of electrons with helium and with atoms heavier than helium.

I. INTRODUCTION

In recent years, rigorous stationary upper and lower bounds have been obtained on diagonal and off-diagonal bound-state matrix elements for rather broad classes of quantum-mechanical operators.[1,2] In a previous paper[2] we showed how some of these bounds could be used to obtain a rigorous stationary upper bound on the scattering length for the problem of collisions of positrons with atoms (or ions) whose wave functions are not exactly known. The starting point is the stationary upper bound on the positron-atom scattering length, which is expressed in terms of a trial scattering wave function. Asymptotically, this trial scattering wave function is the product of a (known) trial function of the projectile coordinates and the exact target ground-state wave function. When the latter is known, the bound is calculable.[3] When the target ground-state wave function is *not* known precisely—as is the case for all atomic systems other than the hydrogen isoelectronic sequence—the bound is only a formal one, since it contains bound-state matrix elements containing the imprecisely known target ground-state wave function. The problem of obtaining a stationary bound on the scattering length in such cases reduces to one of obtaining stationary bounds on these imprecisely known bound-state matrix elements. It was shown in Ref. 2—for the case of positron scattering—that this indeed could be done. Rigorous stationary upper bounds on all such matrix elements were derived and these were used, in turn, to obtain rigorous stationary upper bounds on positron-atom scattering lengths.

Although a calculable stationary upper bound on electron-atom scattering lengths is available for the target ground-state wave function precisely known, the method could not immediately be extended to electron-atom scattering lengths for the target ground-state wave functions imprecisely known, because of the appearance of exchange integrals, which cannot be bounded by the techniques used to bound the direct integrals.

It will be our principal task in this paper to obtain rigorous stationary upper bounds on the various types of exchange integrals which occur in electron-atom scattering. (Stationary *lower* bounds are no harder to obtain, but such lower bounds are not useful in the present context.) We will first write down, in Sec. II, the formal stationary upper bound on the scattering length in terms of calculable integrals, plus direct and exchange integrals containing the imprecisely known target wave functions. Stationary upper (and lower) bounds on the direct integrals were derived in Ref. 2. Stationary bounds on the exchange integrals will be given in Sec. III, thus enabling us to replace the formal stationary upper bound of Sec. II by a calculable stationary upper bound.

In addition to the obvious application to low-energy scattering, the techniques described below and in Ref. 2 are useful in still another way, in that they can be applied, after suitable choice of trial function, to bound not just A itself, but $A - A_B$, where A_B is the Born approximation scattering length. According to the forward dispersion relation,[4] this can be related to the integral of the total cross section over all momenta, and so provides a powerful consistency check on higher-energy measurements as well. The possibility of using dispersion relations in this way has recently been exploited for a number of scattering problems, including positron-helium scattering, by

Bransden, Macdowell, and co-workers.[5] Such results can be sharpened by use of variational bounds on, rather than simply estimates of, $A - A_B$.

II. EXPLICIT FORM OF THE FORMAL BOUND ON THE e^--He SCATTERING LENGTH

For simplicity of notation we will limit our discussion initially to the problem of bounding the electron-helium scattering length. The techniques are readily applicable to electrons incident with zero energy on heavier atoms as well, as will be discussed in Sec. IV. The problem of scattering by ions, with replusive asymptotic Coulomb potentials—which was discussed for the positron case in Ref. 2—does not entail any fundamentally new problems, and can also be handled by these techniques.

Consider, then, the problem of an electron incident at zero energy and zero relative angular momentum on a helium atom in its ground state. (We shall always use the phrase "scattering length" to imply that we are concerned with incident electrons having relative orbital angular momentum $L=0$; however, the results can be extended to $L>0$.) Making the almost certainly correct assumption that there is no He^- bound state, a bound on the scattering length is given by[3]

$$A \leq A_t + (m/2\pi\hbar^2)I, \tag{2.1}$$

where

$$I \equiv \int \Psi_t (H - \epsilon_1)\Psi_t \, d\tau_{123}. \tag{2.2}$$

In Eq. (2.2), H is the total (spin-independent) Hamiltonian for the system, ϵ_1 is the helium ground-state energy, and $d\tau_{123}$ stands for the 3-particle volume element $d\vec{r}_1\, d\vec{r}_2\, d\vec{r}_3$. The inner product over spin functions is to be understood. We consider a trial function for use in (2.2) of the form

$$\Psi_t = 3^{-1/2}[u_t(1)\psi(2,3)\chi(1,2,3) - u_t(2)\psi(1,3)\chi(2,1,3) - u_t(3)\psi(2,1)\chi(3,2,1)]. \tag{2.3}$$

Here ψ represents the exact (unknown) spatially symmetric space part of the helium ground-state wave function satisfying $\int \psi^2(i,j)\, d\vec{r}_i\, d\vec{r}_j = 1$ and u_t represents a trial scattering function component which satisfies the boundary conditions

$$\begin{aligned} &u_t(i) \to \text{const}, \quad r_i \to 0; \\ &u_t(i) \sim (A_t - r_i)/r_i, \quad r_i \sim \infty, \end{aligned} \tag{2.4}$$

where A_t is the trial scattering length. (To obtain the scattering length for nonzero orbital angular momentum L, the boundary conditions (2.4) need only be replaced by the boundary conditions appropriate to zero-energy scattering at relative orbital angular momentum L.[6]) Arbitrarily choosing the spin projection of the incident electron to be positive, the function $\chi(1,2,3)$ in (2.3) may be taken to be the doublet spin function

$$\chi_{1/2,1/2}(1,2,3) = 2^{-1/2}\alpha(1)[\alpha(2)\beta(3) - \beta(2)\alpha(3)]. \tag{2.5}$$

Equation (2.3) does not represent the most general type of trial function that one might wish to employ. One could add a term of the form

$$\mathcal{A}\Phi_t(1,2,3)\chi(1,2,3), \tag{2.6}$$

where Φ_t is any known quadratically integrable function over the 3-particle configuration space and $\mathcal{A}$ is the antisymmetrization operator. Inclusion of the term (2.6) in (2.3) would, when employed in (2.2), result in the appearance of additional terms; those which are unknown would be typically of the form

$$\int \psi(1,2)\xi(1,2,3)\, d\tau_{123}, \tag{2.7}$$

where $\xi(1,2,3)$ is a known, quadratically integrable function. After performing the integration over the space coordinates of particle 3, expression (2.7) reduces in form to that of the inner product of a known quadratically integrable function with an imprecisely known bound-state wave function. Stationary bounds for quantities of this type are readily obtained by methods described in Ref. 2. It will accordingly suffice for our purposes to limit discussion to trial functions of the form (2.3).

If (2.3) is substituted into (2.2), the result can be expressed in the form

$$I = (I_1 + I_2) - (J_1 + J_2), \tag{2.8}$$

where

$$I_1 = \int \psi(1,2)u_t(3)\left(-\frac{2}{r_3} + \frac{1}{r_{13}} + \frac{1}{r_{23}}\right) \times u_t(3)\psi(1,2)\, d\tau_{123}, \tag{2.9}$$

$$I_2 = \int \psi(1,2)u_t(3)T_3 u_t(3)\psi(1,2)\, d\tau_{123}, \tag{2.10}$$

$$J_1 = \int \psi(1,3)u_t(2)\left(-\frac{2}{r_3} + \frac{1}{r_{13}} + \frac{1}{r_{23}}\right) \times u_t(3)\psi(1,2)\, d\tau_{123}, \tag{2.11}$$

$$J_2 = \int \psi(1,3)u_t(2)T_3 u_t(3)\psi(1,2)\, d\tau_{123}, \tag{2.12}$$

and where

$$T_i \equiv -(\hbar^2/2m)\nabla_i^2 \tag{2.13}$$

is the kinetic-energy operator for the ith electron.

We must now face the fact that the helium ground-state wave function ψ is not precisely

known. I_1 and I_2—after the integral over the coordinate $\vec{r}_3$ is performed—are of the form $(\psi, W\psi)$ where W is known, and stationary upper (and lower) bounds for quantities of this type are given in Ref. 2. J_1 and J_2, on the other hand, are exchange integrals. Techniques for bounding quantities of this type comprise the subject matter of Secs. III and IV.

III. STATIONARY BOUNDS ON EXCHANGE INTEGRALS: ELECTRON-HELIUM SCATTERING

We first note that both J_1 and J_2 can be written in the form

$$J_n = \int \psi(1,3) U_n(1,2,3) \psi(1,2)\, d\tau_{123}, \quad n = 1, 2 \tag{3.1}$$

where, by comparison with Eqs. (2.11) and (2.12), we have

$$U_1(1,2,3) = u_t(2)\left(-\frac{2}{r_3} + \frac{1}{r_{13}} + \frac{1}{r_{23}}\right) u_t(3), \tag{3.2a}$$

$$U_2(1,2,3) = u_t(2) T_3 u_t(3). \tag{3.2b}$$

In discussions which are valid for both $n = 1$ and $n = 2$, we will drop the subscript n on J_n and U_n. Now let $\psi_v(i,j)$ be a variational approximation[7] to the exact helium ground-state wave function $\psi(i,j)$, where i, j are chosen from among 1, 2, and 3. Let $|\psi(i,j)\rangle$ be the helium ground-state ket for particles i and j, let

$$Q(i,j) = 1 - |\psi(i,j)\rangle\langle\psi(i,j)| \tag{3.3a}$$

be the operator which projects off the ground state, and let

$$S = \int \psi(i,j)\psi_v(i,j)\, d\vec{r}_i\, d\vec{r}_j \tag{3.3b}$$

be the overlap of ψ and ψ_v. An identity for the wave function in terms of these entities is readily seen to be

$$\psi(i,j) = \frac{\psi_v(i,j) - Q(i,j)\psi_v(i,j)}{S}. \tag{3.4}$$

If this is substituted into (3.1) the result can be written

$$J = \frac{K_v - K_Q - K_Q' + K_{QQ}}{S^2}, \tag{3.5}$$

where

$$K_v = \int \psi_v(1,3) U(1,2,3) \psi_v(1,2)\, d\tau_{123}, \tag{3.6}$$

$$K_Q = \int \psi_v(1,3) U(1,2,3) \{Q(1,2)\psi_v(1,2)\}\, d\tau_{123}, \tag{3.7}$$

$$K_Q' = \int \{Q(1,3)\psi_v(1,3)\} U(1,2,3) \psi_v(1,2)\, d\tau_{123}, \tag{3.8}$$

$$K_{QQ} = \int \{Q(1,3)\psi_v(1,3)\} U(1,2,3) \times \{Q(1,2)\psi_v(1,2)\}\, d\tau_{123}. \tag{3.9}$$

When necessary, we will write the subscript $n (= 1$ or 2) on J and on each of the four K quantities in Eq. (3.5). (Note that the Q's always operate only on the adjacent ψ_v's.) The unknown quantity S^2 which appears in (3.5) has been studied extensively in the literature,[8] and stationary upper and lower bounds for it are well known. We may therefore treat S henceforth as a known quantity, with the understanding that it must be replaced by the appropriate stationary bound wherever it appears. The only unknown in the foregoing equations (3.6)–(3.9) is then the projection operator Q.

We now consider in turn each of the four integrals in Eqs. (3.6)–(3.9). The first of these, K_v of Eq. (3.6), is calculable as it stands and represents a stationary approximation to J. The remaining three terms are of second order or higher. The first of these, K_Q of (3.7), we rewrite in the obviously equivalent form

$$K_Q = \int [\psi_v(1,3) F_2^{-1}(2) F_3(3) U(1,2,3)] \times [F_2(2) F_3^{-1}(3) \{Q(1,2)\psi_v(1,2)\}]\, d\tau_{123}, \tag{3.10}$$

where we have introduced the function $F_j(j) \equiv F_j(r_j)$. We wish to apply the Schwarz inequality to integrals such as (3.10), with the integrand partitioned in the manner indicated by the square brackets. The purpose of the F's in (3.10), and in similar integrals that will occur later on, is to assure that the two factors that result are finite. More generally, we could have introduced an $f(i,j)$ having this property instead of the separable form $F_i^{-1}(i) F_j(j)$. However, it is to be noted that terms of the type K_Q and K_Q' are second-order quantities, because of the appearance of $Q\psi_v$. (The quantities K_{QQ} are *fourth*-order quantities.) The particular choice of F's can therefore be expected not to be critical, except insofar as the resulting bound is relatively easy to obtain. The emphasis will therefore be placed on finding F's which keep down the amount of calculational effort required. The separable form given does indeed appear to be the simplest, and the form of $F_j^2(r_j)$ suggested by the form of the integrals to be bounded is that of a polynomial in r_j. [The choice $F_j(r_j)$ proportional to $e^{\beta r_j}$ leads to difficulties in obtaining a bound.] Most often, it will be found necessary to calculate the integral $\int u_t^2(j) F_j^{-2}(j)\, d\vec{r}_j$. Since u_t approaches a constant asymptotically, $F_j^{-2}(r_j)$ must fall off faster than

r_j^{-3}. Moreover, the requirement that the integrals in which it appears converge means, of course, that $F_j^2(j)$ must not increase too rapidly with r_j. A reasonable and simple choice therefore appears to be

$$F_j^2(j) = 1 + \alpha_j r_j^4 . \tag{3.11}$$

(The constant term is necessary since F^{-1} must be finite at the origin.) The number α_j can be varied to produce the best bound for the given form of F.

At this point we introduce the notation

$$\mathfrak{D}_{ij}(B) \equiv \int \{Q(i,j)\psi_v(i,j)\} B \{Q(i,j)\psi_v(i,j)\}\, d\vec{r}_i\, d\vec{r}_j \tag{3.12}$$

for any operator B. The indices i and j indicate that the integral is only over $\vec{r}_i$ and $\vec{r}_j$, even if B is a function of $\vec{r}_k$ as well as of $\vec{r}_i$ and $\vec{r}_j$. We proceed with the derivation of stationary bounds on the real number[9] J, by noting that since—as we have just seen—the real number K_Q is a second-order quantity, then $|K_Q|$ will also, of course, be a second-order quantity. Hence, use of the bound $K_Q \leq |K_Q|$ in (3.5) will still yield a stationary bound on J. We now apply the Schwarz inequality to $|K_Q|$ and write as a (formal) upper bound on K_Q

$$K_Q \leq \| \psi_v(1,3) F_2^{-1}(2) F_3(3) U(1,2,3) \| \times \left[\int F_3^{-2}(3)\, d\vec{r}_3 \right]^{1/2} \mathfrak{D}_{12}^{1/2}(F_2^2(2)), \tag{3.13a}$$

where, for arbitrary g,

$$\|g\| \equiv (g,g)^{1/2}$$

represents the norm of the function g. The properties of $F_j(j)$ discussed above guarantee that the first two factors on the right-hand side of (3.13a) are finite. All the quantities appearing in these two factors are known and calculable. We note, furthermore, that—by virtue of the fact that ψ_v is a variational estimate of ψ—the remaining factor in (3.13a), the $\mathfrak{D}^{1/2}$ factor, is a second-order quantity. If we can find a simple bound on this $\mathfrak{D}^{1/2}$ factor, i.e., a bound which is still a second-order quantity, then use of such a bound in (3.13a) will result in a simple upper bound on K_Q. Replacement of K_Q by such a bound in (3.5) will result in a stationary bound on J—provided the same is done for K_Q' and K_{QQ}. (These latter will be considered shortly.)

Simple bounds on quantities such as

$$\mathfrak{D}_{12}(F_2^2(2)) = \mathfrak{D}_{12}(1) + \alpha_2 \mathfrak{D}_{12}(r_2^4)$$

were first derived in a slightly different context by Aranoff and Percus[10]; some of these are rederived and some new results are derived elsewhere.[2,11] The simple bounds on $\mathfrak{D}_{ij}(r_j^q)$ and $\mathfrak{D}_{ij}(r_{ij}^s)$ that will be needed in order to complete the bound on J are tabulated for convenience in Appendix A, where some new results are also obtained. Thus, if we replace the $\mathfrak{D}^{1/2}$ factor in Eq. (3.13a) by the simple upper bound

$$[\mathfrak{D}_{12}^{(+)}(F_2^2(2))]^{1/2} = [\mathfrak{D}_{12}^{(+)}(1) + \alpha_2 \mathfrak{D}_{12}^{(+)}(r_2^4)]^{1/2},$$

where $\mathfrak{D}_{12}^{(+)}(1)$ and $\mathfrak{D}_{12}^{(+)}(r_2^4)$ are given in Appendix A, the result will be the required simple upper bound on the second-order quantity K_Q. (We will use the notation $C^{(+)}$ to denote an upper bound on some number C.)

Equation (3.13a) is valid for both K_{Q1} and K_{Q2}; however, in the latter case it is possible to improve on this result by recognizing that the integral

$$\int [T_3 u_t(3)]^2\, d\vec{r}_3$$

exists. This enables us to choose $F_3(3) = 1$, so that by partitioning (3.10) somewhat differently we obtain

$$K_{Q2} \leq \| \psi_v(1,3) F_2^{-1}(2) u_t(2) \| \times \left(\int [T_3 u_t(3)]^2\, d\vec{r}_3 \right)^{1/2} \mathfrak{D}_{12}^{1/2}(F_2^2(2)). \tag{3.13b}$$

In general, it is clear that the partition of the integral (3.10) is not uniquely determined, either for K_{Q1} or K_{Q2}. For example, it is possible in the case of K_{Q1} to make use of the properties of the interaction potential (in a way exactly analogous to the treatment of K_{QQ1} in Appendix B) in order to derive a bound on K_{Q1} that is alternative to that given in (3.13a). However, because K_Q is a second-order quantity, the exact choice of partition is probably not critical.

The above techniques for obtaining bounds, and other remarks concerning K_Q, apply equally well to K_Q', since the two are similar in form.

It remains therefore to obtain a simple upper bound on K_{QQ}. At this point it is convenient to distinguish from the start between two types of J integrals, viz., J_1 and J_2 of Eqs. (2.11) and (2.12), respectively. Thus, to obtain a stationary upper bound on J_1, we need to obtain a simple upper bound on K_{QQ1}, where

$$K_{QQ1} = \int \{Q(1,3)\psi_v(1,3)\} u_t(2)(-2r_3^{-1} + r_{13}^{-1} + r_{23}^{-1})\, u_t(3) \{Q(1,2)\psi_v(1,2)\}\, d\tau_{123}$$
$$= \int \eta(1,3,2)(-r_3^{-1} \times 2 + r_{13}^{-1/2} + r_{13}^{-1/2} \times r_{23}^{-1/2} \times r_{23}^{-1/2}) \eta(1,2,3)\, d\tau_{123} \tag{3.14}$$

and where, in turn

$$\eta(1,3,2) \equiv \{Q(1,3)\psi_v(1,3)\}F_3(3)F_2^{-1}(2)u_t(2). \qquad (3.15)$$

Applying the Schwarz inequality separately to each of the three terms in the last form of (3.14), with the partitioning of the integrand into two factors denoted by the position of the multiplication sign, one obtains

$$K_{QQ_1} \leq 2\left[\int u_t^2(2)F_2^{-2}(2)u_t^2(3)F_3^{-2}(3)\,d\vec{r}_2\,d\vec{r}_3\right]^{1/2}\{[\mathfrak{D}^{(+)}(1/r_i^2)+\alpha_3\mathfrak{D}^{(+)}(r_i^2)]^{1/2}[\mathfrak{D}^{(+)}(1)+\alpha_2\mathfrak{D}^{(+)}(r_i^4)]^{1/2}$$
$$+[\mathfrak{D}^{(+)}(1/r_{ij})+\alpha_3\{\mathfrak{D}^{(+)}(r_i^8)\mathfrak{D}^{(+)}(1/r_{ij}^2)\}^{1/2}]^{1/2}[\mathfrak{D}^{(+)}(1/r_{ij})+\alpha_2\{\mathfrak{D}^{(+)}(r_i^8)\mathfrak{D}^{(+)}(1/r_{ij}^2)\}^{1/2}]^{1/2}\}, \qquad (3.16)$$

where the $\mathfrak{D}^{(+)}(r^q)$ are given in Appendix A and represent upper bounds on $\mathfrak{D}_{ij}(r_i^q)$. (In order to simplify the writing, we drop the subscripts on $\mathfrak{D}$ and $\mathfrak{D}^{(+)}$ whenever no confusion can arise.) In obtaining the right-hand side of (3.16) we have, for example, used the fact that, for $\vec{r}_3$ fixed,

$$\mathfrak{D}_{12}\left(\frac{1+\alpha_2 r_2^4}{r_{13}}\right) \leq \mathfrak{D}^{(+)}\left(\frac{1}{r_{ij}}\right)+\alpha_2\left[\mathfrak{D}^{(+)}(r_i^8)\mathfrak{D}^{(+)}\left(\frac{1}{r_{ij}^2}\right)\right]^{1/2}$$

for any value of $\vec{r}_3$. This follows from the fact that an upper bound on $\mathfrak{D}_{ij}(1/r_{ij}^s)$ for $s=1,2$ is also an upper bound on $\mathfrak{D}_{ij}(1/r_{ik}^s)$ for arbitrary $\vec{r}_k$. [See Appendix A, particularly Eqs. (A1) and (A3).] The partition of the integral K_{QQ_1} indicated in (3.14) is not unique; however, since K_{QQ} is a fourth-order term, the choice of partition is probably not critical. [An alternative bound on K_{QQ_1}, which does not involve $\mathfrak{D}(r_i^8)$, is given in Appendix B.]

In a similar way, we have

$$K_{QQ_2} = \int \{Q(1,3)\psi_v(1,3)\}u_t(2)F_2^{-1}(2)\times[T_3u_t(3)]$$
$$\times F_2(2)\{Q(1,2)\psi_v(1,2)\}\,d\tau_{123},$$

where, in line with the discussion given in connection with Eq. (3.13b), we have chosen $F_3(3)=1$. Thus we have

$$K_{QQ_2} \leq \left\{\int u_t^2(2)F_2^{-2}(2)\,d\vec{r}_2\times\mathfrak{D}(1)\right.$$
$$\left.\times\int[T_3u_t(3)]^2\,d\vec{r}_3\times[\mathfrak{D}(1)+\alpha_2\mathfrak{D}^{(+)}(r_i^4)]\right\}^{1/2}. \qquad (3.17)$$

We have now found simple bounds on all the unknown (second-order or higher) integrals of (3.5) and hence stationary bounds on the integrals J_1 and J_2 of Eq. (2.8). When the techniques of Ref. 2 are used to obtain stationary bounds on I_1 and I_2, the resulting stationary bound on I yields a stationary bound on the scattering length according to (2.1).

We note in passing that in cases where the computational effort involved in obtaining a variational approximation ψ_v to the true helium ground-state wave function is felt not to be warranted, all of the foregoing bounds are valid when ψ_v is replaced by an arbitrary normalized trial function ψ_t. However, if this is done, the bounds will contain first-order error terms; that is, they will no longer be stationary.

IV. EXTENSION TO MORE COMPLICATED SYSTEMS

We begin with a few general remarks concerning the application of the foregoing to atomic systems beyond helium. In the general case, when the spin S of the target differs from zero, there will be two scattering lengths, associated with the two values $S\pm\frac{1}{2}$ of the total spin of the target plus electron. The total spin of the system will be reflected in the form of the trial function Ψ_t, and a separate calculation of the type indicated above must be performed for each of the two possible values. (As always, we ignore all spin interactions; it should not be difficult to include them.)

Secondly, we note that the number of factors $F_j(j)F_j^{-1}(j)$ by which the integrand should be multiplied prior to partition should be the minimum number such that the two integrals which appear after application of Schwarz's inequality remain finite. As in the foregoing example, this number is just *two*, regardless of the number of electrons. Thus, each of the integrals occurring in the N-electron problem will be identical in form (with different multiplicative factors) with those occurring above, with $\psi_v(1,2)$ replaced by $\psi_v(1,2,\ldots,N)$, etc.; it is also clear that the $\mathfrak{D}$ terms which will occur are identical to those which occurred in (3.16) and (3.17); no new $\mathfrak{D}$ forms will appear.

Finally, we note that in cases where the ion, formed by the addition of an electron to the target, has a bound state, the procedure must be modified so that the effect of the bound state is "subtracted out," in a manner described previously[12] in a different context.

It is clear that extensions to the case of nonzero projectile orbital angular momentum go through just as in the case of helium, *provided* the target ground state has zero orbital angular momentum. (Note that conservation of energy requires the initial and final target states—and hence the initial and final target orbital angular momenta—to be the same.) When the target has nonzero orbital angular momentum (or more generally, when spin-

dependent or tensor forces are present)—and regardless of the orbital angular momentum of the projectile—the problem becomes a multichannel one. In the zero-energy limit, formal bounds on linear combinations of elements of the reaction matrix, in which matrix elements involving the exact target wave functions appear, have been given previously.[13] The question of obtaining bounds on such matrix elements when the target wave function is unknown requires separate investigation although in the atomic case, at least, it appears that the methods developed here can be applied to the more general multichannel problem.

To see explicitly how the many-electron case works out, consider an N-electron atom with spin $S_{\text{target}}=0$, so that there is effectively only one scattering length. (As noted above, the only difference in the more general case of nonzero spin is that there are two.) We also assume $L_{\text{target}}=0$ to avoid multichannel complications. A suitable trial function can be written as

$$\Psi_t=(N+1)^{-1/2}\left(1-\sum_{i=1}^{N}P_{i,N+1}\right)\times[\xi(1,2,\ldots,N)u_t(N+1)\alpha(N+1)]+\Phi_t(1,2,\ldots,N+1), \tag{4.1}$$

where P_{jk} is the operator which interchanges the jth and kth particles, ξ is the total (space+spin) normalized antisymmetrized ground-state atomic wave function, and u_t has the asymptotic form indicated in (2.4). As before, we are temporarily considering $\xi(1,2,\ldots,N)$, the exact target wave function, as known. In general, it will be of the form of a sum of products of space and spin coordinates

$$\xi(1,2,\ldots,N)=\sum_{\beta}\phi_{\beta}(1,2,\ldots,N)\times\chi_{\beta}(1,2,\ldots,N); \tag{4.2a}$$

similarly ξ_v in Eq. (4.3) below will be of the form

$$\xi_v(1,2,\ldots,N)=\sum_{\beta}\phi_{\beta v}(1,2,\ldots,N)\times\chi_{\beta}(1,2,\ldots,N), \tag{4.2b}$$

but the exact form of Eqs. (4.2) is not relevant for the purposes of the present discussion.

The function Φ_t appearing in (4.1) is some suitably chosen antisymmetrized function of the space and spin coordinates of the $N+1$ particles and represents distortion of the target by the projectile. It falls off faster than $1/r_i$ for all r_i, and therefore all the matrix elements in which it appears [after substitution of (4.1) into (2.2) and use of the N-particle analog of (3.4)], are either known or can be bounded by previous techniques. The remaining matrix elements are each of a form which can be written either as

$$\int\xi_v(1,2,\ldots,N)U(1,2,\ldots,N+1)\times[Q\xi_v(i_1,i_2,\ldots,i_N)]\,d\tau_{12\ldots N+1} \tag{4.3a}$$

or

$$\int[Q\xi_v(1,2,\ldots,N)]U(1,2,\ldots,N+1)\times[Q\xi_v(i_1,i_2,\ldots,i_N)]\,d\tau_{12\ldots N+1}, \tag{4.3b}$$

where $i_1,i_2,\ldots,i_{N+1}$ represents some permutation of $1,2,\ldots,N+1$ and where $U(1,2,\ldots,N+1)$ represents a product of three factors: $u_t(N+1)$ on the left, followed by either the kinetic-energy operator T_{N+1} or the interaction potential

$$\frac{-N}{r_{N+1}}+\sum_{j=1}^{N}\frac{1}{r_{N+1,j}},$$

and finally $u_t(i_{N+1})$ on the right. [The argument of the Q's in Eq. (4.3) is of course the same as the ξ_v's on which they operate.]

It is clear that after multiplying $u_t(N+1)$ by $[F^{-1}(N+1)F(i_{N+1})]$ and $u_t(i_{N+1})$ by $[F^{-1}(i_{N+1})F(N+1)]$, bounds on (4.3) can be obtained exactly as described in Sec. III.

V. SUMMARY OF CALCULATIONS NECESSARY TO OBTAIN A STATIONARY UPPER BOUND ON THE e^--ATOM SCATTERING LENGTH

In order to replace the formal stationary bound of Eq. (2.1) by a calculable stationary bound, stationary bounds on the four quantities I_1, I_2, J_1, and J_2 must be obtained. [See Eqs. (2.8)–(2.12).] The first two of these are direct integrals, and techniques for bounding these have been given in Ref. 2. Specifically, the bound on I_1 and I_2 is given by Eq. (4.13) of Ref. 2, except that the interaction potential will be of the opposite sign. [The choice of trial function indicated by Eq. (2.3) of the present paper is equivalent to the choice $\chi_t=0$ in Eq. (4.13) of Ref. 2. Such a choice is not at all necessary, as indicated by the discussion of Eq. (2.6) above.]

To obtain stationary bounds on J_1 and J_2, it is first necessary to obtain a variational approximation ψ_v to the true target ground-state wave function ψ [e.g., Eq. (2.27) of Ref. 7]. Then K_{v1} and K_{v2} [Eq. (3.6)] can be computed. To bound the remaining terms in (3.5), it is necessary to calculate $\|\psi_v(1,3)F_2^{-1}(2)F_3(3)U_1(1,2,3)\|$ and $\|\psi_v(1,3)F_2^{-1}(2)\times U_2(1,2,3)\|$ where $F_j(j)$ is given by (3.11) and where U_1 and U_2 are given by (3.2a) and (3.2b), respectively. The integrals

$$\int F_j^{-2}(j)\, d\vec{r}_j\,,$$

$$\int u_t^2(j) F_j^{-2}(j)\, d\vec{r}_j$$

must also be calculated, as well as stationary bounds on the overlap S, and on ϵ_1. Finally, simple upper bounds on the quantities $\mathfrak{D}(r_i^q)$ for $q=-2$, 2, 4, and 8 and on $\mathfrak{D}(1/r_{ij}^s)$ for $s=1$ and 2 must be obtained. Methods for doing this are given in Appendix A. [The necessity of obtaining a bound on $\mathfrak{D}(r^8)$ may be circumvented by means of an alternative procedure given in Appendix B.]

It might be worth noting that the direct integrals can also be bounded by the methods of the present paper, using the *identical* techniques used for the exchange integrals. [A moment's consideration of Eqs. (2.9) and (2.10) shows that, for example, the F factors would have to be introduced in exactly the same way, and so forth.] It is not yet clear whether such a treatment of the direct integrals would offer any advantage over the method of Ref. 2.

APPENDIX A: BOUNDS ON $\mathfrak{D}_{ij}(r_i^q)$

In order to utilize the bounds derived in Sec. III, we must obtain simple upper bounds on the quantities $\mathfrak{D}_{ij}(r_i^q)$, for $q=-2$, 0, 2, 4, and 8 as well as on the quantities $\mathfrak{D}(1/r_{ij}^s)$ for $s=1$ and 2. We must also show that an upper bound on $\mathfrak{D}_{ij}(1/r_{ij}^2)$ is an upper bound on $\mathfrak{D}_{ij}(1/r_{ik}^2)$ for arbitrary $\vec{r}_k$. [Note that, because of the indistinguishability of the electrons, we have $\mathfrak{D}_{ij}(r_i^q)=\mathfrak{D}_{ij}(r_j^q)$ for $i,j=1,2,3$.]

In the remainder of this Appendix we shall drop the subscripts ij on $\mathfrak{D}$ wherever no confusion can arise. The formulas obtained will, in fact, apply equally well to the problem of heavier atoms with N electrons discussed in Sec. IV, provided it is understood that the $\mathfrak{D}$'s are defined by the obvious N-electron generalization of (3.12).

The bounds on $\mathfrak{D}(r_i^q)$ and on $\mathfrak{D}(r_{ij}^q)$ for negative values of q proceed along identical lines: One writes down, for example, the commutation relations[10]

$$\frac{1}{r_{ik}} = \frac{i}{2\hbar}\left(\vec{p}_i\cdot\frac{\vec{r}_{ik}}{r_{ik}} - \frac{\vec{r}_{ik}}{r_{ik}}\cdot\vec{p}_i\right), \tag{A1}$$

$$\frac{1}{r_i^2} = \frac{i}{\hbar}\left(\vec{p}_i\cdot\frac{\vec{r}_i}{r_i^2} - \frac{\vec{r}_i}{r_i^2}\cdot\vec{p}_i\right), \tag{A2}$$

$$\frac{1}{r_{ik}^2} = \frac{i}{\hbar}\left(\vec{p}_i\cdot\frac{\vec{r}_{ik}}{r_{ik}^2} - \frac{\vec{r}_{ik}}{r_{ik}^2}\cdot\vec{p}_i\right). \tag{A3}$$

Considering both sides of each of Eqs. (A1)–(A3) as the argument of a $\mathfrak{D}$ function, and applying Schwarz's inequality to each of the right-hand sides, we obtain

$$\mathfrak{D}_{ij}(1/r_{ik}) \le \left(\frac{1}{\hbar}\right)\mathfrak{D}^{1/2}(1)\mathfrak{D}^{1/2}(p_i^2), \tag{A4}$$

$$\mathfrak{D}^{1/2}(1/r_i^2) \le \left(\frac{2}{\hbar}\right)\mathfrak{D}^{1/2}(p_i^2), \tag{A5}$$

$$\mathfrak{D}_{ij}^{1/2}(1/r_{ik}^2) \le \left(\frac{2}{\hbar}\right)\mathfrak{D}_{ij}^{1/2}(p_i^2). \tag{A6}$$

$\mathfrak{D}(1)$ may be obtained directly from (3.4) (or its many-electron generalization). We find

$$\mathfrak{D}(1) = (1 - S^2). \tag{A7}$$

[In (A4) and (A7) 1 is the unit operator.]

Because of the indistinguishability of the electrons, we have

$$\mathfrak{D}(p_i^2) \le (2m/N)\mathfrak{D}(t), \tag{A8}$$

where

$$t = \sum_{i=1}^{N} T_i$$

is the kinetic-energy operator of the target atom. A simple upper bound on $\mathfrak{D}(t)$ is given by[10,2]

$$\begin{aligned}\mathfrak{D}^{1/2}(t) &\le [\mathfrak{D}^{(+)}(t)]^{1/2} \\ &= \tfrac{1}{2}\{(1-S^2)^{1/2}b + [(1-S^2)b^2 \\ &\qquad + 4\,|\,\epsilon_t - S^2\epsilon_1\,|\,]^{1/2}\},\end{aligned} \tag{A9}$$

where ϵ_1 is the ground-state energy of the target atom (or the appropriate bound), ϵ_t is the expectation value of the target Hamiltonian with respect to ψ_v, and the number b—for the case of an N-electron atom of nuclear charge Z—is given by

$$b = (mN/2\hbar^2)^{1/2}(2Z + N - 1)e^2, \tag{A10}$$

where e is the electronic charge. Explicitly, Eqs. (A4)–(A6) become, in terms of (A9) and (A10),

$$\mathfrak{D}(1/r_{ik}) \le [(1-S^2)(2m/N\hbar^2)\mathfrak{D}^{(+)}(t)]^{1/2}, \tag{A11}$$

$$\mathfrak{D}(1/r_i^2) \le (8m/N\hbar^2)\mathfrak{D}^{(+)}(t), \tag{A12}$$

$$\mathfrak{D}(1/r_{ik}^2) \le (8m/N\hbar^2)\mathfrak{D}^{(+)}(t). \tag{A13}$$

Note that in verifying Eqs. (A1) and (A3), the vector $\vec{r}_k$ plays no role; thus Eqs. (A11) and (A13) verify the validity of the contention made in the first paragraph of this Appendix.

In order to obtain a bound on $\mathfrak{D}(r_i^q)$ for positive q's, we proceed along slightly different lines than those followed previously.[10,11,2] The reason is that the previous methods appear difficult to use for $q>4$: The commutator of $\vec{r}r^{(q-1)/2}$ with H is equal to a quantity which can be related to $r^{(q-1)/2}$. In Eq. (E8) of Ref. 11, for example, the product of the two commutators in the $\mathfrak{D}$ term can thus be related to r^{q-2}. However, the powers of r occur multiplied by powers of momenta, and the Schwarz

inequality must be applied to separate the two. After this is done, the remaining expression involves a term in r^{2q-4}. Thus, the expression gives useful information if and only if $2q-4 \leq q$, that is, if $q \leq 4$. The following method will be seen to be applicable to all even powers of q, and hence to odd (and fractional) powers as well, by virtue of the relationship

$$\mathfrak{D}(r_i^q) \leq \mathfrak{D}^{1/2}(r_i^{2\sigma})\mathfrak{D}^{1/2}(r_i^{2\tau}),$$

where $q=\sigma+\tau$.

We begin by considering the more general problem of obtaining a bound on $\mathfrak{D}(A^2)$, where A^2 is an operator expressible in the form

$$\vec{A}^\dagger \cdot \vec{A} = A^2 \tag{A14}$$

and where $\vec{A}$ is a vector operator of odd parity. Using the N-particle analog of (3.4) one may readily verify, using commutator notation, that

$$\mathfrak{D}(\vec{A}^\dagger \cdot (h-\epsilon_1)\vec{A}) = \mathfrak{D}(\vec{A}^\dagger \cdot [h, \vec{A}]) + (Q\psi_v, A^2(h-\epsilon_1)\psi_v), \tag{A15}$$

where h is the Hamiltonian for the atom (or ion), ϵ_1 is the ground-state energy, and we have used $(h-\epsilon_1)\psi = 0$. We now proceed to treat the first term on the right-hand side of (A15) in a manner very similar to that employed in obtaining simple bounds on $(\psi, A^2\psi)$ in Sec. IV A of Ref. 11. (Excited states may be correspondingly handled by methods similar to those of Sec. IV C of Ref. 11.) We write

$$\begin{aligned}\mathfrak{D}(\vec{A}^\dagger \cdot (h-\epsilon_1)\vec{A}) &\equiv \langle Q\psi_v | \vec{A}^\dagger \cdot (h-\epsilon_1)\vec{A} | Q\psi_v\rangle \\ &= \sum_{n=1}^{\infty} \langle Q\psi_v | \vec{A}^\dagger (h-\epsilon_1) | \psi_n\rangle\langle\psi_n | \vec{A} | Q\psi_v\rangle \\ &= \sum_{n=2}^{\infty} (\epsilon_n - \epsilon_1)\langle Q\psi_v | \vec{A}^\dagger | \psi_n\rangle\langle\psi_n | \vec{A} | Q\psi_v\rangle \\ &\geq (\epsilon_2 - \epsilon_1) \sum_{n=2}^{\infty} \langle Q\psi_v | \vec{A}^\dagger | \psi_n\rangle\langle\psi_n | \vec{A} | Q\psi_v\rangle .\end{aligned} \tag{A16}$$

We now assume that ψ_v has been chosen to have the same parity as $\psi(\equiv\psi_1)$. Since $\vec{A}$ is of odd parity, it follows that $\langle Q\psi_v | \vec{A} | \psi\rangle = 0$. The sum in (A16) can then be extended to include the value $n=1$, and the sum can then be evaluated by closure. (A16) can therefore be written

$$\mathfrak{D}(A^2) \leq (\epsilon_2 - \epsilon_1)^{-1}\mathfrak{D}(\vec{A}^\dagger \cdot [h-\epsilon_1]\vec{A}). \tag{A17}$$

We couple this with the observation that

$$\begin{aligned}\mathfrak{D}(\vec{A}^\dagger \cdot [h, \vec{A}] - [h, \vec{A}^\dagger] \cdot \vec{A}) &\equiv \mathfrak{D}([\vec{A}^\dagger, [h, \vec{A}]) \\ &= 2\,\mathrm{Re}\mathfrak{D}(\vec{A}^\dagger \cdot [h, \vec{A}]),\end{aligned} \tag{A18}$$

and that, for all operators $\vec{A}$ that we shall consider, $\vec{A}^\dagger \cdot [h, \vec{A}]$ will be real. Inserting Eqs. (A15) and (A18) into Eq. (A17), applying Schwarz's inequality to the last term in Eq. (A15), and using Eq. (A7), we obtain the inequality

$$\mathfrak{D}(A^2) \leq (\epsilon_2 - \epsilon_1)^{-1}\{\tfrac{1}{2}\mathfrak{D}([\vec{A}^\dagger, [h, \vec{A}]]) + (1-S^2)^{1/2}\,\|A^2(h-\epsilon_1)\psi_v\|\}. \tag{A19}$$

The usefulness of (A19) lies in the fact that the second term involves only known functions, while the argument of the first term reduces to something quite simple for many operators of interest. Specifically, after a moderate amount of commutative algebra, one finds, on choosing

$$\vec{A}^\dagger = \vec{A} = r_i^{l-1}\vec{r}_i, \quad l = 1, 2, \ldots, \tag{A20a}$$

that[11]

$$[\vec{A}, [h, \vec{A}]] = c_l(\hbar^2/m)r_i^{2l-2}, \tag{A20b}$$

where

$$c_1 = 3, \quad c_2 = 6, \quad c_3 = 11, \quad c_4 = 18, \ldots . \tag{A21}$$

Since we then have $A^2 = r_i^{2l}$, Eq. (A19) becomes

$$\mathfrak{D}(r_i^{2l}) \leq (\epsilon_2 - \epsilon_1)^{-1}[(c_l\hbar^2/2m)\mathfrak{D}(r_i^{2l-2}) + (1-S^2)^{1/2}\,\|r_i^{2l}(h-\epsilon_1)\psi_v\|]. \tag{A22}$$

The set of Eqs. (A21) and (A22), with the choices $l=4, 3, 2, 1$, bounds $\mathfrak{D}(r_i^q)$ for $q=8, 6, 4, 2$ in terms of calculable numbers plus $\mathfrak{D}(1)$ which can be bounded by using (A7) and bounding S.

This completes the information necessary to bound all of the quantities $\mathfrak{D}(r^q)$ which are needed in order to calculate the bounds in Sec. IV.

APPENDIX B: ALTERNATIVE BOUND ON ONE OF THE EXCHANGE INTEGRALS

As mentioned previously, the partition of the various exchange integrals, leading to the bounds of Sec. III, is not unique, and other choices are possible. It is not *a priori* clear that a particular choice will be superior to all others in every case; the alternative bounds presented in this Appendix are specifically constructed to avoid the necessity of computing the upper bound on $\mathfrak{D}(r_i^8)$ that occurs in Eq. (3.16). We will still need a bound on $\mathfrak{D}(r_i^4)$, so that the calculational effort saved will not be very great. The principal advantage is that the bound on $\mathfrak{D}(r_i^8)$, although formally of second order,

may tend to be rather large numerically for all but the most accurate wave functions. (For extremely accurate wave functions, it *is* clear that the details of partition are irrelevant.) The principal disadvantage is that the exact form of the bound will be different for different trial scattering wave functions.

We are concerned, then, with integrals of the form (3.14). We write the interaction potential as the sum of two terms

$$\left(-\frac{1}{r_3}+\frac{1}{r_{13}}\right)+\left(-\frac{1}{r_3}+\frac{1}{r_{23}}\right), \tag{B1}$$

so that (3.14) breaks up into the sum of two integrals, one of which can be written

$$K^{(a)}_{QQ_1}=\int\{Q(1,3)\psi_v(1,3)\}u_t(2)f^{-1}\times\left(-\frac{1}{r_3}+\frac{1}{r_{23}}\right)fu_t(3)\{Q(1,2)\psi_v(1,2)\}\,d\tau_{123}, \tag{B2}$$

where f remains to be chosen. It will be clear that the other integral, corresponding to the first of the two terms in expression (B1), can be treated in an identical manner, so we will confine our attention to (B2).

If we apply the Schwarz inequality to (B2), partitioning the integral as suggested by the multiplication sign, we obtain

$$K^{(a)}_{QQ_1}\leq\|u_t(2)f^{-1}Q(1,3)\psi_v(1,3)\|\times\|\left(-\frac{1}{r_3}+\frac{1}{r_{23}}\right)fu_t(3)Q(1,2)\psi_v(1,2)\|\,. \tag{B3}$$

We must choose f so that both factors on the right-hand side converge. For simplicity, we take f to be

$$f=F_2(2)F_3^{-1}(3) \tag{B4}$$

and note that, the integral

$$g(r_2)\equiv\int\left(-\frac{1}{r_3}+\frac{1}{r_{23}}\right)^2u_t^2(3)(1+\alpha_3r_3^n)^{-1}d\vec{r}_3$$

converges even for $n=0$, but for our purposes it will be convenient to choose $n=2$. In order for the first factor on the right-hand side of (B3) to converge, $F_2(2)$ must fall off faster than r_2^3. The simplest choice therefore appears to be

$$f=(1+\alpha_2r_2^4)^{1/2}(1+\alpha_3r_3^2)^{1/2}\,. \tag{B5}$$

With this choice, the second factor on the right-hand side of (B3) becomes

$$\mathfrak{D}_{12}^{1/2}[(1+\alpha_2r_2^4)g(r_2)]\,. \tag{B6}$$

We note that $g(r_2)$ vanishes at $r_2=0$, and behaves as $1/r_2$ at large r_2. $g(r_2)$ will be everywhere bounded by some number $g_{\max}\geq 0$. Then, since $(1+\alpha_2r_2^4)$ is always positive, a simple bound on (B6) will be given by $g_{\max}^{1/2}$ times a simple bound on $\mathfrak{D}_{12}^{1/2}(1+\alpha_2r_2^4)$, which we previously saw how to obtain.

It can now be seen that a simple bound on the integral (B2) will be given by

$$K^{(a)}_{QQ_1}\leq\left(g_{\max}(1-S^2)[1-S^2+\alpha_2\mathfrak{D}^{(+)}(r_2^4)]\times[\mathfrak{D}^{(+)}(1)+\alpha_3\mathfrak{D}^{(+)}(r_3^2)]\int\frac{u_t^2(2)}{1+\alpha_2r_2^4}\,d\vec{r}_2\right)^{1/2}. \tag{B7}$$

This bound is a simple bound which does not involve $\mathfrak{D}^{(+)}(r_t^8)$; it is, moreover, calculable in terms of previously discussed bounds. It is also clear that the other half of the integral (3.14) can be bounded in exactly the same way.

The bound (B7) was derived primarily as an example, to show the sorts of manipulations that can be performed on the exchange integrals of Sec. III, to obtain variants of the bounds on these integrals that were obtained in that section.

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