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Quasiparticle integral equations for the electron-hydrogen system

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Electron-hydrogen binding energy and scattering observables below the first excitation threshold are calculated with three-body integral equations reduced to effective two-body Lippmann-Schwinger-type equations by means of the quasiparticle method. The effective potentials occurring in this formulation are determined in lowest-order and in first-order quasi-Born approximation (QBA). In first-order QBA, our results are closely related to those obtained in the static exchange approximation. Polarization effects are only partly contained in the low-order quasi-Born-approximation terms considered, a fact discussed in the detailed analysis of our results.

I. INTRODUCTION

Coupled integral equations of the type proposed by Faddeev[1] have been widely used in nuclear three-body theory. There, due to the short range of the two-body interactions, various efficient expansion schemes have been developed which allow the reduction of the original relations to manageable effective two-body equations. It is the aim of the present paper to study the applicability of this approach to electron-atom scattering problems, especially the applicability to elastic electron-hydrogen collisions.

Until now only a few attempts have been made to work with such techniques in the latter field,[2–7] but standard treatments, such as variational,[8–12] polarized-orbital,[13] and close-coupling methods,[14–18] have been applied with considerable success.[19] By contrasting our results with those obtained by means of these conventional methods, considerable insight into the advantages and shortcomings of coupled integral equations when applied to situations with long-ranged Coulomb forces may be gained.

As mentioned, an essential step for the use of coupled three-body integral equations in practice consists of reducing them to effective two-body relations which, after partial-wave decomposition, become one-dimensional and, thus, amenable to numerical calculations. Introducing Faddeev-type integral equations for adequately chosen transition operators, this has been achieved in an exact and general way by Alt, Grassberger, and Sandhas (AGS).[20–24] These equations represent the basis of the following calculations of electron-hydrogen binding and elastic scattering.

The effective potentials occurring in this quasiparticle approach can be expanded into a series called the "quasi-Born series." In what follows, the lowest-order (0.QBA) and the first-order (1.QBA) quasi-Born approximation are taken into account.

The high symmetry of Faddeev-type equations allows, in particular, incorporation of the Pauli principle, and hence exchange effects, in a natural and reliable manner. On the other hand, the characteristic polarization effect due to virtual excitations of the hydrogen target cannot be expected to be included satisfactorily in 1.QBA. This supposition is supported by a comparison of our results with those obtained by means of the above-mentioned conventional methods.

The paper is organized as follows. In Sec. II the essential aspects of the quasiparticle method are recalled and the special approximations used in this paper are described. Section III contains the formalism specialized to the electron-hydrogen problem, including symmetrization and partial-wave decomposition. Details of the numerical treatment are explained in Sec. IV. There we also present our results and compare them with those obtained by standard techniques.

II. EFFECTIVE TWO-BODY EQUATIONS

To fix our notation and to make the paper self-contained, we first briefly recapitulate the quasiparticle formalism and describe in detail the two lowest-order quasi-Born approximations.

A. Quasiparticle method

Let us consider three particles α,β,γ interacting via pure Coulomb potentials. We denote the relative momentum between β and γ by $\vec{p}_\alpha$ and the corresponding reduced mass by μ_α. The relative momentum between the third particle α and the center of mass of the (β,γ) subsystem is denoted by $\vec{k}_\alpha$ and the reduced mass of the respective two fragments by M_α. The total interaction is given by a sum of two-body Coulomb potentials V_α, where the index α indicates that the interaction takes place between particles β and γ $(\beta,\gamma\neq\alpha)$.

Physical scattering processes in which a projectile α collides with a neutral two-body bound system (β,γ), leading to an outgoing configuration of a free particle β and a neutral two-body bound system (γ,α), are described by the transition amplitudes

$$\mathscr{T}_{\beta n,\alpha m}(\vec{k}'_\beta,\vec{k}_\alpha)=\langle\vec{k}'_\beta|\langle\psi_{\beta n}|U_{\beta\alpha}(E+i0)|\psi_{\alpha m}\rangle|\vec{k}_\alpha\rangle\ , \tag{2.1}$$

with the energies being restricted by the on-the-energy-shell condition

$$E'_{\beta n}=\frac{(k'_\beta)^2}{2M_\beta}+\hat{E}_{\beta n}=E_{\alpha m}=\frac{k_\alpha^2}{2M_\alpha}+\hat{E}_{\alpha m}=E\ . \tag{2.2}$$

Here $|\psi_{\alpha m}\rangle$ is the bound-state wave function of the (β,γ) subsystem with binding energy $\hat{E}_{\alpha m}$. The index m denotes collectively all quantum numbers of the bound state. The free movement of particle α relative to this bound state is represented by plane waves $|\vec{k}_\alpha\rangle$. The three-body transition operators $U_{\beta\alpha}$ occurring in (2.1) are given by the Faddeev-type Alt-Grassberger-Sandhas (AGS) equations[20]

$$U_{\beta\alpha}(z)=\bar{\delta}_{\beta\alpha}G_0^{-1}(z)+\sum_{\gamma=1}^{3}\bar{\delta}_{\beta\gamma}T_\gamma(z)G_0(z)U_{\gamma\alpha}(z)\ , \tag{2.3}$$

where $G_0(z)=(z-H_0)^{-1}$ is the resolvent of the free three-body Hamiltonian H_0, and $\bar{\delta}_{\beta\alpha}=1-\delta_{\beta\alpha}$. The two-body Coulomb T operator of the γ subsystem, acting in the whole three-body space, fulfills the Lippmann-Schwinger (LS) equation

$$T_\gamma(z)=V_\gamma+V_\gamma G_0(z)T_\gamma(z)\ . \tag{2.4}$$

Although the three-body problem is solved in principle by (2.3), the numerical treatment of these equations is not an easy task, because they are two dimensional after partial-wave decomposition. However, it has been shown by Alt, Grassberger, and Sandhas[20–24] that Eqs. (2.3) can be reduced to exact effective two-body equations (which are one dimensional after partial-wave decomposition) for off-shell extensions of the transition amplitudes (2.1). These equations, in other words, hold for amplitudes which are not restricted by the on-shell condition (2.2).

The starting point of this quasiparticle approach is the splitting of the subsystem T operator (2.4) into a sum of separable terms T_γ^s and the rest T'_γ,

$$\begin{aligned}T_\gamma(z)&=T_\gamma^s(z)+T'_\gamma(z)\\&=\sum_{r,s=1}^{N_\gamma}|\gamma r;z\rangle\Delta_{\gamma,rs}(z)\langle\underline{\gamma s;z}|+T'_\gamma(z)\ .\end{aligned} \tag{2.5}$$

The separable terms have to be constructed so that they contain the bound-state poles and other dominant contributions (quasiparticles) of T_γ; in other words, that T'_γ becomes as small as possible. This requirement provides some constraints on the otherwise arbitrary "form factors" $|\gamma r;z\rangle$ and $\langle\underline{\gamma s;z}|$ and "propagators" $\Delta_{\gamma,rs}(z)$. In the particular case of a bound-state pole this implies that at least one term of T_γ^s reproduces the pole denominator [via $\Delta_{\gamma,rs}(z)$] and the correct residue of T_γ. Special choices which fulfill these requirements are discussed below [cf. Eqs. (2.11)–(2.16)]. Inserting (2.5) into the AGS equations (2.3) and sandwiching them between $\langle\vec{k}'_\beta|\langle\underline{\beta n;z}|G_0(z)$ and $G_0(z)|\alpha m;z\rangle|\vec{k}_\alpha\rangle$, one immediately obtains exact effective two-body equations of matrix Lippmann-Schwinger form:

$$\mathscr{T}_{\beta n,\alpha m}(\vec{k}'_\beta,\vec{k}_\alpha;z)=\mathscr{V}_{\beta n,\alpha m}(\vec{k}'_\beta,\vec{k}_\alpha;z)+\sum_{\gamma=1}^{3}\sum_{r,s}\int d^3k''_\gamma\,\mathscr{V}_{\beta n,\gamma r}(\vec{k}'_\beta,\vec{k}''_\gamma;z)\hat{\Delta}_{\gamma,rs}\left[z-\frac{(k''_\gamma)^2}{2M_\gamma}\right]\mathscr{T}_{\gamma s,\alpha m}(\vec{k}''_\gamma,\vec{k}_\alpha;z)\ . \tag{2.6}$$

The effective transition amplitudes and potentials are given by

$$\mathscr{T}_{\beta n,\alpha m}(\vec{k}'_\beta,\vec{k}_\alpha)=\langle\vec{k}'_\beta|\langle\underline{\beta n}|G_0U_{\beta\alpha}G_0|\alpha m\rangle|\vec{k}_\alpha\rangle\ , \tag{2.7}$$

and

$$\mathscr{V}_{\beta n,\alpha m}(\vec{k}'_\beta,\vec{k}_\alpha)=\langle\vec{k}'_\beta|\langle\underline{\beta n}|G_0U'_{\beta\alpha}G_0|\alpha m\rangle|\vec{k}_\alpha\rangle\ , \tag{2.8}$$

respectively, the $U'_{\beta\alpha}$ being defined as solutions of the AGS equations with T_γ replaced by T'_γ,

$$U'_{\beta\alpha}=\bar{\delta}_{\beta\alpha}G_0^{-1}+\sum_{\gamma=1}^{3}\bar{\delta}_{\beta\gamma}T'_\gamma G_0U'_{\gamma\alpha}\ . \tag{2.9}$$

In the latter relations we have suppressed the evident z dependence and will do so also in the following if no confusion is to be expected. As mentioned above, $T_\gamma(z)$ is an operator in the three-body space. It is related to the genuine two-body transition operator $\hat{T}_\gamma(z)$ which acts in the two-body space of particles $\alpha,\beta\neq\gamma$, only, via

$$\langle\vec{k}'_\gamma|T_\gamma(z)|\vec{k}_\gamma\rangle=\delta(\vec{k}'_\gamma-\vec{k}_\gamma)\hat{T}_\gamma\left[z-\frac{k_\gamma^2}{2M_\gamma}\right]\ , \tag{2.10}$$

and similar relationships hold true for the other quantities in (2.5). A consequence of this is that instead of the propagator $\Delta_{\gamma,rs}(z)$, its two-body restriction $\hat{\Delta}_\gamma(z-k_\gamma^2/2M_\gamma)$ occurs in (2.6). Comparison with (2.1) shows that only those elements (2.7) correspond to the physical amplitudes (2.1) for which the form factors $|\alpha m;z\rangle$ satisfy the on-shell restrictions

$$G_0(E_{\alpha m})|\alpha m;z=E_{\alpha m}\rangle|\vec{k}_\alpha\rangle=|\psi_{\alpha m}\rangle|\vec{k}_\alpha\rangle\ , \tag{2.11}$$

and analogous ones for $\langle\underline{\beta n;z}|$. Other separable terms, introduced in (2.5) in order to get the correction T'_γ sufficiently small, lead to elements (2.7) which do not correspond to any physical transition process.

It is a characteristic feature of this reduction procedure that it provides us with exact effective two-body equations which, as in the genuine two-body case, are one dimensional after partial-wave decomposition. In other words, the original three-body equations are replaced by relations well suited for practical applications. Let us mention that Eqs. (2.3) and hence (2.6) not only yield the scattering observables, but, solving their homogeneous versions, determine also the bound-state problem.

Until now the reduction scheme has been kept completely general. For its application special choices of the form factors and of the propagators in (2.5) are needed.

One possibility consists in splitting first the potential V_γ according to

$$V_\gamma = V^s_\gamma + V'_\gamma = \sum_{r=1}^{N_\gamma} |\chi_{\gamma r}\rangle \lambda_{\gamma r} \langle \chi_{\gamma r}| + V'_\gamma \tag{2.12}$$

into a sum of separable terms and a nonseparable rest V'_γ (this splitting may be made in a z-dependent way). Then, via (2.4), a corresponding splitting of T_γ of the form (2.5) is obtained, with the rest amplitude T'_γ being defined as a solution of

$$T'_\gamma = V'_\gamma + V'_\gamma G_0 T'_\gamma \ . \tag{2.13}$$

The form factors in T^s_γ are related to the form factors $|\chi_{\gamma r}\rangle$ in V^s_γ by

$$|\gamma r\rangle = (1 + T'_\gamma G_0)|\chi_{\gamma r}\rangle \ , \tag{2.14}$$

and

$$\langle \underline{\gamma r}| = \langle \chi_{\gamma r}|(1 + G_0 T'_\gamma) \ , \tag{2.15}$$

respectively, and the propagator matrix Δ_γ is given by

$$(\Delta_\gamma{}^{-1})_{rs} = \delta_{rs}\lambda_{\gamma r}^{-1} - \langle \chi_{\gamma r}|(G_0 + G_0 T'_\gamma G_0)|\chi_{\gamma s}\rangle \ . \tag{2.16}$$

Of course, those $|\chi_{\gamma r}\rangle$ corresponding to bound states have to be chosen such that the form factors (2.14) associated with them fulfill the requirement (2.11).

The concept of starting from a splitting (2.12) of the potential in order to obtain a corresponding splitting of T_γ is suggested by the existence of several systematical methods for choosing V^s_γ which, at least for short-ranged potentials, lead rather quickly to sufficiently small correction terms V'_γ and hence to small rest amplitudes T'_γ.[23,25] It is the aim of the present investigation to study whether a splitting of this type can be found which also in the Coulomb case leads to sufficiently small rest terms. In Sec. III the choice used in this paper will be discussed in detail.

It should, however, be emphasized that the quasiparticle approach is by no means restricted to expansion schemes of the potential. Any alternative method leading to an adequate separation (2.5) may be used as well. In Ref. 21, e.g., the kernel of the AGS equations has been split by multiplying with projections P_γ and Q_γ on different parts of the spectrum, i.e., by writing

$$G_0 T_\gamma G_0 = G_0 V_\gamma G_\gamma(\mathsf{P}_\gamma + \mathsf{Q}_\gamma) = G_0 T^s_\gamma G_0 + G_0 T'_\gamma G_0 \ . \tag{2.17}$$

Or, equivalently, representing the same kernel in the form $G_\gamma V_\gamma G_0$, we may multiply from the left with the above sum of projections. For details and further choices we refer to Ref. 21. There, also the relationship with the Feshbach formalism is exhibited. Although such choices may be of interest in the Coulomb case too, they will not be studied in the present investigation.

B. Quasi-Born approximation

The exact definitions of the effective potentials (2.8) and the propagators $\hat{\Delta}_{\gamma,rs}$ given by (2.16) provide us with an adequate starting point for different approximation schemes as, e.g., the separable expansion method or the quasi-Born approximation (QBA). This has been discussed in detail in Ref. 23. We briefly recall the most important aspects of this discussion.

In the separable expansion method one chooses the number N_γ of separable terms in (2.12) so large that V'_γ, and thus T'_γ, too, can be neglected. Although this procedure results in very simple effective potentials, it has the disadvantage that even for short-ranged two-body interactions the dimension of the matrices in (2.6) is usually comparatively high. This becomes much more serious in the Coulomb case[3,4] where the potential cannot be expected to be well approximated, if at all, by a reasonably low number of separable terms.[26]

In the quasi-Born-approximation method the number N_γ of separable terms is kept as small as possible. That means only terms corresponding to dominant subsystem structures are introduced. Of course, the rest amplitude T'_γ can no longer be neglected but has to be taken into account, e.g., perturbatively. By iterating (2.9)

$$U'_{\beta\alpha} = \bar{\delta}_{\beta\alpha} G_0^{-1} + \sum_{\gamma=1}^{3} \bar{\delta}_{\beta\gamma}\bar{\delta}_{\gamma\alpha} T'_\gamma + \cdots \ , \tag{2.18}$$

and inserting this expansion in (2.8), we obtain the quasi-Born-approximation series of the effective potential

$$\mathscr{V}_{\beta n,\alpha m}(\vec{k}'_\beta, \vec{k}_\alpha) = \bar{\delta}_{\beta\alpha} \langle \vec{k}'_\beta | \langle \beta n | G_0 | \alpha m \rangle | \vec{k}_\alpha \rangle + \sum_{\gamma=1}^{3} \bar{\delta}_{\beta\gamma}\delta_{\gamma\alpha} \langle \vec{k}'_\beta | \langle \underline{\beta n} | G_0 T'_\gamma G_0 | \alpha m \rangle | \vec{k}_\alpha \rangle + \cdots \ . \tag{2.19}$$

In lowest order (0.QBA), which corresponds to setting $T'_\gamma = 0$, we have

$$\mathscr{V}^{(0)}_{\beta n,\alpha m}(\vec{k}'_\beta, \vec{k}_\alpha) = \bar{\delta}_{\beta\alpha} \langle \vec{k}'_\beta | \langle \chi_{\beta n} | G_0 | \chi_{\alpha m} \rangle | \vec{k}_\alpha \rangle \ , \tag{2.20}$$

as in the separable expansion method.

In the 1.QBA of the effective potential the corrections linear in T'_γ have to be considered in addition. Thus the 1.QBA consists of the nondiagonal terms ($\beta \neq \alpha$),

$$\mathscr{V}^{(1)}_{\beta n,\alpha m}(\vec{k}'_\beta, \vec{k}_\alpha) = \mathscr{V}^{(0)}_{\beta n,\alpha m}(\vec{k}'_\beta, \vec{k}_\alpha) + \sum_{\gamma=1}^{3} \langle \vec{k}'_\beta | \langle \chi_{\beta n} | G_0 T'_\gamma G_0 | \chi_{\alpha m} \rangle | \vec{k}_\alpha \rangle \ , \tag{2.21}$$

and the diagonal terms ($\beta = \alpha$),

$$\mathscr{V}^{(1)}_{\alpha n,\alpha m}(\vec{k}'_\alpha, \vec{k}_\alpha) = \sum_{\gamma=1}^{3} \bar{\delta}_{\gamma\alpha} \langle \vec{k}'_\alpha | \langle \chi_{\alpha n} | G_0 T'_\gamma G_0 | \chi_{\alpha m} \rangle | \vec{k}_\alpha \rangle \tag{2.22}$$

(see Fig. 1). The question of convergence of the quasi-Born expansion for short-ranged potentials has been investigated in Refs. 23 and 25.

Besides the low dimension of the matrix equation (2.6), the quasi-Born method is characterized by the fact that all subsystem partial-wave contributions which are not contained explicitly in T^s_γ enter the effective potentials via T'_γ. However, the computation of the effective potentials in 1.QBA becomes much more time consuming.

III. SPECIALIZATION TO THE ELECTRON-HYDROGEN SYSTEM

In the following sections we apply the general formalism of Sec. II to the scattering of electrons off hydrogen atoms.

A. Choice of form factors

In this section we work in the two-particle space only. Since no confusion is to be expected, the labeling with a hat, as used in Eq. (2.10), is suppressed. However, when going over to the three-body space, the momentum δ function and the energy shift occurring there must be added (see, e.g., Ref. 20).

According to (2.12) the subsystem interactions have to be approximated by separable terms such that the rest V'_α can be taken into account perturbatively. Weinberg's "ideal choice"[27] is well-known to work efficiently in the short-range case. The calculations of Ball, Chen, and Wong[3] show that in the Coulomb case the expansion into Sturmian functions leads to a very slowly convergent or even nonconvergent series. Hence we use only the first term of this expansion needed to simulate via T^s_α the subsystem ground-state pole. With this choice our 0.QBA is identical with the 1*s* approximation of Refs. 3 and 4 which allows comparison with our results. The use of just this choice of T^s_α is also suggested by the results of Refs. 3 and 4. According to these references the zeroth order is already a good approximation for *S* waves in the spin-singlet channel, which means that at least in this case it is justified to take into account T'_α perturbatively. In the other cases the first term of the Sturmian expansion is not a good approximation. Here it only serves as a means to reduce the dimension of the three-body equations. Consequently the correction due to T'_α should be remarkable. To study whether the first order correction in T'_α leads to a sufficient accuracy is the aim of the following numerical investigations in Sec. IV.

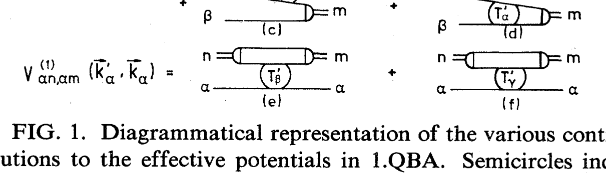

FIG. 1. Diagrammatical representation of the various contributions to the effective potentials in 1.QBA. Semicircles indicate the form factors.

As discussed, Sturmian functions are used to construct T^s_α. They are defined as energy-dependent eigenstates of the two-body *LS* kernel G_0V_α, normalized to unity, for arbitrary two-particle energy E_α,

$$G_0(E_\alpha)V_\alpha\,|\,\psi_{\alpha n}(E_\alpha)\rangle=\eta_{\alpha n}(E_\alpha)\,|\,\psi_{\alpha n}(E_\alpha)\rangle\ . \tag{3.1}$$

Then the "ideal choice" form factors are given by

$$|\,\chi_{\alpha n}(E_\alpha)\rangle=V_\alpha\,|\,\psi_{\alpha n}(E_\alpha)\rangle\ , \tag{3.2}$$

and the strength parameters in (2.12) are fixed via

$$\lambda_{\alpha n}(E_\alpha)\langle\chi_{\alpha n}(E_\alpha)\,|\,\psi_{\alpha m}(E_\alpha)\rangle=\delta_{nm}\ . \tag{3.3}$$

An important property of this choice is that the rest potential V'_α defined via (2.12) acts on the form factors according to

$$V'_\alpha G_0(E_\alpha)\,|\,\chi_{\alpha n}(E_\alpha)\rangle=0\ . \tag{3.4}$$

It should be noted that for this choice the on-shell condition (2.11) is automatically fulfilled.

The infinitely many eigenvalues are all positive (negative) for attractive (repulsive) Coulomb potentials as long as $E_\alpha\leq 0$. If E_α coincides with one of the hydrogen binding energies $E_{\alpha n}$, the corresponding Sturmian function is just the respective bound-state wave function, and $\eta_{\alpha n}(E_{\alpha n})$ equals 1 in the attractive, and -1 in the repulsive case. This in particular means that, at a fixed negative energy, $|\,\eta_{\alpha n}\,|\geq 1$ can occur only for a *finite* number of eigenvalues. To obtain in the attractive case a sufficiently small rest term T'_α, at least those Sturmian functions have to be incorporated in T^s_α for which $\eta_{\alpha n}\geq 1$ within the energy range under consideration. Then the poles of $T_\alpha(E_\alpha)$ at $E_\alpha=E_{\alpha n}$ show up solely in T^s_α. In the repulsive case we may similarly construct T^s_α from all Sturmian functions belonging to large negative eigenvalues, $\eta_{\alpha n}\leq -1$. This is, however, less compelling because of the absence of (dominant) bound-state poles. It is, however, important if the additional approximation

$$T'_\alpha\simeq V'_\alpha \tag{3.5}$$

is made which otherwise would not be justifiable. In the following we restrict ourselves to subsystem energies below the first excited state $n=2$. Hence, according to this prescription only one separable term has to be introduced in each of the attractive potentials. Correspondingly, in the repulsive potential we also take one separable term representing an electron-electron quasiparticle (for this terminology, see Ref. 27).

In coordinate space the two-body interactions are

$$V_\alpha(\vec{r}_\alpha)=\mp\frac{e^2}{r_\alpha}\ , \tag{3.6}$$

and the corresponding eigenvalue equations (3.1) read

$$\left[\Delta_\alpha-\frac{2\kappa_\alpha\gamma_\alpha}{\eta_\alpha(E_\alpha)r_\alpha}-\kappa_\alpha^2\right]\psi_\alpha(\vec{r}_\alpha,E_\alpha)=0\ . \tag{3.7}$$

Here the Coulomb parameter is defined by $\gamma_\alpha=\mp\mu_\alpha e^2/\kappa_\alpha$ and κ_α is given by $\kappa_\alpha=(-2\mu_\alpha E_\alpha)^{1/2}$. The minus sign always refers to the electron-proton subsystem and the plus sign to the electron-electron subsystem. The relative coordinate between the particles β and γ is denoted by $\vec{r}_\alpha$. From the solution of (3.7) one obtains for the eigenvalues

$$\eta_{\alpha n}(E_\alpha)=-\frac{\gamma_\alpha}{n}, \quad n=1,2,3,\ldots . \tag{3.8}$$

The corresponding normalized eigenfunctions are

$$\psi_{\alpha,nlm}(\vec{r}_\alpha,E_\alpha)=\varphi_{\alpha,nl}(r_\alpha,E_\alpha)Y_{lm}(\Omega_{\vec{r}_\alpha}) ,$$

$$l=0,1,\ldots,n-1, \quad m=-l,\ldots,l ,$$

with

$$\varphi_{\alpha,nl}(r_\alpha,E_\alpha)=\left[(2\kappa_\alpha)^3\frac{(n-l-1)!}{2n[(n+l)!]^3}\right]^{1/2} \times\exp(-\kappa_\alpha r_\alpha)(2\kappa_\alpha r_\alpha)^l L_{n-l-1}^{2l+1}(2\kappa_\alpha r_\alpha) , \tag{3.9}$$

the L_{n-l-1}^{2l+1} being the Laguerre polynomials. In contrast to the hydrogen bound-state problem, normalizable solutions of (3.7) exist for each energy because the interactions (3.6) appear there as being modified by energy-dependent factors $\eta_{\alpha n}(E_\alpha)$. At the binding energies of the hydrogen atom, (3.7) becomes the usual bound-state Schrödinger equation with $\eta_{\alpha n}=1$, and the solutions (3.9) are then the bound-state wave functions of the hydrogen atom.

From (3.6) and (3.9) one finds the form factors (3.2) in momentum space by Fourier transformation, the first one being given by

$$\chi_{\alpha,100}(\vec{p}_\alpha,E_\alpha)=\mp\frac{\sqrt{2}\kappa_\alpha^{3/2}e^2}{\pi(p_\alpha^2+\kappa_\alpha^2)} . \tag{3.10}$$

A general expression for the parameters $\lambda_{\alpha n}$ can be calculated from (3.3),

$$\lambda_{\alpha n}(E_\alpha)=\mp\frac{n}{\kappa_\alpha e^2} , \tag{3.11}$$

and the propagator (2.16) becomes

$$\Delta_{\alpha,nm}(E_\alpha)=\delta_{nm}\frac{\lambda_{\alpha n}}{1-\eta_{\alpha n}}=\delta_{nm}\frac{n^2}{\mu_\alpha e^4\mp ne^2\kappa_\alpha} . \tag{3.12}$$

Equation (3.12) shows explicitly that all bound states which are contained in the separable parts of (2.5) ($\alpha=1$ or 2) give rise to poles with residues equal to 1 at the corresponding binding energies.

B. Electron-hydrogen integral equations

In the following we use atomic units (a.u.), i.e., energies are measured in units of e^2/a_0, a_0 being the Bohr radius. We also insert for the reduced masses the values $\mu_1=\mu_2=1$, $\mu_3=\frac{1}{2}$, and $M_1=M_2=1$, $M_3=2$. Let us consider an incoming electron "1" which collides with a hydrogen atom in the ground state. Then the total energy in a.u. is $E=\frac{1}{2}(k_1^2-1)$, and from (3.8) it follows for the first attractive eigenvalue ($\alpha=1$ or 2) that $\eta_{\alpha 1}(E)\geq 1$ in the elastic scattering region $-\frac{1}{2}\leq E<-\frac{1}{8}$. Hence, in agreement with the discussion following Eq. (3.4), we build up the separable part of the interaction V_α with the corresponding form factor (3.10) and the parameter $\lambda_{\alpha 1}$. That is, we explicitly take into account the dominant hydrogen ground state in the effective propagators of Eqs. (2.6). Further inspection of (3.8) shows that for three-body energies $-\frac{1}{4}\leq E<-\frac{1}{8}$ also the magnitude of the first repulsive eigenvalue $\eta_{31}(E)$ becomes larger than one. In order to guarantee that in the elastic scattering region the absolute values of *all* eigenvalues of the rest kernel $G_0V'_\alpha$ are smaller than one, we extract the corresponding separable term from the repulsive interaction, too.

As usual, we neglect the proton spin, and choose as spin basis the eigenstates of the total spin S. Thus, we distinguish between a spin-singlet ($S=0$) and a spin-triplet ($S=1$) channel described by corresponding amplitudes $\mathcal{T}_{\beta\alpha}^S$. Due to conservation of the total spin, these two channels are decoupled and we are left with three coupled equations for each of them.

Due to the fact that the incoming electron "1" and the target electron "2" are indistinguishable, we have to consider the symmetrized amplitude

$$\mathcal{T}^S(\vec{k}',\vec{k})=\mathcal{T}_{11}^S(\vec{k}',\vec{k})-(-1)^{1-S}\mathcal{T}_{21}^S(\vec{k}',\vec{k}) \tag{3.13}$$

being composed of the direct and the exchange amplitudes. In complete analogy to (3.13), symmetrized effective potentials have to be used in the final equations.

Since in our calculations the separable parts of the two-body interactions (quasiparticles) have been chosen to contain only s-wave components, as discussed after Eq. (3.5), the total angular momentum is given by the angular momentum L between the third particles relative to the respective quasiparticles. Expanding the amplitude (3.13) into Legendre polynomials $P_L(x)$, the corresponding partial-wave amplitudes $\mathcal{T}_{\beta\alpha}^{SL}$ are defined by

$$\mathcal{T}_{\beta\alpha}^S(\vec{k}',\vec{k})=\frac{1}{4\pi}\sum_{L=0}^{\infty}(2L+1)\mathcal{T}_{\beta\alpha}^{SL}(k',k)P_L(\cos\theta) , \tag{3.14}$$

with θ being the scattering angle. After completing the partial-wave decomposition of the effective potentials in analogy to (3.14), one finally arrives at a single one-dimensional equation for each triplet partial-wave amplitude,

$$\mathcal{T}^{1L}(k',k;E)=\mathcal{V}^{1L}(k',k;E)+\int_0^\infty dk''(k'')^2\mathcal{V}^{1L}(k',k'';E)\hat{\Delta}_1(E-\tfrac{1}{2}(k'')^2)\mathcal{T}^{1L}(k'',k;E) \tag{3.15}$$

and at two coupled one-dimensional equations for each singlet partial-wave amplitude,

$$\mathscr{T}^{0L}(k',k;E)=\mathscr{V}^{0L}(k',k;E)+\int_0^\infty dk''(k'')^2\mathscr{V}^{0L}(k',k'';E)\hat{\Delta}_1(E-\tfrac{1}{2}(k'')^2)\mathscr{T}^{0L}(k'',k;E)$$
$$+2\int_0^\infty dk''(k'')^2\mathscr{V}^{L}_{13}(k',k'';E)\hat{\Delta}_3(E-\tfrac{1}{4}(k'')^2)\mathscr{T}^{L}_{31}(k'',k;E)\,, \tag{3.16}$$

$$\mathscr{T}^{L}_{31}(k',k;E)=\mathscr{V}^{L}_{31}(k',k;E)+\int_0^\infty dk''(k'')^2\mathscr{V}^{L}_{31}(k',k'';E)\hat{\Delta}_1(E-\tfrac{1}{2}(k'')^2)\mathscr{T}^{0L}(k'',k;E)$$
$$+\int_0^\infty dk''(k'')^2\mathscr{V}^{L}_{33}(k',k'';E)\hat{\Delta}_3(E-\tfrac{1}{4}(k'')^2)\mathscr{T}^{L}_{31}(k'',k;E)\,. \tag{3.17}$$

The propagators occurring in (3.15)—(3.17) are given by

$$\hat{\Delta}_1(E-\tfrac{1}{2}(k'')^2)=\frac{1}{1-[(k'')^2-2E]^{1/2}}\,, \tag{3.18}$$

and

$$\hat{\Delta}_3(E-\tfrac{1}{4}(k'')^2)=\frac{2}{1+2[(k'')^2/4-E]^{1/2}}\,. \tag{3.19}$$

The effective potentials are described in detail in the Appendix.

Let us add some comments. Equation (3.18) shows explicitly that the bound-state pole at the two-body energy $\hat{E}_1=-\frac{1}{2}$ leads to a branch cut in (3.15)—(3.17) for three-body energies $E\geq-\frac{1}{2}$. Since in the singlet channel an electron-electron quasiparticle can be formed [see the comments following Eq. (3.5)], the corresponding transition amplitude $\mathscr{T}_{31}$ has to be taken into account, which gives rise to a higher dimension of the matrix equation in this case. We furthermore notice that the diagonal term $\mathscr{V}^{(1)}_{33}$ arising in 1.QBA admits the decomposition [see (A7)]

$$\mathscr{V}^{(1)}_{33}(\vec{k}'_3,\vec{k}_3)=-\frac{8\{[(k'_3)^2-4E](k_3^2-4E)\}^{1/4}}{\pi^2\{[(k'_3)^2-4E]^{1/2}+(k_3^2-4E)^{1/2}\}^3(\vec{k}'_3-\vec{k}_3)^2}+\tilde{\mathscr{V}}^{(1)}_{33}(\vec{k}'_3,\vec{k}_3)\,. \tag{3.20}$$

The first term contains the Coulomb potential $-1/\pi^2(\vec{k}'_3-\vec{k}_3)^2$ between the proton and the electron-electron subsystem which in coordinate space reads as $v_3(\vec{\rho}_3)=-2/\rho_3$, $\vec{\rho}_3$ being the corresponding relative coordinate. It is due to this singularity in (3.20), which arises from the infinite range of v_3, that the numerical treatment of the singlet channel requires much more effort than the triplet case, where an analogous term is forbidden by the Pauli principle.

IV. RESULTS AND DISCUSSION

In this section we give details of the numerical treatment and compare our results with those obtained by other methods.

A. Numerical methods

The integral equations (3.15)—(3.17) have been transformed to matrix equations by means of Gauss-Legendre quadrature rules and solved numerically by the Gauss-Jordan algorithm. We furthermore make the additional approximation $T'_\alpha=V'_\alpha$ ($\alpha=1,2,3$) which allows the evaluation of all effective potentials in 1.QBA analytically.[28] For the strong nuclear interactions this has been shown to work very well.[23] In the present case, due to the smallness of the electric force, this approximation should be justified even better in the repulsive electron-electron subsystem.[29] Remarkable corrections, however, are to be expected in the attractive electron-proton subsystems (when going to higher orders of the quasi-Born expansion) due to virtual target excitations contained in T'_α. The order of magnitude of this polarization effect is discussed below (see Fig. 16) and will be studied more thoroughly in a subsequent publication. A first report of these results has been given in Ref. 30.

After partial-wave decomposition, our effective potentials are essentially given by combinations of Legendre polynomials of the second kind and their derivatives. Due to this fact the numerical calculations required not much computing time. For instance, one singlet partial-wave amplitude in 1.QBA took 80 sec of CPU (central processing unit) time on an IBM model 370/168 computer for the claimed accuracy.

In order to determine the three-body binding energy of H^- from the homogeneous version of (3.16) and (3.17), the zero of the determinant of $1-\mathscr{K}$, $\mathscr{K}$ being the kernel of (3.16) and (3.17), has been evaluated. To calculate the transition amplitudes in the elastic scattering region, the propagator-pole singularities have been regularized by a subtraction method. Stability has been found, for instance, in the singlet channel in 1.QBA, to four decimal places with 48 mesh points.

Numerical problems arose from the Coulomb singularity in the diagonal part (3.20) of the effective interaction. It has been treated by the following subtraction method. The integral equation (3.17) is reduced to a nonsingular equation plus some singular integrals by splitting the kernel $\mathscr{K}$ into the sum

$$\mathscr{K}=\mathscr{K}^{(\mathrm{c.m.})}+\mathscr{K}'\,, \tag{4.1}$$

where the contribution of the center-of-mass Coulomb potential $v_3=-2/\rho_3$ is contained in $\mathscr{K}^{(\mathrm{c.m.})}$. The rest term $\mathscr{K}'$ consists of the shorter-ranged parts only, and thus does not give rise to numerical problems. A simple algebraic manipulation leads to the nonsingular equation

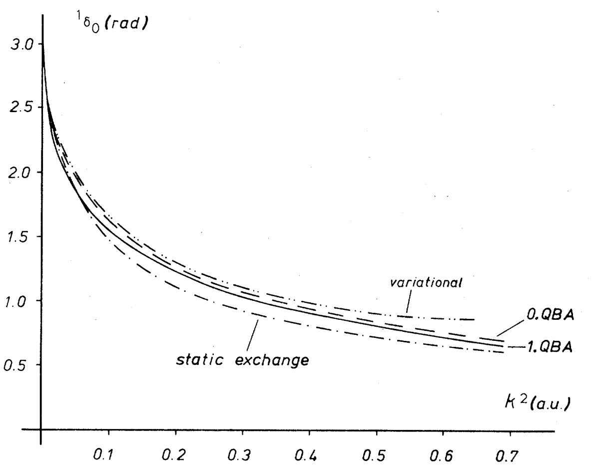

FIG. 2. Singlet S-wave elastic electron-hydrogen phase shifts as a function of k^2 in 0.QBA and in 1.QBA. For comparison variational (Ref. 9) and SEA results (Ref. 14) are included.

$$\mathcal{T}(k_i)=\mathcal{V}(k_i)+\sum_{j\neq i} w_j\mathcal{K}(k_i,k_j)\mathcal{T}(k_j)+\left\{\mathcal{H}(k_i)-\sum_{j\neq i} w_j\mathcal{K}^{(\mathrm{c.m.})}(k_i,k_j)+w_i\mathcal{K}'(k_i,k_i)\right\}\mathcal{T}(k_i)\,, \tag{4.2}$$

where w_i are the weights belonging to the discrete Gauss points k_i. For simplicity we suppressed the second variable in $\mathcal{T}$ and $\mathcal{V}$. The singular integrals

$$\mathcal{H}(k_i)=\int_0^\infty dk'\mathcal{K}^{(\mathrm{c.m.})}(k_i,k') \tag{4.3}$$

have been determined with a k_i-dependent integration mesh, adapted to the special form of the integrand.

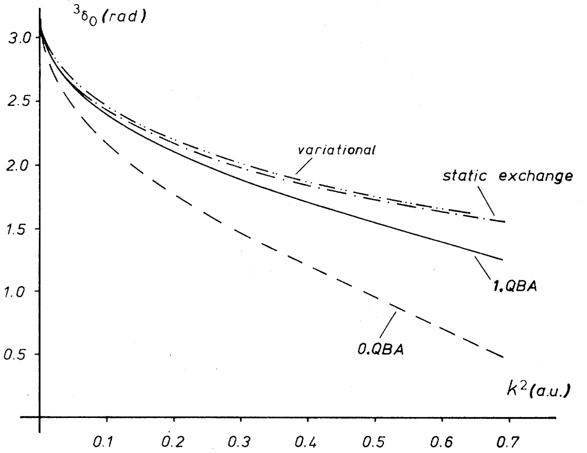

FIG. 3. As in Fig. 2, but for the triplet channel.

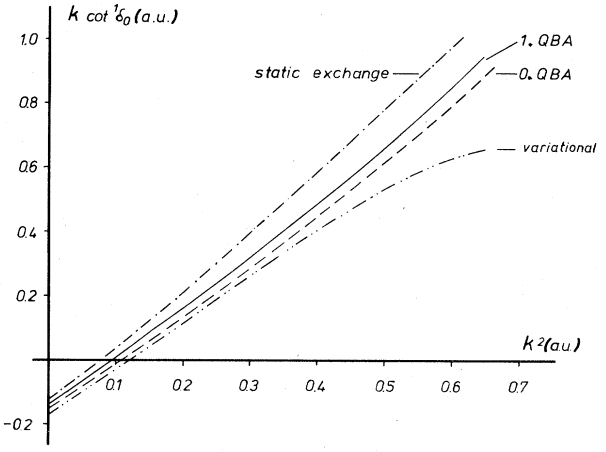

FIG. 4. Plot of $k\cot{}^1\delta_0$ vs k^2 in 0.QBA and in 1.QBA. References as in Fig. 2.

B. Phase shifts, scattering lengths, and three-body binding energy

In Figs. 2 and 3 we have plotted the singlet ($^1\delta_0$) and triplet ($^3\delta_0$) S-wave phase shifts, and in Figs. 4 and 5 the corresponding results for $k\cot^{2S+1}\delta_0$, in 0.QBA and in 1.QBA. For comparison we also show the values obtained by variational methods[9] and the static exchange approximation (SEA).[14] The 1.QBA is related[31] to the SEA. Both have in common that they contain only the hydrogen ground-state explicitly and allow for electron exchange processes, but differ completely in the off-shell treatment of their respective effective potentials.

In Table I we present our results for the H^- binding energy E_B and for the singlet (^1a) and the triplet (^3a) scattering lengths, in 0.QBA and in 1.QBA. For comparison we include the corresponding values obtained by variational methods,[8,9] close-coupling approximations,[14–16] and integral equation techniques[2–6] as well as an experi-

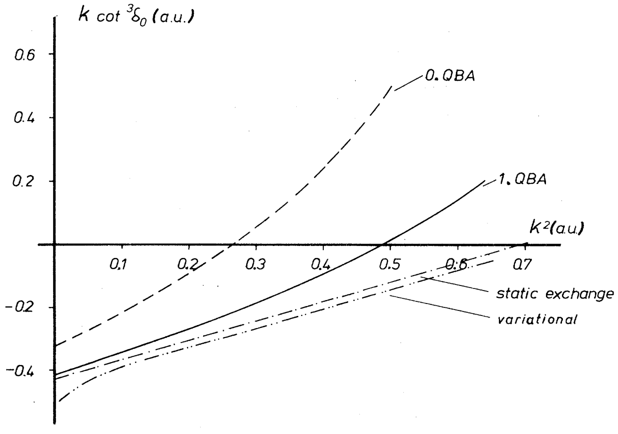

FIG. 5. Same as in Fig. 4, but for the triplet channel.

TABLE I. H$^-$ binding energy, and singlet and triplet scattering lengths in 0.QBA and in 1.QBA. Comparison is made with results obtained by other techniques and with an experimental value for the three-body binding energy.

	0.QBA	1.QBA		
E_B (a.u.)	−0.5255	−0.5172	−0.62[a]	−0.525[b]
			−0.5315[c]	−0.52775[d]
			−0.543[e]	−0.52773[f]
${}^1a$ (a_0)	6.32	7.22	4.0[a]	5.965[g]
			6.337[h]	8.095[i]
			5.6[e]	7.5[j]
				6.742[k]
${}^3a$ (a_0)	3.12	2.43	2.7[a]	1.769[g]
			3.112[h]	2.35[i]
			2.2[e]	2.33[j]
				1.893[k]

[a] Separable approximation, Ref. 2.
[b] Separable approximation, Ref. 6.
[c] Separable expansion, Ref. 3.
[d] Variational, Ref. 8.
[e] Reference 5.
[f] Experiment, Ref. 32.
[g] Variational, Ref. 9.
[h] Separable approximation, Ref. 4.
[i] Static exchange, Ref. 14.
[j] Close coupling ($1s$-$2s$), Ref. 15.
[k] Close coupling ($1s$-$2s$-$2p$), Ref. 16.

mental value for the three-body binding energy.[32] Tables II and III list the S-wave phase shifts. Here, in addition, a close-coupling calculation[18] has been included which simulates the full effect of the electric dipole polarizability of the hydrogen ground state by means of a pseudostate.

In 0.QBA, our singlet phase shifts come very close to the variational results,[9] and the singlet scattering length looks quite reasonable, even compared to a three-state close-coupling calculation.[16] For the H$^-$ binding energy the agreement of this lowest-order approximation with variational[8] and experimental[32] results is particularly good. This has already been found in the rank-one approximation of Ref. 3, which coincides with our 0.QBA. Thus the binding of the second electron to the hydrogen atom can be well described by a pure exchange potential.

Although the singlet results in 1.QBA deviate more from the variational values they are still acceptable. Of particular interest is the agreement (cf. Table II) between the 1.QBA singlet phase shifts and those obtained by a close-coupling calculation[18] which incorporates polarization effects due to the virtual excitation of the target electron into higher bound states and the continuum, using the $2\bar{p}$ pseudostate given in Ref. 33. Investigation of the various parts of the effective potential (see Fig. 1) reveals that each of them is the origin of a sizable correction to the 0.QBA. However, a complicated cancellation mechanism makes the overall correction small as compared to the individual contributions, and repulsive, thereby increasing the deviation from the variational results. Consequently, the higher QBA's must again provide some more attraction, a behavior which is reminiscent of the oscillatory convergence found in the separable expansion method.[3,4]

The triplet S-wave phase shifts in 0.QBA are much smaller than the variational results, especially at higher energies, and the corresponding scattering length is too large. This is not surprising since the electron-electron interaction is completely neglected in this approximation; i.e., the presence of the second electron is taken into account only indirectly via the Pauli principle. Since the first-order corrections are dominated by the repulsive Coulomb interaction between the electrons, the 0.QBA is considerably improved by adding these effectively attractive corrections in 1.QBA. At low energies the agreement between the 1.QBA and other theoretical results is now quite reasonable. However, the discrepancies become larger with increasing energy, indicating that the 1.QBA needs further improvement at higher energies. This could have been anticipated since the magnitude of the largest eigenvalue of the rest kernel $G_0 V'_\alpha$, which determines the convergence of the QBA series, approaches unity as we come close to the first excitation threshold.

In Figs. 6–9 we compare the P- and D-wave singlet (${}^1\delta_1, {}^1\delta_2$) and triplet (${}^3\delta_1, {}^3\delta_2$) phase shifts with the corresponding variational[10,11] and SEA (Ref. 14) results. In 0.QBA the effective potential gives no contribution at all to triplet scattering whereas in the singlet case only the effective electron exchange interaction is operative. It is, therefore, not surprising that the lowest-order QBA is in-

TABLE II. Singlet S-wave elastic electron-hydrogen phase shifts at various electron momenta k. Results obtained in 0.QBA and in 1.QBA are compared with the SEA (Ref. 14), the $1s$-$2\bar{p}$ pseudostate close-coupling (Ref. 18), and variational results (Ref. 9).

k	0.QBA	1.QBA	SEA	$1s$-$2\bar{p}$	Variational
0.1	2.5367	2.4651	2.396		2.553
0.2	2.0480	1.9608	1.870		2.0673
0.3	1.6800	1.6035	1.508	1.637	1.6964
0.4	1.3993	1.3373	1.239		1.4146
0.5	1.1801	1.1301	1.031	1.131	1.202
0.6	1.0055	0.9642	0.8690	0.959	1.041
0.7	0,8633	0.8280	0.7441	0.829	0.930
0.8	0.7445	0.7126	0.6512	0.734	0.886

TABLE III. Triplet S-wave elastic electron-hydrogen phase shifts at various electron momenta k computed in 0.QBA and in 1.QBA as compared with the SEA (Ref. 14), the $1s$-$2\bar{p}$ pseudostate close-coupling (Ref. 18), and variational results (Ref. 9).

k	0.QBA	1.QBA	SEA	$1s$-$2\bar{p}$	Variational
0.1	2.8299	2.8994	2.908		2.9388
0.2	2.5205	2.6612	2.679		2.7171
0.3	2.2149	2.4304	2.461	2.498	2.4996
0.4	1.9130	2.2082	2.257		2.2938
0.5	1.6122	1.9939	2.070	2.102	2.1046
0.6	1.3068	1.7834	1.901	1.930	1.9329
0.7	0.9852	1.5683	1.749	1.776	1.7797
0.8	0.6231	1.3319	1.614	1.639	1.643

sufficient for $L \geq 1$. The P- and D-wave phase shifts are determined to a large extent by the higher subsystem states which are not contained in the 0.QBA. Indeed, a considerable improvement is achieved by incorporating the latter at least partially via the 1.QBA. The close agreement between the 1.QBA and the SEA (Ref. 14) D-wave phase shifts in both spin channels and over the whole energy range, which can be seen most clearly by comparing the corresponding numerical values in Table IV, is remarkable.

The P- and D-wave phase shifts are very sensitive to the various diagrams of Fig. 1. In contrast to the singlet S wave, the corresponding contributions now add up to a relatively large total 1.QBA correction. However, the 1.QBA phase shifts are still smaller than the variational results and, for the reason mentioned above, the discrepancy becomes more pronounced for higher energies. By calculating the first-order effective potentials with the full T'_α instead of making the approximation $T'_\alpha \simeq V'_\alpha$, the influence of the higher subsystem states can easily be investigated within the quasiparticle approach.^{23} Indeed, when the difference $T'_\alpha - V'_\alpha$ is approximated by a sum of separable terms the corrections arising from each of them can be calculated separately. First numerical estimates^{34} confirm the expectation that the approximation $T'_\alpha \simeq V'_\alpha$ becomes worse with increasing energy, especially when approaching the first excitation threshold. The D wave in particular is strongly influenced by the hydrogenic $2p$ state, reflecting the fact that the polarizability of the hydrogen ground state, to which this subsystem state contributes substantially, becomes more important for larger L.

C. Differential and total cross sections

All cross sections in this section are given in units of πa_0^2, where a_0 denotes the Bohr radius. Because of the fast convergence of the partial-wave series (see Table V) all scattering amplitudes could be determined sufficiently accurately with less than 10 partial waves. The singlet and triplet contributions to the differential cross section,

$$\frac{d\sigma^{(S)}}{d\Omega} = \pi \left| \sum_{L=0}^{\infty} (2L+1)\mathcal{T}^{SL}(k,k;E)P_L(\cos\theta) \right|^2 , \tag{4.4}$$

are plotted separately in Figs. 10—13 for two different energies of the incoming electron. For comparison we include the SEA cross sections determined from the corresponding S-, P-, and D-wave phase shifts given in Refs. 14 and 15.

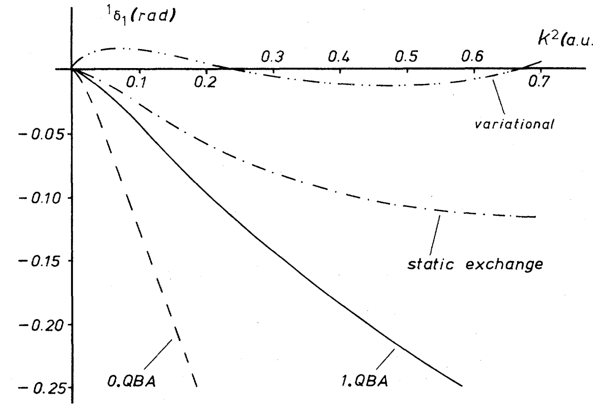

FIG. 6. Singlet P-wave elastic electron-hydrogen phase shifts as a function of k^2 in 0.QBA and in 1.QBA, as compared with variational (Ref. 10) and SEA results (Ref. 14).

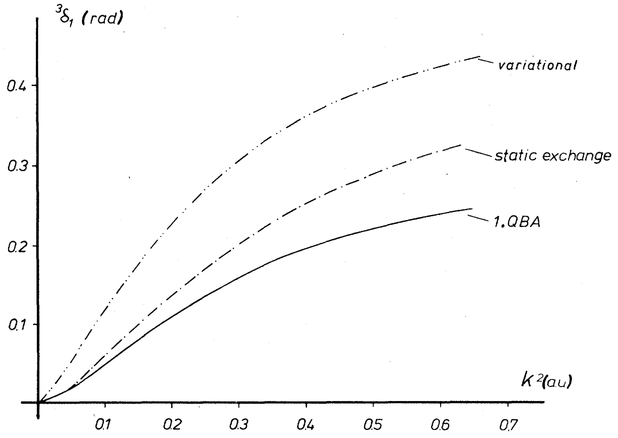

FIG. 7. Triplet P-wave elastic electron-hydrogen phase shifts as a function of k^2 in 1.QBA. References as in Fig. 6.

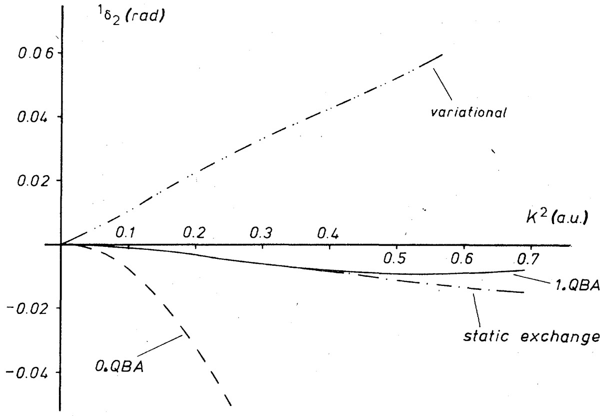

FIG. 8. As in Fig. 6, but for the D wave. The variational results are from Ref. 11.

TABLE IV. Singlet and triplet D-wave elastic electron-hydrogen phase shifts as a function of the electron momentum k. Comparison is made between the 1.QBA and the SEA (Ref. 14).

$^{2S+1}\delta_L$	k	1.QBA	SEA
	0.3	−0.0006	−0.0005
	0.4	−0.0019	−0.0017
$^{1}\delta_2$	0.5	−0.0041	−0.0039
	0.6	−0.0066	−0.0070
	0.7	−0.0084	−0.0106
	0.8	−0.0083	−0.0139
	0.3	0.0008	0.0008
	0.4	0.0028	0.0029
$^{3}\delta_2$	0.5	0.0068	0.0070
	0.6	0.0130	0.0135
	0.7	0.0213	0.0223
	0.8	0.0309	0.0327

As the energy increases, the singlet cross section in 1.QBA becomes smaller for all scattering angles (cf. Figs. 10 and 12). Although lying always below the 1.QBA, the SEA result shows a similar behavior. The difference between these two approximations comes mainly from the difference between the corresponding P-wave phase shifts. The inclusion of the partial waves $L \geq 3$ in the 1.QBA cross section is less substantial because of the fast convergence of the partial-wave series. The 0.QBA is determined essentially by the effective electron exchange potential. Since the latter is insufficient to produce reasonable singlet phase shifts for $L > 0$ (see Figs. 6 and 8), it can be anticipated that the shape of the cross section in 1.QBA is more realistic than that in 0.QBA.

As mentioned already, the triplet differential cross section in 0.QBA contains only an S-wave contribution and, thus, is isotropic (see Figs. 11 and 13). In 1.QBA the total shape of the angular distribution is much more sensitive to a variation of the energy than in the singlet channel. However, we find a good agreement with the SEA results. The strong reduction of the cross section in the forward direction at very low energies is caused by the P wave, which dominates the scattering in this energy region. Toward higher energies the D wave also becomes important (even more than in the singlet channel, as a comparison of Figs. 8 and 9 shows). Hence, the cross section becomes smaller at large scattering angles and slightly larger in the forward direction. The minimum, mainly produced by destructive interference of the S, P, and D wave, is shifted towards larger angles. The discrepancy between the 1.QBA and the SEA in this case can be attributed essentially to the different S- and P-wave phase shifts.

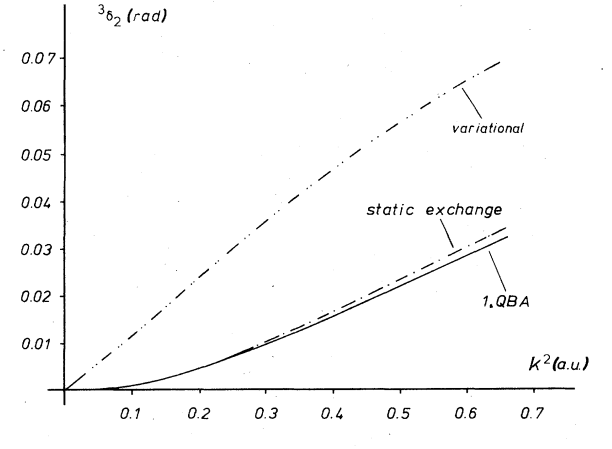

FIG. 9. As in Fig. 7, but for the D wave. References as in Fig. 8.

In Figs. 14—16 we compare the total differential cross section,

$$\frac{d\sigma}{d\Omega}=\frac{1}{4}\frac{d\sigma^{(0)}}{d\Omega}+\frac{3}{4}\frac{d\sigma^{(1)}}{d\Omega}\ , \tag{4.5}$$

in different approximations and at various energies with experimental results.[35] For energies less than 3 eV the large experimental cross section at large scattering angles (see Fig. 14) can be explained by the dominance of electron exchange. Our separable approximation (0.QBA) gives reasonable results for $\theta > 120°$, demonstrating that the scattering in this region can be well described by a pure exchange potential. At smaller scattering angles however, higher subsystem states and consequently

TABLE V. Example of convergence of the partial-wave series (3.14) in 1.QBA. The elastic electron-hydrogen singlet and triplet amplitude in forward direction at an electron momentum $k=0.8$ is tabulated as a function of the number N_L of partial waves included.

N_L	$\mathrm{Re}\mathscr{T}^0$	$\mathrm{Im}\mathscr{T}^0$	$\mathrm{Re}\mathscr{T}^1$	$\mathrm{Im}\mathscr{T}^1$
1	−0.015 66	−0.013 54	−0.007 28	−0.029 89
2	0.008 60	−0.020 20	−0.029 35	−0.035 33
3	0.009 92	−0.020 22	−0.034 24	−0.035 48
4	0.009 59	−0.020 22	−0.035 11	−0.035 49
5	0.009 45	−0.020 22	−0.035 26	−0.035 49
6	0.009 42	−0.020 22	−0.035 28	−0.035 49
7	0.009 41	−0.020 22	−0.035 28	−0.035 49

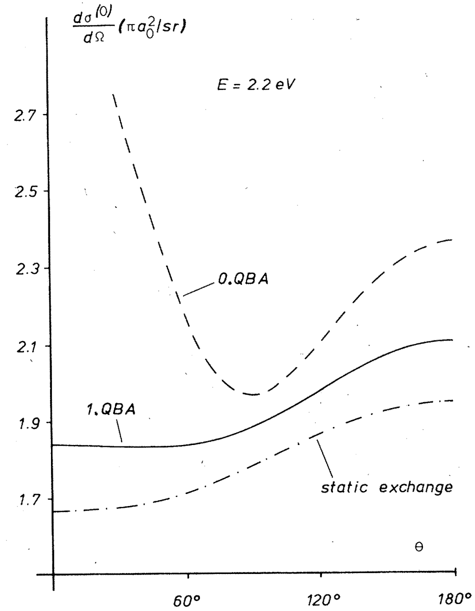

FIG. 10. Singlet contribution to the differential cross sections for elastic electron-hydrogen scattering in 0.QBA and in 1.QBA. Comparison is made with the SEA (calculated from the phase shifts of Refs. 14 and 15).

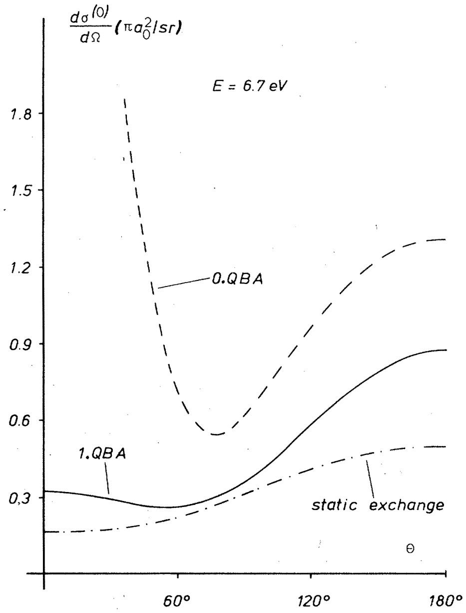

FIG. 12. As in Fig. 10, but for higher electron bombarding energy.

higher-order QBA contributions are important to reproduce the experimental results. Here the 1.QBA differs considerably from the 0.QBA and reproduces the experimental data much better. For a further improvement of the 1.QBA at very low energies presumably an improvement of the *P*- and *D*-wave phase shifts would be sufficient.

With increasing energy the experimental cross section becomes smaller for $\theta > 60°$ whereas it grows rapidly at small scattering angles (see Fig. 15). In contrast, due to the behavior of its triplet contribution, the differential cross section in 0.QBA decreases at all angles more rapidly than the 1.QBA and lies finally almost everywhere outside of the experimental errors. Furthermore, the minimum (in this approximation determined only by the singlet contribution) changes its position in the opposite direction as compared to the experiment.

The results obtained in 1.QBA, on the other hand, decrease at large scattering angles in the same way as the experimental values and lie at all energies well within the experimental errors. Furthermore, the position of the minimum is shifted in the right direction, i.e., toward

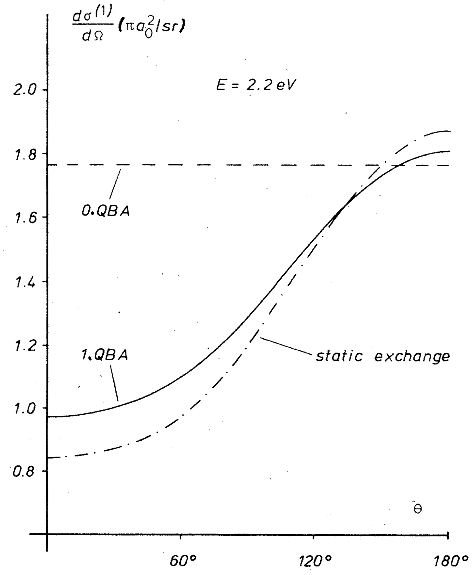

FIG. 11. Same as in Fig. 10, but for the triplet channel.

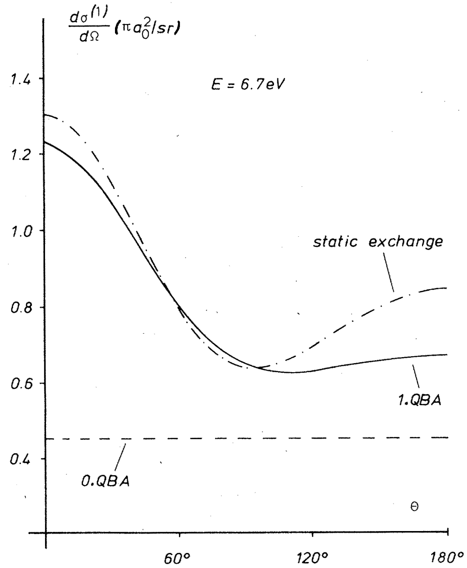

FIG. 13. Same as in Fig. 12, but for the triplet channel.

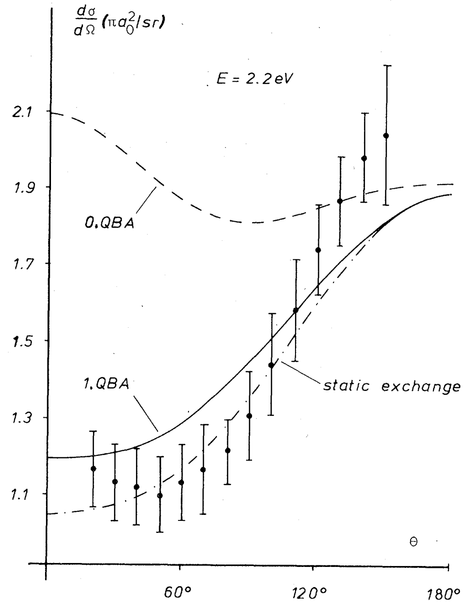

FIG. 14. Full differential cross section for elastic electron-hydrogen scattering in 0.QBA (dashed line) and in 1.QBA (solid line). Also shown are the SEA values (obtained from the phase shifts of Refs. 14 and 15) (dashed-dotted line) and the experimental results of Ref. 35.

larger angles (caused by the triplet contribution). In the forward direction, the 1.QBA changes only slowly and lies even for intermediate energies much below the experimental cross section. Since an improvement of the S-, P-, and D-wave phase shifts leads only to a comparatively small modification of the 1.QBA cross section, it becomes evident that a better incorporation of the higher subsystem states via higher order QBA contributions is necessary to describe the scattering at small angles correctly.

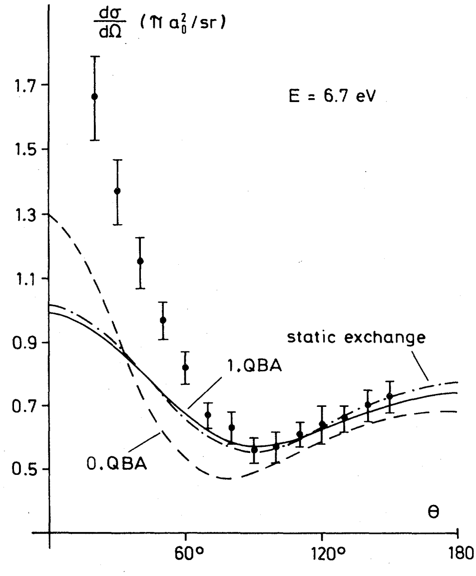

FIG. 15. Same as in Fig. 14, but for higher electron bombarding energy.

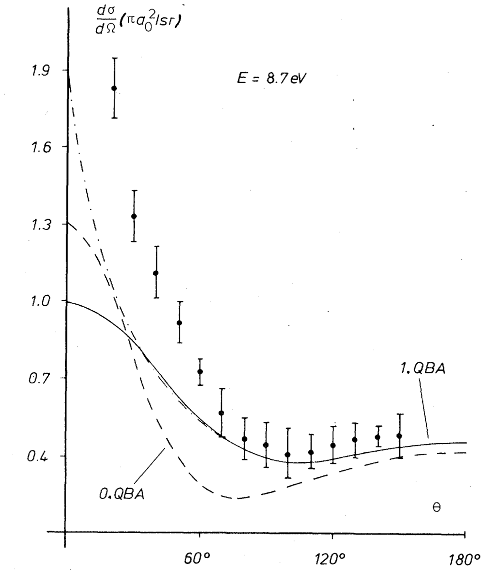

FIG. 16. Full differential cross section for elastic electron-hydrogen scattering in 0.QBA (dashed line) and in 1.QBA (solid line), as compared with the experimental results of Ref. 35. The dashed-dotted line has been determined by using the 1.QBA phase shifts for $L=0$, 1, and 2 and the phase shifts (4.6) for $L>2$.

For the energies considered, the polarizability of the hydrogen atom by the field of the incoming electron is a significant effect, which influences the scattering primarily at small angles.[35] The phase shifts for larger angular momenta are dominated by the induced polarization potential,[36] which is given by $-\alpha_d/2\rho^4$, with the dipole polarizability of the hydrogen ground state being $\alpha_d = 4.5a_0^3$. In order to get some idea of what might be expected from an inclusion of this effect we replaced for $L \geq 3$ the 1.QBA results by the phase shifts obtained from the asymptotic formula[37]

$$\tan\delta_L = \frac{\pi\alpha_d k^2}{(2L+3)(2L+1)(2L-1)} . \tag{4.6}$$

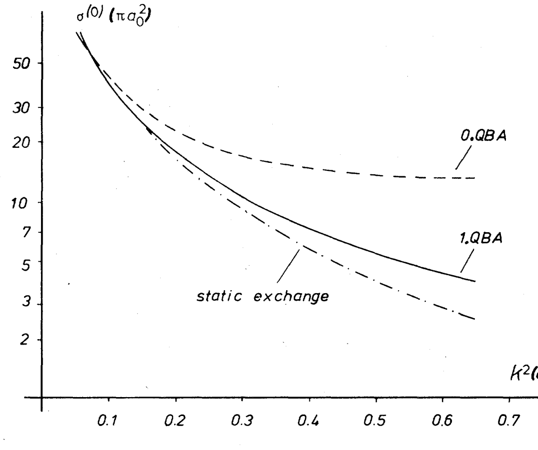

FIG. 17. Singlet contribution to the total cross sections for elastic electron-hydrogen scattering vs k^2 in 0.QBA and in 1.QBA. For comparison the SEA results are included.

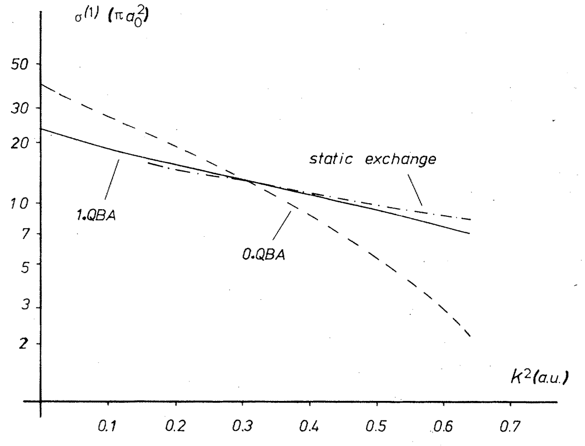

FIG. 18. As in Fig. 17, but for the triplet channel.

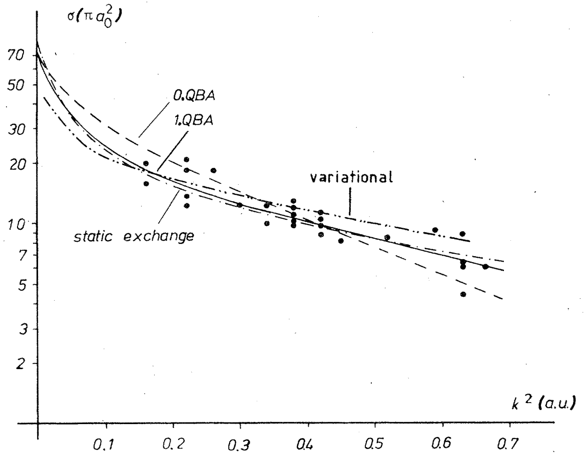

FIG. 19. Total cross section for elastic electron-hydrogen scattering vs k^2 in 0.QBA and in 1.QBA, as compared with the SEA (Ref. 14) and the experimental results of Ref. 38. Also shown are the variational values (obtained from the phase shifts of Refs. 9–12).

Figure 16 shows the difference between the cross section calculated in this way and by means of the 1.QBA. Since also the lowest partial waves need further improvement, a full agreement with the experimental data can, of course, not be expected. However, the improvement for $\theta < 30°$ is considerable.

Figures 17 and 18 display the singlet and triplet contributions to the total cross section,

$$\sigma^{(S)} = 4\pi^2 \sum_{L=0}^{\infty} (2L+1) \, | \mathcal{T}^{SL}(k,k;E) |^2 \, , \tag{4.7}$$

as a function of k^2 in different approximations. Our total elastic cross sections,

$$\sigma = \tfrac{1}{4}\sigma^{(0)} + \tfrac{3}{4}\sigma^{(1)} \, , \tag{4.8}$$

are plotted in Fig. 19 and compared with the SEA, variational, and experimental results.[38] As can be seen from these figures and from Table VI, our total cross sections in 0.QBA and in 1.QBA are comparable to those obtained by standard techniques and agree well with the experimental data. The agreement between the corresponding triplet contributions in 1.QBA and in the SEA is most remarkable (see Fig. 18).

In conclusion, we can say that the QBA method turns out to be a useful procedure for the treatment of the electron-hydrogen problem. As compared to our 0.QBA, the 1.QBA represents a much more realistic description of the experimental cross sections over the whole energy range below the first excitation threshold. Whereas the short-range effects are well reproduced in this approximation, the treatment of the polarization effects is still unsatisfactory and has to be improved by calculating higher-order QBA contributions.

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APPENDIX

In this appendix we have collected the analytic expressions of the effective potentials used in our numerical calculations. As (a) of Fig. 1 shows, in the 0.QBA only exchange diagrams are considered. By inserting the form factors (3.10) into (2.20), one ends up with the simple expression

TABLE VI. Total cross sections for elastic electron-hydrogen scattering in 0.QBA and in 1.QBA at various electron momenta k, as compared with some close-coupling results (Refs. 14, 15, and 18).

k	0.QBA	1.QBA	SEA	1s-2s	1s-2$\bar{p}$
0.1	60.57	56.47	62.1	62.3	
0.2	45.24	37.46	37.8	37.8	
0.3	32.70	25.53	24.5	24.9	24.17
0.4	23.56	18.54	17.5	18.0	
0.5	16.75	14.08	13.3	13.8	14.68
0.6	11.57	10.90			11.93
0.7	7.64	8.39			9.68
0.8	4.80	6.25	6.74	7.17	7.85

$$\mathcal{V}^{(0)}_{\beta\alpha}(\vec{k}'_\beta,\vec{k}_\alpha;E)=\pm\bar{\delta}_{\beta\alpha}\frac{4\mu_\alpha^2(\tilde{p}'_\beta\tilde{p}_\alpha)^{3/2}}{\pi^2\mu_\beta(p_\alpha^2+\tilde{p}_\alpha^2)^3}\,, \tag{A1}$$

where the relative momentum $\vec{p}_\alpha$ is a linear combination of the external momenta, $\vec{p}_\alpha=\vec{k}'_\beta+\mu_\alpha/m_\gamma\vec{k}_\alpha$. Here we introduced for convenience the abbreviations

$$\tilde{p}_\alpha=\left[\frac{\mu_\alpha}{M_\alpha}k_\alpha^2-2\mu_\alpha E\right]^{1/2}, \tag{A2}$$

and $\tilde{p}'_\beta$ defined in an analogous way. The minus sign in (A1) has to be taken if $\alpha=1$. We should mention that the general expression (A1) can also be used to investigate other three-body Coulomb systems, such as (e^+,e^-,e^+), (e^+,e^-,p), (p,e^-,p), . . . (see Ref. 6).

The nondiagonal terms in 1.QBA (2.21) contain in addition to the lowest-order contributions those which are linear in T'_γ. These correction terms have a much more complicated structure than the 0.QBA. In order to reduce their complexity we made the approximation

$$T'_\gamma\simeq V'_\gamma=V_\gamma-V_\gamma^s\,. \tag{A3}$$

Since the contributions (c) and (d) of Fig. 1 vanish with our special choice of form factors, we have to consider only the analytical representation of (b). Using (A3), we write it as

$$\mathcal{V}'_{\beta\alpha}=\mathcal{V}^{(1)}_{\beta\alpha}-\mathcal{V}^{(0)}_{\beta\alpha}=\bar{\delta}_{\beta\alpha}\bar{\delta}_{\gamma\beta}\bar{\delta}_{\gamma\alpha}(\mathcal{V}^{(c\gamma)}_{\beta\alpha}-\mathcal{V}^{(s\gamma)}_{\beta\alpha})\,, \tag{A4}$$

where the two-body Coulomb potential V_γ is contained in $\mathcal{V}^{(c\gamma)}_{\beta\alpha}$, and the separable part V_γ^s of the two-body interaction in $\mathcal{V}^{(s\gamma)}_{\beta\alpha}$. With the special choice for V_γ^s discussed in Sec. III A and the abbreviations (A2) we obtain

$$\mathcal{V}^{(c\gamma)}_{\beta\alpha}(\vec{k}'_\beta,\vec{k}_\alpha;E)=\frac{4\mu_\beta\mu_\alpha(\tilde{p}'_\beta\tilde{p}_\alpha)^{3/2}}{\pi^4}\int d^3K\frac{1}{(\vec{p}'_\gamma-\vec{p}_\gamma)^2[(p'_\beta)^2+(\tilde{p}'_\beta)^2]^2(p_\alpha^2+\tilde{p}_\alpha^2)^2}\,, \tag{A5}$$

and

$$\mathcal{V}^{(s\gamma)}_{\beta\alpha}(\vec{k}'_\beta,\vec{k}_\alpha;E)=\frac{16\mu_\beta^2\mu_\alpha^2(\tilde{p}'_\beta\tilde{p}_\alpha)^{3/2}}{\pi^4\mu_\gamma}\int d^3K\frac{K^2/M_\gamma-2E}{[(p'_\beta)^2+(\tilde{p}'_\beta)^2]^3(p_\alpha^2+\tilde{p}_\alpha^2)^3}\,, \tag{A6}$$

where

$$\vec{p}'_\beta=\vec{K}+\frac{\mu_\beta}{m_\alpha}\vec{k}'_\beta,\quad \vec{p}_\alpha=-\vec{K}-\frac{\mu_\alpha}{m_\beta}\vec{k}_\alpha,\quad \vec{p}'_\gamma=-\vec{k}'_\beta-\frac{\mu_\gamma}{m_\alpha}\vec{K},\quad \vec{p}_\gamma=\vec{k}_\alpha+\frac{\mu_\gamma}{m_\beta}\vec{K}\,.$$

In addition to the nondiagonal terms, the 1.QBA contains the diagonal contributions depicted in (e) and (f) of Fig. 1. From (2.22) one obtains, in analogy to (A4), in the approximation (A3) the decomposition

$$\mathcal{V}^{(1)}_{\beta\alpha}=\delta_{\beta\alpha}\sum_\gamma\bar{\delta}_{\gamma\alpha}(\mathcal{V}^{(c\gamma)}_{\alpha\alpha}-\mathcal{V}^{(s\gamma)}_{\alpha\alpha})\,. \tag{A7}$$

The explicit expressions are

$$\mathcal{V}^{(c\gamma)}_{\alpha\alpha}(\vec{k}'_\alpha,\vec{k}_\alpha;E)=\mp\frac{4\mu_\alpha^2(\tilde{p}'_\alpha\tilde{p}_\alpha)^{3/2}}{\pi^4(\vec{k}'_\alpha-\vec{k}_\alpha)^2}\int d^3K\frac{1}{[(p'_\alpha)^2+(\tilde{p}'_\alpha)^2]^2(p_\alpha^2+\tilde{p}_\alpha^2)^2}\,, \tag{A8}$$

and

$$\mathcal{V}^{(s\gamma)}_{\alpha\alpha}(\vec{k}'_\alpha,\vec{k}_\alpha;E)=\mp\frac{16\mu_\alpha^4(\tilde{p}'_\alpha\tilde{p}_\alpha)^{3/2}}{\pi^4\mu_\gamma}\int d^3K\frac{K^2/M_\gamma-2E}{[(p'_\alpha)^2+(\tilde{p}'_\alpha)^2]^3(p_\alpha^2+\tilde{p}_\alpha^2)^3}\,, \tag{A9}$$

with the relative momenta $\vec{p}'_\alpha,\vec{p}_\alpha$ being given as

$$\vec{p}'_\alpha=-\vec{K}-\frac{\mu_\alpha}{m_\beta}\vec{k}'_\alpha\,,$$

and

$$\vec{p}_\alpha=-\vec{K}-\frac{\mu_\alpha}{m_\beta}\vec{k}_\alpha\,.$$

The minus (plus) sign has to be taken for V_γ being attractive (repulsive). The representation (A8) shows clearly the Coulomb singularity for $\vec{k}'_\alpha=\vec{k}_\alpha$ discussed in Sec. III B.

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