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Electron-hydrogen quasiparticle calculations including the polarization effect

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The quasiparticle treatment of the electron-hydrogen problem performed in a recent publication is extended. It is shown that the characteristic polarization effect is essentially contained in the third-order quasi-Born approximation of the effective interaction, i.e., in an order which has not been considered in the aforementioned investigation. Instead of incorporating the corresponding contributions exactly, phenomenological polarization potentials proposed in the literature are used in the present calculations. With an adequate choice of the cutoff parameter in these expressions, almost perfect agreement between theory and experiment is achieved. The dependence on this parameter is studied. Comparison of our method with other procedures is being made.

I. INTRODUCTION

Recently it has been shown that systems of integral equations with Faddeev-type coupling, which have been used primarily in the three-nucleon problem, also represent a promising tool for treating low-energy electron-hydrogen collisions.[1] The quasiparticle formalism[2–5] in particular, developed by Alt, Grassberger, and Sandhas (AGS), turned out to be most adequate in this context, for the effective potentials occurring in this approach can be determined by means of a Born-like expansion. This is particularly relevant in the Coulomb case, where the usual separable approximation techniques of short-range theory fail.[6]

In Ref. 1 the two lowest orders of the quasi-Born expansion, denoted as zeroth- and first-order quasi-Born approximations (0.QBA and 1.QBA), have been taken into account. Going up to this order is known to lead in the nuclear case to rather accurate results.[5] In the electron-hydrogen problem passable agreement between theory and experiment has been achieved for large scattering angles only. Remarkable differences, however, showed up in forward direction.

These properties are qualitatively understandable. Due to the highly symmetric coupling of the equations employed, the Pauli principle is incorporated in a reliable way. Hence, in the backward direction, where Pauli exchange terms play an important role, good results are to be expected. For small angles another effect becomes more essential, namely the virtual excitation of the hydrogen target into an infinity of bound states and into the electron-proton continuum. This long-ranged polarization effect, which is responsible for the pronounced forward peak,[7–12] is practically not contained in 0.QBA and 1.QBA.

It is the *third*-order quasi-Born approximation where such contributions essentially show up. With some additional approximations the corresponding terms, in fact, take the form derived in conventional approaches for the polarization effect.[13] Hence, in order to reduce the discrepancies mentioned, the 3.QBA should be taken into account. To do this exactly would be an extremely complicated task. We therefore replace the correct expressions by simple phenomenological polarization potentials suggested in the literature,[14] which depend on a cutoff parameter.

Some general comments on our method may be helpful. In integral-equation approaches based on single (or less symmetrically coupled) equations, the polarization effect, which concerns the nonexchange terms only, can easily be taken care of. But the incorporation of the Pauli principle is a nontrivial task. Just the opposite is true within the Faddeev formalism. There, the characteristic symmetry of the coupled equations implies that the Pauli principle can be built in naturally. The treatment of the polarization effect, however, is less evident. Our present approach overcomes this complication. It, indeed, allows the taking into account of *both* effects in a satisfactory way.

In what follows these statements will be substantiated in detail for the differential cross section *below* the first excitation threshold. In Sec. II the formal aspects of the problem are discussed. Our numerical results are given in Sec. III. In particular, we show that almost perfect agreement between theory and experiment is achieved when adding to the effective interaction of Ref. 1 the above-mentioned phenomenological polarization potentials with optimized cutoff parameter. The sensitivity on this parameter is studied. Furthermore, we compare our results with those obtained by means of alternative methods.

II. FORMALISM

The quasiparticle approach, specialized to the electron-hydrogen problem, has been described in detail in Ref. 1. Hence, we can restrict ourselves to those of its aspects which are of relevance in the present context.

Adequate off-shell extensions $\mathcal{T}_{\beta\alpha}(\mathbf{k}'_\beta,\mathbf{k}_\alpha)$ of the electron-hydrogen scattering amplitudes satisfy the exact set of relations[2]

$$\mathscr{T}_{\beta\alpha}(\mathbf{k}'_\beta,\mathbf{k}_\alpha)=\mathscr{V}_{\beta\alpha}(\mathbf{k}'_\beta,\mathbf{k}_\alpha)+\sum_{\gamma=1}^{3}\int d^3k''_\gamma\,\mathscr{V}_{\beta\gamma}(\mathbf{k}'_\beta,\mathbf{k}''_\gamma)\times\Delta_\gamma(k''_\gamma)\mathscr{T}_{\gamma\alpha}(\mathbf{k}''_\gamma,\mathbf{k}_\alpha) \tag{2.1}$$

which, considered as a matrix equation, evidently shows the structure of the two-body Lippmann-Schwinger equation. The effective potentials occurring here are *exactly* given by

$$\mathscr{V}_{\beta\alpha}(\mathbf{k}'_\beta,\mathbf{k}_\alpha)=\langle\mathbf{k}'_\beta|\ \langle\bar{\beta}|G_0U'_{\beta\alpha}G_0|\alpha\rangle\ |\mathbf{k}_\alpha\rangle\ , \tag{2.2}$$

with $U'_{\beta\alpha}$ being defined by the set of coupled AGS equations

$$U'_{\beta\alpha}=\bar{\delta}_{\beta\alpha}G_0^{-1}+\sum_{\gamma=1}^{3}\bar{\delta}_{\beta\gamma}T'_\gamma G_0U'_{\gamma\alpha}\ . \tag{2.3}$$

In order to obtain these relations, the electrons had to be considered as distinguishable particles e_1 and e_2. The electron-proton and the electron-electron subsystems (e_1p), (e_2p), and (e_1e_2) are denoted by α (β or γ)$=1$, 2, and 3, respectively. As usual these indices also label the corresponding two-fragment channels, and $\mathbf{k}_\alpha$ ($\mathbf{k}_\beta$ or $\mathbf{k}_\gamma$) are the relative momenta between the fragments. The free three-particle resolvent is given by G_0, and $\bar{\delta}_{\beta\alpha}=(1-\delta_{\beta\alpha})$ represents the anti-Kronecker symbol.

The essential step in deriving the effective two-body equations (2.1) is the splitting

$$T_\gamma=|\gamma\rangle\Delta_\gamma\langle\bar{\gamma}|+T'_\gamma \tag{2.4}$$

of the three subsystem transition operators T_γ. One standard way of constructing such decompositions consists in decomposing first the subsystem potentials according to

$$V_\gamma=|\chi_\gamma\rangle\lambda_\gamma\langle\chi_\gamma|+V'_\gamma\ . \tag{2.5}$$

In Ref. 1, the form factor $|\chi_\gamma\rangle$ has been chosen as

$$|\chi_\gamma\rangle=V_\gamma|\psi_\gamma\rangle\ , \tag{2.6}$$

with $|\psi_\gamma\rangle$ being the eigenfunction of the two-body Lippmann-Schwinger (LS) kernel, which belongs to the respective biggest eigenvalue η_γ. This provides $|\gamma\rangle=|\chi_\gamma\rangle$ and $\langle\bar{\gamma}|=\langle\chi_\gamma|$ for the form factors in (2.4). Since $|\psi_\gamma\rangle$ is normalized to unity, we have $\Delta_\gamma=\lambda_\gamma/(1-\eta_\gamma)$ for the propagator. The rest amplitude T'_γ in the above decomposition satisfies the two-body operator LS equation

$$T'_\gamma=V'_\gamma+V'_\gamma G_0T'_\gamma\ . \tag{2.7}$$

For $\gamma=1$, 2, the Sturmian functions $|\psi_\gamma\rangle$ are related to the hydrogen ground state. The separable term in the splitting (2.4) thus represents the corresponding bound-state pole behavior of T_γ. For energies below the first excitation threshold, the rest T'_γ, therefore, can be expected to be fairly small, and the same should be true for $\gamma=3$. This suggests solving (2.3) by iteration, a procedure leading to the quasi-Born approximations $\mathscr{V}^{(n)}_{\beta\alpha}$ of the effective potential (2.2). Up to the order $n=3$, these approximations are given by

$$\mathscr{V}^{(0)}_{\beta\alpha}=\bar{\delta}_{\beta\alpha}\langle\chi_\beta|G_0|\chi_\alpha\rangle\ , \tag{2.8}$$

$$\mathscr{V}^{(1)}_{\beta\alpha}=\mathscr{V}^{(0)}_{\beta\alpha}+\sum_{\gamma}\bar{\delta}_{\beta\gamma}\bar{\delta}_{\gamma\alpha}\langle\chi_\beta|G_0T'_\gamma G_0|\chi_\alpha\rangle\ , \tag{2.9}$$

$$\mathscr{V}^{(2)}_{\beta\alpha}=\mathscr{V}^{(1)}_{\beta\alpha}+\sum_{\gamma,\epsilon}\bar{\delta}_{\beta\gamma}\bar{\delta}_{\gamma\epsilon}\bar{\delta}_{\epsilon\alpha}\langle\chi_\beta|G_0T'_\gamma G_0T'_\epsilon G_0|\chi_\alpha\rangle\ , \tag{2.10}$$

$$\mathscr{V}^{(3)}_{\beta\alpha}=\mathscr{V}^{(2)}_{\beta\alpha}+\sum_{\gamma,\epsilon,\eta}\bar{\delta}_{\beta\gamma}\bar{\delta}_{\gamma\epsilon}\bar{\delta}_{\epsilon\eta}\bar{\delta}_{\eta\alpha}\times\langle\chi_\beta|G_0T'_\gamma G_0T'_\epsilon G_0T'_\eta G_0|\chi_\alpha\rangle\ . \tag{2.11}$$

In Ref. 1 only the 0.QBA and the 1.QBA potentials $\mathscr{V}^{(0)}_{\beta\alpha}$ and $\mathscr{V}^{(1)}_{\beta\alpha}$, respectively, have been taken into account, with T'_γ being approximated additionally by V'_γ. The discrepancies between theory and experiment found in this reference, however, indicate that important contributions to the effective potential are contained in higher orders. Indeed, as we will see, the essential effect of target polarizability shows up just in the 3.QBA elastic potential.

Let e_1 be the incoming electron. Then in $\mathscr{V}^{(3)}_{11}$ a term

$$\mathscr{V}^{P}_{11}=\langle\chi_1|G_0(T'_2+T'_3)G_0T'_1G_0(T'_2+T'_3)G_0|\chi_1\rangle\ , \tag{2.12}$$

occurs, where T'_1 represents the rest-transition operator of the (e_2,p) subsystem, which still contains all *excited* target states, including the continuum. Hence, (2.12) plays the role of a polarization potential. To exhibit this point more clearly, we recall that, close to the ground-state pole, we have[15]

$$G_0T'_1G_0\underset{z\to E_1}{\sim}G_0T_1G_0-|\psi_1\rangle\frac{1}{z-E_1}\langle\psi_1|=G_1Q_1-G_0\ . \tag{2.13}$$

Here Q_1 is the projection onto the whole spectrum with the exception of the ground state. This shows that for such energies $\mathscr{V}^{P}_{11}$ contains essentially a contribution of the form

$$\tilde{\mathscr{V}}^{P}_{11}=\mathop{\sum\!\!\!\!\!\!\int}_{n\neq1}\langle\psi_1|(V_2+V_3)|\psi_{1n}\rangle\frac{1}{z-E_{1n}}\times\langle\psi_{1n}|(V_2+V_3)|\psi_1\rangle\ , \tag{2.14}$$

where $|\psi_{1n}\rangle$ denotes the bound (and continuum) states in subsystem 1, and $|\psi_{11}\rangle$ has been abbreviated as before by $|\psi_1\rangle$. This expression evidently is of the conventional form of the *polarization potential* derived in other approaches.[13]

Let us add some comments. In the above argumentation we have fully ignored the 2.QBA, and only part of the 3.QBA has been taken into account in $\mathscr{V}^{P}_{11}$. Furthermore, we have replaced $(T'_2+T'_3)$ by $(V'_2+V'_3)$ and then by (V_2+V_3). Moreover, as mentioned already, $\mathscr{V}^{P}_{11}(z)$ approaches $\tilde{\mathscr{V}}^{P}_{11}(z)$ only close to the energy shell. Inspection of the neglected terms, however, indicates that this is justified. In fact, some of the terms omitted are governed by overlap integrals between differing Sturmian functions which, according to the considerations of Refs. 5 and 16, should be negligible even if these functions do not belong to the same subsystem. The other neglected contributions are similar to lower-order terms, being multiplied, however, by factors which are small due to the smallness of the electric coupling constant. Of course, detailed estimates would be necessary to rigorously confirm these arguments, a task far beyond the scope of the present investigations.

However, there is no need to go through such details, as the only conclusion we draw from the present considerations is that an essential part of the dominant polarization effect is contained in the 3.QBA term (2.12) which, therefore, should be added to the effective potential used in Ref. 1. To compute $\mathscr{V}^P$, or even the simplified form $\tilde{\mathscr{V}}^P$, is of course not an easy task. But, in the energy region below the first excitation threshold, where the adiabatic approximation ought to be justified, simple phenomenological polarization potentials proposed in the literature[14] may be used instead of (2.12) or (2.14). In the calculations presented in the following we have chosen

$$\mathscr{V}^{P1}_{11}(r_1)=-\alpha/2(r_1^2+d^2)^2 \tag{2.15}$$

and

$$\mathscr{V}^{P2}_{11}(r_1)=-\alpha r_1^2/2(r_1^2+d^2)^3 \, . \tag{2.16}$$

Note that for large distances of electron e_1 from the hy-

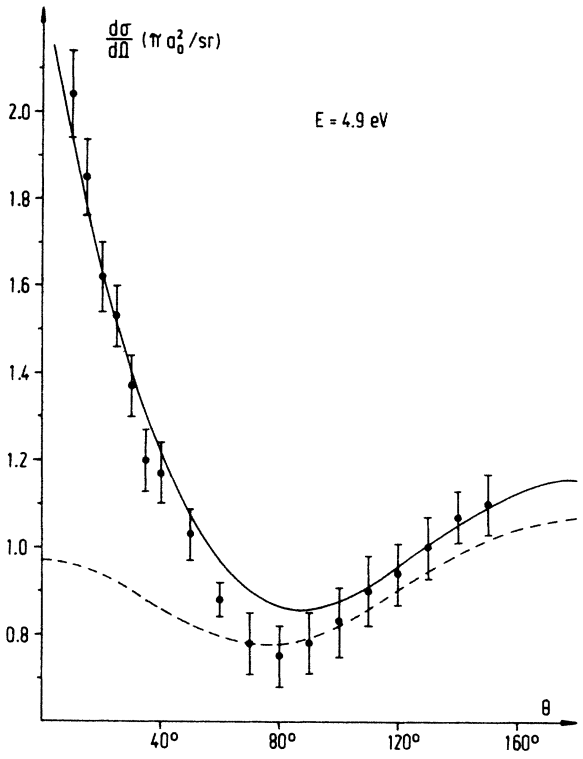

FIG. 2. Same as in Fig. 1, but for $E=4.9$ eV.

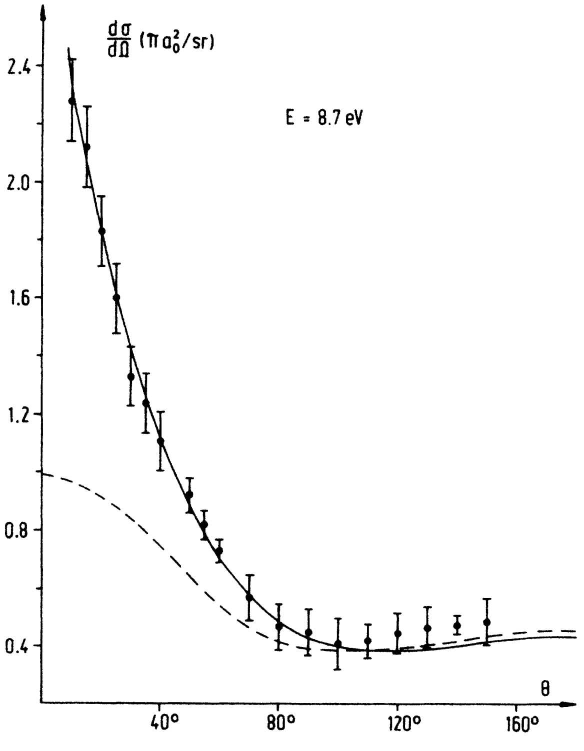

FIG. 1. Differential cross section at laboratory energy $E=8.7$ eV for elastic electron-hydrogen scattering in 1.QBA (dashed line) and after having incorporated the polarization potential $\mathscr{V}^{P1}$ (solid line). The experimental data are taken from Ref. 7.

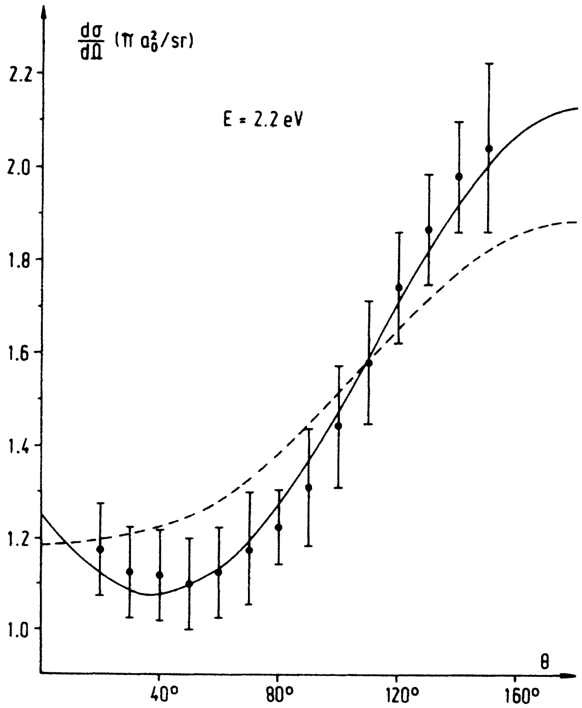

FIG. 3. Same as in Fig. 1, but for $E=2.2$ eV.

drogen target, i.e., for large values of r_1, both potentials show the asymptotic behavior $-\alpha/2r_1^4$ which, in adiabatic approximation, follows rigorously from (2.14). Here $\alpha = 4.5a_0^3$, with a_0 the Bohr radius, denotes the dipole polarizability of the target, and d is a cutoff parameter (see below).

III. RESULTS

We have solved the integral equations (2.1), after symmetrization and partial wave decomposition, in the way described in Ref. 1. But now, the polarization potentials (2.15) or (2.16), which in momentum space read

$$\mathcal{V}^{P1}(\mathbf{k}',\mathbf{k}) = -\frac{\alpha \exp(-|\mathbf{k}'-\mathbf{k}|d)}{16\pi d} \tag{3.1}$$

and

$$\mathcal{V}^{P2}(\mathbf{k}',\mathbf{k}) = -\frac{\alpha(3-|\mathbf{k}'-\mathbf{k}|d)\exp(-|\mathbf{k}'-\mathbf{k}|d)}{64\pi d}, \tag{3.2}$$

have been added to the first-order quasi-Born approximation of the effective potential.

Figs. 1–3 show the electron-hydrogen differential cross sections for laboratory energies $E = 8.7$, 4.9, and 2.2 eV, respectively. The dashed curves are the 1.QBA calculations of Ref. 1, the solid curves show the results obtained after having incorporated $\mathcal{V}^{P1}(\mathbf{k}',\mathbf{k})$. The d parameter has been chosen to provide an optimal fit to the experimental data. In Figs. 1 and 2 this has been achieved for $d = 1.80$ and in Fig. 3 for $d = 1.53$. Practically the same curves are obtained when using $\mathcal{V}^{P2}$ instead of $\mathcal{V}^{P1}$, but the optimal choices of the parameter are $d = 1.36$ for both $E = 8.7$ and 4.9 eV and $d = 1.04$ for $E = 2.2$ eV. Inclusion of the polarization effect, hence, yields a remarkable improvement over the 1.QBA results, leading to almost perfect agreement between theory and experiment.

This improvement becomes particularly evident by inspection of the singlet (${}^1\delta_L$) and triplet (${}^3\delta_L$) phase shifts obtained in different approximations or approaches. In Tables I–III the 0.QBA and the 1.QBA results for $L = 0$, 1, and 2 are compared with those obtained after having included $\mathcal{V}^{P1}$ and $\mathcal{V}^{P2}$. Moreover, comparison is made with variational results,[8] which usually are considered to be most accurate.

In Table IV we compare our $L = 3$ phase shifts with variational results,[9] and for $L = 3$, 4, and 5 with the δ_L provided by the asymptotic formula[17]

$$\tan\delta_L = \frac{\pi\alpha k^2}{(2L+3)(2L+1)(2L-1)} . \tag{3.3}$$

For increasing L the difference between singlet and triplet phase shifts evidently vanishes. Furthermore, it turns out that ${}^1\delta_5$ and ${}^3\delta_5$ fairly agree with the phase shift given by Eq. (3.3). For $L \geq 5$ the δ_L provided by this formula, therefore, have been used in computing the cross sections with inclusion of the polarization effect. The number of phase shifts taken into account has been increased until the partial-wave series remained stable.

As mentioned, the cutoff parameter d has been chosen to yield an optimal least-squares fit to the experimental cross sections. For $E = 8.7$ eV we found $d = 1.80$. In order to demonstrate the dependence on this parameter, the cross sections obtained for different values of d are shown in Fig. 4.

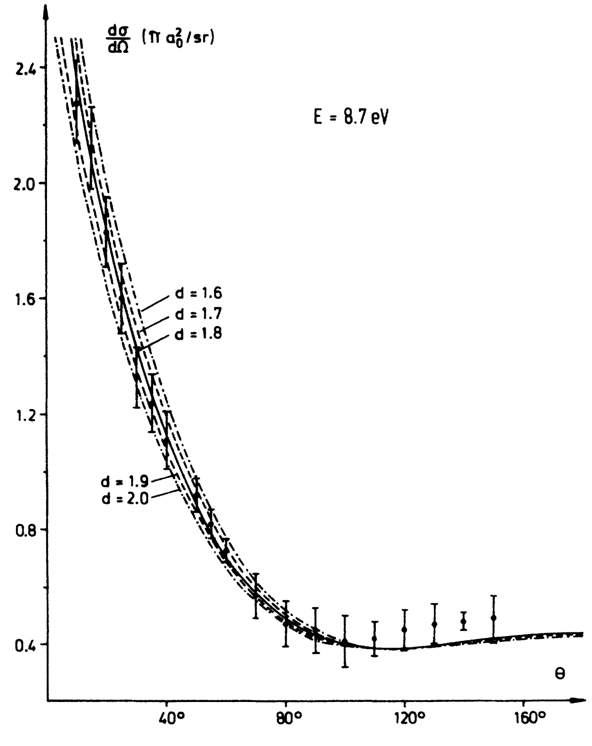

FIG. 4. Solid curve ($d = 1.80$) and experimental data of Fig. 1 compared with cross sections obtained for different values of the cutoff parameter d.

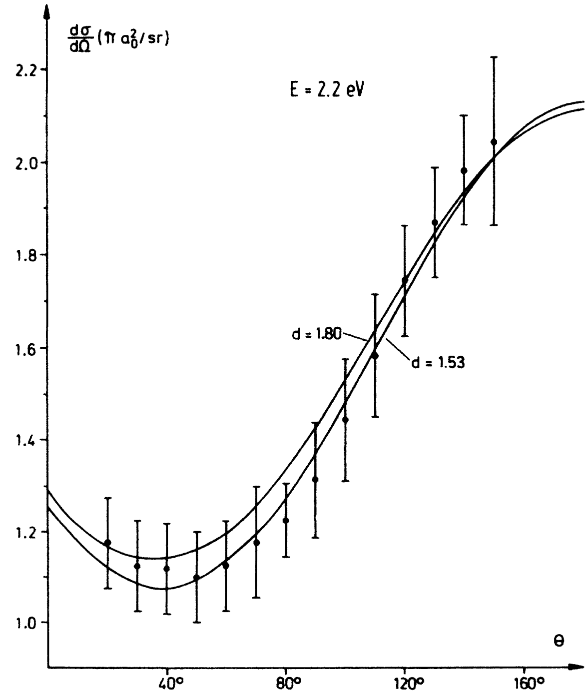

FIG. 5. Solid curve ($d = 1.53$) and experimental data of Fig. 3 compared with cross section obtained for $d = 1.80$.

TABLE I. Singlet and triplet elastic electron-hydrogen phase shifts for $L=0$, 1, and 2 at $E=8.7$ eV.

	${}^1\delta_0$	${}^3\delta_0$	${}^1\delta_1$	${}^3\delta_1$	${}^1\delta_2$	${}^3\delta_2$
0.QBA	0.7445	0.6231	−0.7548		−0.1845	
1.QBA	0.7126	1.3319	−0.2682	0.2417	−0.0083	0.0309
$P1$ ($d=1.80$)	1.1011	1.3929	−0.1618	0.3785	0.0397	0.0805
$P2$ ($d=1.36$)	0.9981	1.3954	−0.1587	0.3792	0.0417	0.0826
variational[a]	0.886	1.643	−0.004	0.427	0.0745	0.0697

[a]Reference 8.

TABLE II. Singlet and triplet elastic electron-hydrogen phase shifts for $L=0$, 1, and 2 at $E=4.9$ eV.

	${}^1\delta_0$	${}^3\delta_0$	${}^1\delta_1$	${}^3\delta_1$	${}^1\delta_2$	${}^3\delta_2$
0.QBA	1.0055	1.3068	−0.4631		−0.0865	
1.QBA	0.9642	1.7834	−0.1679	0.1829	−0.0066	0.0130
$P1$ ($d=1.80$)	1.3774	1.8432	−0.0858	0.3074	0.0264	0.0471
$P2$ ($d=1.36$)	1.2786	1.8457	−0.0829	0.3103	0.0275	0.0483
variational[a]	1.041	1.9329	−0.009	0.3412	0.0383	0.0424

[a]Reference 8.

TABLE III. Singlet and triplet elastic electron-hydrogen phase shifts for $L=0$, 1, and 2 at $E=2.2$ eV.

	${}^1\delta_0$	${}^3\delta_0$	${}^1\delta_1$	${}^3\delta_1$	${}^1\delta_2$	${}^3\delta_2$
0.QBA	1.3993	1.9130	−0.2133		−0.0207	
1.QBA	1.3373	2.2082	−0.0749	0.0857	−0.0019	0.0028
$P1$ ($d=1.53$)	1.9883	2.2714	−0.0109	0.1874	0.0166	0.0216
$P2$ ($d=1.04$)	2.0212	2.2771	−0.0036	0.2030	0.0174	0.0224
variational[a]	1.4146	2.2938	0.0100	0.1872	0.0183	0.0198

[a]Reference 8.

TABLE IV. Singlet and triplet elastic electron-hydrogen phase shifts for $L=3$, 4, and 5 at $E=8.7$ eV.

	${}^1\delta_3$	${}^3\delta_3$	${}^1\delta_4$	${}^3\delta_4$	${}^1\delta_5$	${}^3\delta_5$
$P1$ ($d=1.80$)	0.0231	0.0256	0.0115	0.0115	0.0064	0.0064
$P2$ ($d=1.36$)	0.0237	0.0263	0.0118	0.0118	0.0065	0.0064
variational[a]	0.0259	0.0263				
O'Malley[b]	0.0287		0.0131		0.0070	

[a]Reference 8.
[b]Reference 17.

TABLE V. Total cross sections for elastic electron-hydrogen scattering in 0.QBA, 1.QBA, and with the two different polarization potentials, as compared with some close-coupling results (Ref. 12), the SEA results (Ref. 18), and variational results (Refs. 8 and 9).

E (eV)	0.QBA	1.QBA	$P1$	$P2$	$1s$-$\overline{2p}$	SEA	variational (S,P,D,F)
2.2	23.56	18.54	18.197	18.271		17.5	18.65
4.9	11.57	10.90	12.881	12.786	11.93		12.27
8.7	4.80	6.25	8.029	7.908	7.85	6.74	8.20

It is a remarkable fact that the optimal value of d turned out to be energy independent in the region, where the polarization effect is particularly dominant, namely for $E=8.7$ and 4.9 eV. At lower energies, however, d had to be reduced in order to get the best fit. Since for $E=2.2$ eV the polarization effect is no longer most important, this probably means that the modification of d serves to cure inaccuracies of the other contributions to the effective potential. We therefore show in Fig. 5 beside the solid curve of Fig. 3, calculated with $d=1.53$, the result obtained without changing d, i.e., by taking $d=1.80$. It turns out that, under the assumption of energy independence of $\mathscr{V}^{P1}$, a reasonable fit is still achieved.

In Table V we present total cross sections computed in our different approximations using the above best fit values of d. For comparison, close-coupling calculations, which include the polarizability by means of a $\overline{2p}$ pseudostate,[12] and cross sections found in static exchange approximation (SEA) are shown.[18] Moreover, variational results[8,9] are given. The remarkable agreement of our results with the latter should be emphasized.

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