Electron-hydrogen quasiparticle calculations with the Temkin-Lamkin polarization potential

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Low-energy electron-hydrogen scattering data are calculated within the quasiparticle approach to Faddeev-type integral equations. The simple phenomenological polarization potentials employed in former applications of this formalism, however, are replaced by the more sophisticated parameter-free Temkin-Lamkin potential. Despite the fact that, in contrast to the former calculations, there is no longer a fitting parameter at our disposal that could be used to optimize the results, the best previous values are reproduced or even slightly improved.

I. INTRODUCTION

The quasiparticle formalism[1-4] developed by Alt, Grassberger, and Sandhas (AGS) for Faddeev-type integral equations has been applied to low-energy electron-hydrogen collisions in two recent publications.[5,6] In Ref. 5 the zeroth- and the first-order quasi-Born approximation of the effective potentials, denoted as 0.QBA and 1.QBA, were taken into account. For large scattering angles, fair agreement between the theoretical and experimental cross sections has been achieved, but the strong forward peak could not be reproduced. As pointed out in Ref. 6, this is due to the neglect of the polarization effect contained in higher-order quasi-Born terms. To calculate these terms exactly would be an extremely complicated task. This suggested that they be replaced by simple phenomenological polarization potentials.[7] With an optimal choice of the cutoff parameter in these expressions, a remarkable improvement of the differential cross sections was achieved. But deviations of the low phase shifts from variational results, while partly reduced, were still evident.

In the present paper, we report on results obtained with the same integral equations employing now, however, instead of the simple polarization potentials used in Ref. 6, the more sophisticated Temkin-Lamkin potential.[8] It will be shown that, despite the fact that there is no longer a fitting parameter at our disposal, the resulting cross sections coincide almost exactly with the ones found in our preceding investigation, and also the phase shifts are only slightly modified. In other words, we arrive in a *parameter-free* manner at the same good agreement between theoretical and experimental cross sections, but the above-mentioned discrepancies concerning the low phase shifts, apart from slight improvements, are also reproduced.

The latter observation is not astonishing. For the Temkin-Lamkin potential, being derived in "adiabatic" approximation, is energy independent, such as the phenomenological expressions of Ref. 7. Deviations similar to the ones found in Ref. 6, therefore, were to be expected *a priori*. We only mention in this context that the characteristic Feshbach resonances cannot show up at all for energy-independent polarization potentials. General arguments and the present detailed results, therefore, indicate that excited subsystem states should be taken into account more explicitly in future applications of the integral equation approach.

Since our calculations are based completely on the formalism and the numerical program used in Ref. 6, it appears justified to restrict the discussion of formal questions given in Sec. II to some few relevant aspects. In Sec. III the new results obtained with the Temkin-Lamkin potential are presented and compared with the ones of Ref. 6 and with variational calculations.

II. FORMALISM

Faddeev-type integral equations are usually reduced to effective two-body Lippmann-Schwinger equations by expanding the two-body amplitudes in their kernel into a series of separable terms. In Ref. 5 only one separable term has been introduced in each subsystem amplitude, the form factors being chosen as Sturmian functions. The nonseparable rest was taken into account in first quasi-Born approximation (1.QBA) in the resulting effective interaction.

As recalled in the introduction, the effect of the target polarizability is not contained in this order of approximation. Phenomenological polarization potentials of the form

$$V^{P1}(\mathbf{k}',\mathbf{k})=-\frac{\alpha\exp(-Qd)}{16\pi d}\ , \tag{2.1}$$

$$V^{P2}(\mathbf{k}',\mathbf{k})=-\frac{\alpha(3-Qd)\exp(-Qd)}{64\pi d}\ , \tag{2.2}$$

therefore, have been added in Ref. 6 to the diagonal elements of the first-order (1.QBA) interaction. Here, α represents the dipole polarizability, d is an open parameter, and $Q=|\mathbf{k}'-\mathbf{k}|$.

In the present investigations, the same formalism is applied. But instead of (2.1) and (2.2), we use the Temkin-Lamkin potential given in coordinate space by[8]

$$V^{\rm pol}(r)=-\frac{1}{r^4}\left[\tfrac{9}{4}-\tfrac{1}{3}e^{-2r}(r^5+\tfrac{9}{2}r^4+9r^3+\tfrac{27}{2}r^2+\tfrac{27}{2}r+\tfrac{27}{4})\right]\ , \tag{2.3}$$

or, after transformation into momentum space, by

$$V^{\rm pol}(\mathbf{k}',\mathbf{k})=\frac{1}{2\pi^2}\left[\frac{3Q^4+\frac{88}{3}Q^2+80}{(4+Q^2)^3}+\frac{9}{8}\left[\frac{\pi}{2}Q-2-Q\arctan\frac{Q}{2}\right]\right]. \quad (2.4)$$

III. RESULTS

Figures 1–3 show the differential cross sections for laboratory energies $E=8.7$, 4.9, and 2.2 eV, respectively. The dotted curves are the 1.QBA calculations of Ref. 5, while the solid curves represent the results achieved after inclusion of the polarization potential (2.4). Comparison with the corresponding figures of Ref. 6 demonstrates that these curves agree almost exactly with the ones obtained for the phenomenological potentials (2.1) and (2.2) after optimizing there the open parameter d.

Inclusion of the polarization effect is of particular relevance with respect to the forward direction, i.e., with respect to the higher partial waves. Table I shows that, for $L \geq 5$, the phase shifts obtained when using the Temkin-Lamkin potential practically coincide with the O'Malley result:[10]

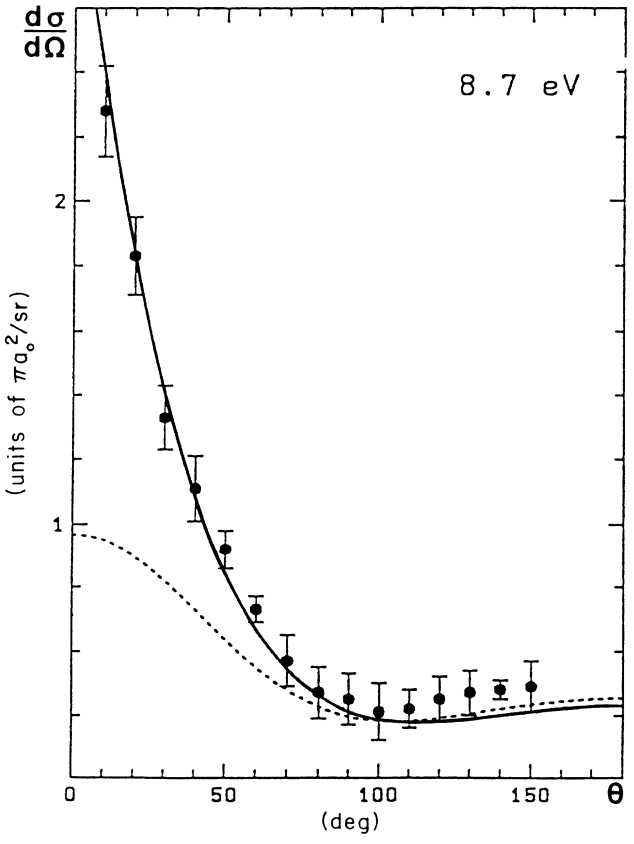

FIG. 1. Differential cross section in atomic units (πa_0^2/sr) at laboratory energy 8.7 eV for elastic electron-hydrogen scattering in 1.QBA (dotted curve) and after having incorporated the polarization potential $V^{\rm pol}$ (solid curve). The experimental data are taken from Ref. 9.

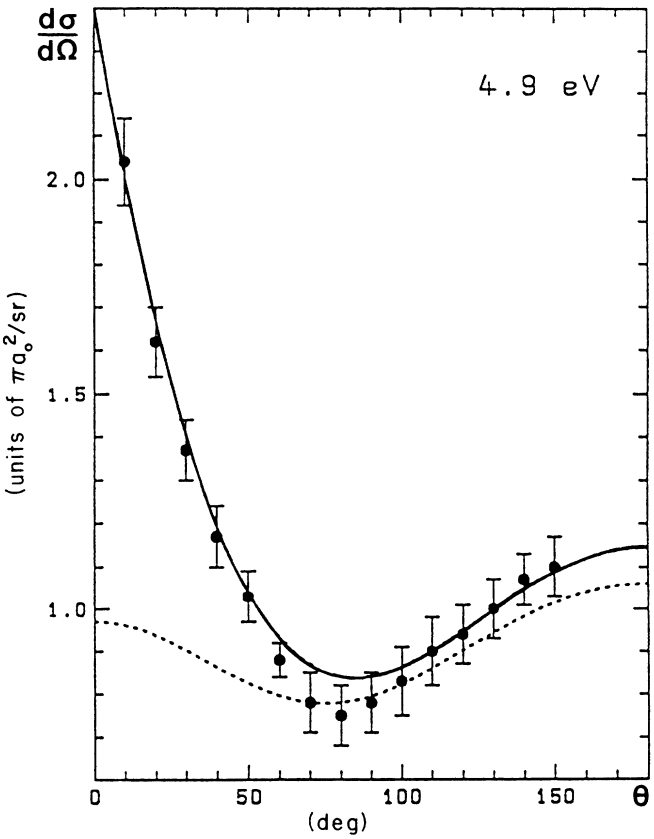

FIG. 2. Same as in Fig. 1, but for $E=4.9$ eV.

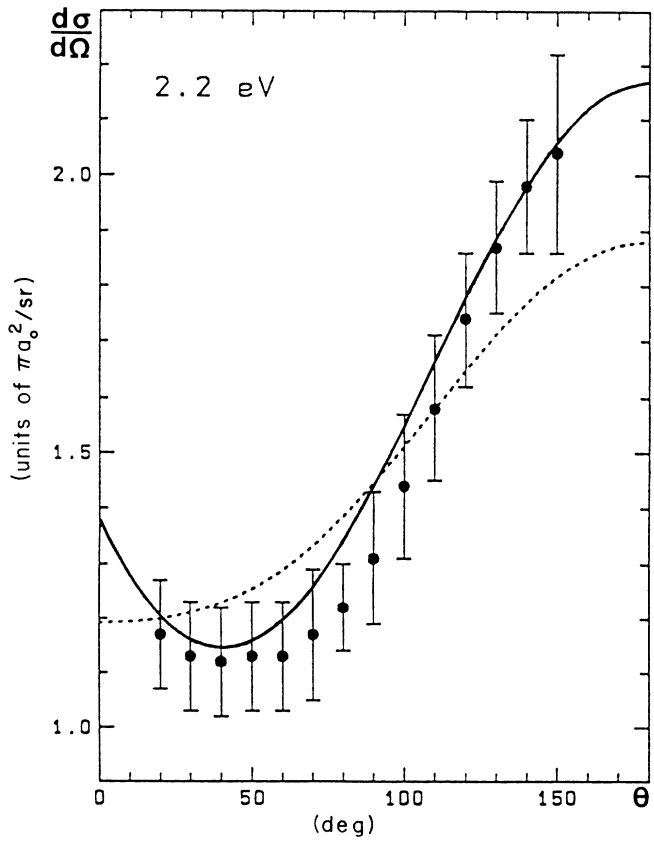

FIG. 3. Same as in Fig. 1, but for $E=2.2$ eV.

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

	$^1\delta_3$	$^3\delta_3$	$^1\delta_4$	$^3\delta_4$	$^1\delta_5$	$^3\delta_5$
V^{pol}	0.0270	0.0295	0.0132	0.0132	0.0071	0.0071
O'Malley[a]	0.0287		0.0131		0.0070	

[a]Reference 10.

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

	$^1\delta_0$	$^3\delta_0$	$^1\delta_1$	$^3\delta_1$	$^1\delta_2$	$^3\delta_2$
1.QBA[a]	0.7126	1.3319	−0.2682	0.2417	−0.0083	0.0309
$P1$ $(d=1.80)$[b]	1.1011	1.3929	−0.1618	0.3785	0.0397	0.0805
$P2$ $(d=1.36)$[b]	0.9981	1.3954	−0.1587	0.3792	0.0417	0.0826
V^{pol}	0.9578	1.4020	−0.1567	0.3731	0.0474	0.0883
Variational[c]	0.886	1.643	−0.004	0.427	0.0745	0.0697

[a]Reference 5.
[b]Reference 6.
[c]Reference 11.

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

	$^1\delta_0$	$^3\delta_0$	$^1\delta_1$	$^3\delta_1$	$^1\delta_2$	$^3\delta_2$
1.QBA[a]	0.9642	1.7834	−0.1679	0.1829	−0.0066	0.0130
$P1$ $(d=1.80)$[b]	1.3774	1.8432	−0.0858	0.3074	0.0264	0.0471
$P2$ $(d=1.36)$[b]	1.2786	1.8457	−0.0829	0.3103	0.0275	0.0483
V^{pol}	1.2338	1.8503	−0.0766	0.3125	0.0321	0.0530
Variational[c]	1.041	1.9329	−0.009	0.3412	0.0383	0.0424

[a]Reference 5.
[b]Reference 6.
[c]Reference 11.

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

	$^1\delta_0$	$^3\delta_0$	$^1\delta_1$	$^3\delta_1$	$^1\delta_2$	$^3\delta_2$
1.QBA[a]	1.3373	2.2082	−0.0749	0.0857	−0.0019	0.0028
$P1$ $(d=1.53)$[b]	1.9883	2.2714	−0.0109	0.1874	0.0166	0.0216
$P2$ $(d=1.04)$[b]	2.0212	2.2771	−0.0036	0.2030	0.0174	0.0224
V^{pol}	1.6313	2.2745	−0.0105	0.1803	0.0181	0.0231
variational[c]	1.4146	2.2938	0.0100	0.1872	0.0183	0.0198

[a]Reference 5.
[b]Reference 6.
[c]Reference 11.

$$\tan\delta_L = \frac{\pi\alpha k^2}{(2L+3)(2L+1)(2L-1)} , \quad (3.1)$$

a property found already for the phenomenological potentials V^{P1} or V^{P2}. As in Ref. 6, the $L \geq 5$ contributions to the cross sections, therefore, could be chosen according to this formula.

In Tables II–IV we compare our present results for the $L=0,1,2$ phase shifts ${}^{2S+1}\delta_L$ with the ones of Ref. 6 and with variational values[11] that are usually considered to be most accurate. Also, for these low partial waves, the improvement of the 1.QBA achieved by incorporating the parameter-free Temkin-Lamkin potential is similar to the one obtained with the phenomenological expressions (2.1) or (2.2) for optimized values of the parameter d. This, on the one hand, appears rather satisfactory; but it also means that the discrepancies to the variational calculations are not removed when replacing V^{P1} or V^{P2} by $V^{\rm pol}$ (only in the singlet-S phase shift the deviations are slightly reduced).

The present approach, therefore, provides, in a *parameter-free* manner, quite accurate results for the differential cross sections and the higher partial waves of electron-hydrogen scattering below the first excitation threshold. The inaccuracies of the low phase shifts found in Ref. 6, however, are not removed when going over to the Temkin-Lamkin polarization potential.

The main conclusion to be drawn from the present investigation, therefore, is that the excited two-body (hydrogen) states should be taken into account more explicitly in the kernel of the integral equations, a requirement leading, of course, to a higher number of coupled quasiparticle equations, i.e., to a considerable increase of the numerical effort.

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