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Semiprecision Calculations of Electron-Hydrogen Resonances

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Reliable calculations of the shift (Δ) and width (Γ) are combined with precision calculations of the unshifted energy ($\mathcal{E}$) to obtain the position and width of the lowest ^1S resonance in e-H scattering. These values together with our previous results for the two higher, ^3P and ^1D, resonances are compared with the previous most-accurate calculations and some differences are noted. Comparison with experiment is also made.

Motivated by recent spectacularly clear experimental observation of the lowest three resonances below the first excitation threshold in electron-hydrogen scattering by Sanche and Burrow,[1] we have completed a calculation of the lowest (^1S) of these resonances. These calculations together with earlier ones for the ^3P and ^1D states, respectively,[2,3] are based on precision Hylleraas calculation[2-4] of the resonant wave function $Q\Phi$, combined with various reasonable physically motivated approximations for the nonresonant continuum Υ. These approximations were basically the exchange- and polarized-orbital approximations.[5] The similarity of the results from both calculations gave some confidence in those results; however, a much more elaborate pseudostate continuum-wave calculation[6] continues to give essentially the same result for the lowest optically allowed ^1P He($2s2p$) autoionization state. This affords much greater confidence in these approximations.

Therefore, we have used the exchange approximation Υ in the present ^1S e-H case for the nonresonant scattering function (P and Q are projection operators[4]).

$$\Upsilon_{\mathrm{ex}} = P\Upsilon_{\mathrm{ex}} = u(r_1/r_1)Y_0(\Omega_1)\phi_0(r_2) + (1 \leftrightarrow 2)\,. \tag{1}$$

The integrodifferential equation is well known and has been solved many times as a function of the incident energy k^2 (in rydbergs—cf. Ref. 5). We have also discussed the resonant Hylleraas-type functions in several papers, including the nontrivial problem of Q projection.[4]

The formulas for the width and the shift are likewise well known.[2] We repeat the formula for the latter to emphasize in the present ^1S application that Δ contains one discrete contribution from the ^1S bound state of H$^-$, which occurs even in the exchange approximation:

$$\Delta = \frac{1}{2\pi}\left(\frac{\Gamma_b}{E - E_{1_S}} + \mathcal{P}\int \frac{\Gamma(E')\,dE'}{E - E'}\right) \tag{2a}$$

(where $\mathcal{P}$ means principal part), which can be written

$$\Delta = \Delta_b + \Delta_c\,, \tag{2b}$$

with

$$\Gamma_b = 2\,|\langle P\Upsilon_{1_S}|H|Q\Phi\rangle|^2\,, \tag{3a}$$

$$\Delta_b = \frac{1}{2\pi}\left(\frac{\Gamma_b}{E - E_{1_S}}\right), \tag{3b}$$

and Υ_{1_S} is the exchange-approximate ^1S wave function of H$^-$ quadratically normalized to unity. [The discrete contributions to Δ in ^1P He($2s2p$) application have been discussed in detail in Ref. 6.] Note $P\Upsilon_{\mathrm{ex}} = \Upsilon_{\mathrm{ex}}$ for bound and continuum solutions.

Table I contains our results for the ^1S resonance. The value of $\mathcal{E}$, where the resonant energy E is related to $\mathcal{E}$ by

$$E = \mathcal{E} + \Delta\,, \tag{4}$$

is a result which goes beyond that calculated in Ref. 4. The shift result has been broken down into its one discrete and its continuum parts [Eqs. (2)]. We see that discrete contribution is not negligible. Comparison of these results is made with three recent ^1S calculations.[7-9] Chung and Chen[7] have used an anomaly-free Kohn variational method which derives from putting

TABLE I. Results (in eV) for the lowest ^1S electron-hydrogen resonance.

	Present	Chung and Chen [a]	Bardsley and Junker [b]	Shimamura [c]
$\mathcal{E}$	9.552 042	9.552 464		
Δ_c	−0.006 653			
Δ_b	+0.001 060 6			
Δ	−0.005 578	−0.003 481 [d]		
E	9.546 468	9.548 98	9.552 05	9.552 25
Γ	0.040 554	0.0411	0.0474	0.0472

[a] Reference 7.
[b] Reference 8.
[c] Reference 9.
[d] Inferred from differencing—cf. text.

TABLE II. Results (in eV) of three lowest resonances in electron-hydrogen scattering.[a]

State	Quantity	GSFC	Burke and Taylor[b]	McGowan *et al.*	Sanche and Burrow[c]	Risley, Edwards, and Geballe[d]
^1S	E	9.5465[e]	9.555	9.56 ± 0.01[f]	9.558 + 0.01	
	Γ	0.0406[e]	0.0475	0.043 ± 0.006[f]	...	0.1710 ± 0.0095[g]
^3P	E	9.733[h]	9.735 05	9.71 ± 0.03[f]	9.738 ± 0.01	
	Γ	0.0063[h]	0.0059	>0.009[f]	0.0056 ± 0.0005	0.5869 ± 0.0099[i]
^1D	E	10.1185[j]	10.1199	10.13 ± 0.015[k]	10.128 ± 0.01	
	Γ	0.010[j]	0.0088		0.0073 ± 0.002	

[a] All results have been corrected to eV using a reduced rydberg 13.598 433 eV and R_∞ = 13.605 826 eV from B. N. Taylor, W. H. Parker, and D. N. Langenberg [Rev. Mod. Phys. 41, 375 (1969)].

[b] Reference 10.

[c] Reference 1.

[d] J. S. Risley, A. K. Edwards, and R. Geballe, in *Abstracts, Seventh International Conference on the Physics of Electronic and Atomic Collision*, edited by L. M. Branscomb *et al.* (North-Holland, Amsterdam, 1971), p. 1047.

[e] This work.

[f] J. W. McGowan, Phys. Rev. 156, 165 (1967).

[g] The entry represents the energy difference between ^3P and ^1S resonances.

[h] Reference 2. Width and shift calculated with polarized-orbital nonresonant function.

[i] Energy difference between ^1D (and/or ^1P) resonance and ^1S resonance [J. S. Risley (private communication)].

[j] Reference 3. Width and shift calculated with polarized-orbital nonresonant function.

[k] J. W. McGowan, E. M. Clarke, and E. K. Curley, Phys. Rev. Lett. 15, 917 (1965); Phys. Rev. Lett. 17, 66 (E) (1966).

their correlation function in Q space. Their value of Δ is inferred by subtracting their resonance energy from their value of QHQ (which uses a configuration-interaction-type wave function and yields a value of $\mathcal{E}$ slightly above our own). Our results agree closely with theirs, whereas they differ more significantly from Bardsley and Junker.[8] That calculation is based on a complex coordinate method (which yields a complex energy whose imaginary part is the width). A similar discrepancy occurs with the results of Shimamura.[9] He used a Schwartz-type Kohn procedure. As Shimamura himself has said, this is an empirical method of avoiding the unphysical singularities. Comparison with our results again suggests that the method of Chung and Chen provides a preferable alternative.

In Table II we summarize our results of the first three resonances and compare them with those of Burke and Taylor and the experimental results. Burke and Taylor[10] have done a scattering calculation and thus they derive E directly from the resonant curve of the phase shift versus k^2. On the other hand, they use 20 Hylleraas-correlation terms (plus $2s$, $2p$ close-coupling states), and it is not clear that this is sufficient for convergence. In fact, our results strongly suggest that it is not. However, because of the nature of our calculation of Δ and Γ we refrain from claiming our results as definitive. Very conservatively, however, we would claim that Δ is correct to within a factor of 2. The convergence of $\mathcal{E}$ is to a minimum of 5 significant figures, so that our value of E should be correct to within 0.003 eV. This is only true for the ^1S resonance. Because of the larger physical size of the higher two states, our Hylleraas Φ together with our calculation of Δ provides a reasonably secure upper bound on E for ^3P and ^1D resonances.

With regard to the experimental results, it is not clear that they are sufficiently accurate yet to distinguish between the various calculations. In fact, Golden[11] has recently argued that in elastic scattering a device which uses an axial magnetic field such as a troichoidal monochromator can have the effect of distorting the observed width from its true value.

It is not our purpose (and not within our competence) to criticize the experimental values. It is hoped, however, that the present calculated results will be of use to experimentalists in assessing their instrumental accuracy as well as in comparisons with theory.

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