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Line-shape parameters for ^1P Feshbach resonances in He and Li$^+$

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The line-shape parameter (q) for the three lowest ^1P autoionization states of He and Li$^+$ below the first excited target (He$^+$, Li^{2+}) level are accurately calculated. In order to do this we rederive a rigorous expression for q in terms of the Feshbach formalism; the formula contains additional terms representing the effect of other resonances on the resonance being calculated. Hylleraas functions are used to calculate $Q\Phi$, and the exchange approximation is used for the nonresonant continuum. Results agree well with the experiment where available. Our previous calculations of positions and widths are not affected; however, it is noted that the energy of the newest experiment of Morgan and Ederer for the lowest ^1P autoionization state of He (60.151 ± 0.01 eV) is such that when it is combined with the older experimental value of Madden and Codling (60.133 ± 0.015 eV), the weighted mean of the two measurements (60.145 ± 0.008 eV) is in exceptional agreement with our previous value (60.145 eV).

I. INTRODUCTION

Over the last many years we have carried out a series of calculations of two-electron autoionization states, trying to use the full potential of the Feshbach formalism[1,2] to obtain significant accuracy. The main object of these investigations was to provide precision checks of the continuum solutions of the Schrödinger equation, of which autoionization states (i.e., resonances) are a part which is particularly well suited to such tests.[3] The applications were confined to two-electron systems (i.e., scattering from one electron targets) for the obvious reason that such systems are amenable to precision calculations and for the not so obvious reason that projection operators—the life blood of the Feshbach formalism[1]—are explicitly available for the one-body targets.[2]

The results of these calculations[4–6] culminating in two recent papers,[7,8] have yielded increasingly satisfactory agreement with experiment. Two discrepancies remained, however, both with respect to the $^1P(2s\,2p)$ autoionization state of He: one was the deviation of the calculated energy value from the central position of that state as measured in the classic vacuum uv absorption experiment of Ref. 9; the second was the deviation from the measured[9] line-shape parameter q. We shall discuss the position measurement briefly at the end; suffice it here to note that a new measurement in the following paper by Morgan and Ederer[10] is now in good accord with our previous result.

This leaves the line-shape parameter discrepancy as the remaining issue to be dealt with. Here the problem is that the translation of the line-shape parameter as introduced by Fano[11] into calculationally unambiguous form within the Feshbach formalism is not completely obvious. Section II is concerned with that. Since only the obvious parts of the formula are what was previously included,[7] Sec. III is devoted to a recalculation of q for the autoionization states mentioned in the abstract.

II. DERIVATION OF q

In the Fano formulation[11] the cross section for an electromagnetic transition described by an operator T (think of the absorption of a photon of energy E) from an initial bound state—which we shall take to be the ground state—to a final continuum state characterized by a resonance at energy E_s is given by the formula

$$\left|\frac{\langle\Psi\,|\,T\,|\,\Psi_g\rangle}{\langle\Psi_0\,|\,T\,|\,\Psi_g\rangle}\right|^2=\frac{(\epsilon+q)^2}{1+\epsilon^2}\ . \tag{1}$$

It is assumed that Ψ is characterized by a resonance at energy E_s and a width Γ_s. In Eq. (1) the scaled energy is defined by

$$\epsilon=(E-E_s)/(\Gamma_s/2) \tag{2}$$

From (1) it is seen that the final additional parameter that is necessary to describe the shape of the line is q, usually called the line-shape parameter. It is our object in this section to give a derivation in terms of the Feshbach formalism[1] (which assumes only nonoverlapping resonances) of a rigorous expression for q from which *ab initio* calculations can be performed, and to do such calculations.

The denominator in the left-hand side (lhs) of Eq. (1) is a transition element from Ψ_g to a nonresonant (scattering) state Ψ_0 which is asymptotically like the fully resonant scattering function Ψ, but lacking an internal part associated with the resonance. (But it does have internal contributions from other resonances, as we shall see.)

It is at this point that the incisiveness and beauty of the Feshbach theory enters, for it is of the essence that it divides the whole wave function into internal pieces $Q\Psi$ and an external part $P\Psi$, at the outset

$$\Psi=P\Psi+Q\Psi\ . \tag{3}$$

Coupled equations for $P\Psi$ and $Q\Psi$ can readily be derived.[1,2] In particular the boundlike part is readily expandable in terms of a well-defined set of functions $\Phi_n = Q\Phi_n$ satisfying

$$QHQ\Phi_n = \mathcal{E}_n \Phi_n \;. \tag{4}$$

Using the relation between $P\Psi$ and $Q\Psi$,

$$Q\Psi = \frac{1}{E - QHQ} QHP\Psi \;, \tag{5}$$

one obtains by inserting a complete Φ_n in Q space in (5)

$$|Q\Psi\rangle = \sum\!\!\!\!\!\!\int_n \frac{|Q\Phi_n\rangle\langle Q\Phi_n | H | P\Psi\rangle}{E - \mathcal{E}_n} \;. \tag{6}$$

[In (6) we mean the sum over the discrete spectrum and integral over the continuous spectrum of (4). Note that below the relevant inelastic threshold, Q is such that the Φ_n are discrete and correspond to real resonances, and above the threshold the spectrum is continuous.] The function $P\Psi$ satisfies the full optical potential Schrödinger equation

$$\left[PHP + \sum\!\!\!\!\!\!\int_n \frac{H_{PQ}|\Phi_n\rangle\langle\Phi_n|H_{QP}}{E - \mathcal{E}_n} - E \right] |P\Psi\rangle = 0 \;, \tag{7}$$

whereas the nonresonant function *is defined* to satisfy the same equation less the resonant ($n = s$) term,

$$\left[PHP + \sum\!\!\!\!\!\!\int_{n\,(\neq s)} \frac{H_{PQ}|\Phi_n\rangle\langle\Phi_n|H_{QP}}{E - \mathcal{E}_n} - E \right] |P\Psi_0^{(s)}\rangle = 0 \;. \tag{8}$$

A formal relation between $P\Psi$ and $P\Psi_0^{(s)}$ can be readily derived[12]

$$|P\Psi_u\rangle = |P\Psi_0^{(s)}\rangle + \frac{G_P^{(s)} H_{PQ}|\Phi_s\rangle\langle\Phi_s|H_{QP}|\Psi_0^{(s)}\rangle}{E - \mathcal{E}_s - \Delta_s} \;, \tag{9}$$

where $G_P^{(s)}$ is Green's function of Eq. (8) which, projected on $\phi_0(r_2)Y_{L0}(\Omega_1)$, satisfies the equation

$$\left\langle \phi_0(r_2)Y_{L0}(r_1) \right| \left[PHP + \sum\!\!\!\!\!\!\int_{n\,(\neq s)} \frac{H_{PQ}|\Phi_n\rangle\langle\Phi_n|H_{QP}}{E - \mathcal{E}_n} - E \right] \left| G_0^{(s)} \right\rangle = -\delta(r_1 - r_1') \;. \tag{10}$$

Δ_s is the shift in the resonance position E_s from $\mathcal{E}_s$ [cf. Eq. (4)],

$$E_s = \mathcal{E}_s + \Delta_s \;, \tag{11}$$

where

$$\Delta_s = \langle\Phi_s | H_{QP} G_P^{(s)} H_{PQ} | \Phi_s\rangle \;. \tag{12}$$

In Eqs. (9) and beyond we have labeled $\Psi = \Psi_u$, because if the solution of (8) is normalized to unit (plane wave) amplitude,

$$\lim_{r_1\to\infty} (P\Psi_0^{(s)}) = \frac{\sin(kr_1 - l\pi/2 + \eta_0)}{kr_1} Y_{L0}(\Omega_1)\varphi_0(r_2) \;, \tag{13}$$

then the solution of (7) defined in Eq. (9) will be differently normalized to

$$\lim_{r_1\to\infty} (P\Psi_u) = \frac{1}{\cos\eta_r} \frac{\sin(kr_1 - l\pi/2 + \eta_0 + \eta_r)}{kr_1} \times Y_{L0}(\Omega_1)\varphi_0(r_2) \;. \tag{14}$$

Both the normalization factor, the width, and the energy dependence of the additional (resonant) part of the phase shift are derivable from Eq. (9),

$$\tan\eta_r = -\frac{\frac{1}{2}\Gamma_s}{E - E_s} \tag{15}$$

and

$$\Gamma_s = 2k \, | \langle P\Psi_0^{(s)}(E_s) | H_{PQ} | \Phi_s\rangle |^2 \;. \tag{16}$$

(Rydberg units are used throughout.)

It is convenient at this point to define the Q-space Green's functions as follows:

$$G_Q = \sum\!\!\!\!\!\!\int_n \frac{|Q\Phi_n\rangle\langle Q\Phi_n|}{E - \mathcal{E}_n} \tag{17}$$

and

$$G_Q^{(s)} = \sum\!\!\!\!\!\!\int_{n\,(\neq s)} \frac{|Q\Phi_n\rangle\langle Q\Phi_n|}{E - \mathcal{E}_n} \;, \tag{18}$$

and to retain "bra-ket" notation explicitly. With these definitions Eq. (6) can be written

$$|Q\Psi_u\rangle = G_Q QH \, |P\Psi_u\rangle \;. \tag{19}$$

Inserting Eqs. (9) and (19) into (3), we have

$$\begin{aligned} |\Psi_u\rangle &= |P\Psi_u\rangle + |Q\Psi_u\rangle \\ &= |P\Psi_0^{(s)}\rangle + \frac{G_P^{(s)} H_{PQ}|\Phi_s\rangle\gamma_s}{E - \mathcal{E}_s - \Delta_s} \\ &\quad + \frac{|Q\Phi_s\rangle\langle\Phi_s|H_{QP}}{E - \mathcal{E}_s} \left[P\Psi_0^{(s)} + \frac{G_P^{(s)} H_{PQ}|\Phi_s\rangle\gamma_s}{E - \mathcal{E}_s - \Delta_s} \right] \\ &\quad + G_Q^{(s)} H_{QP} \, |P\Psi_u\rangle \;, \end{aligned} \tag{20}$$

where

$$\gamma_s = \langle\Phi_s | H_{QP} | \Psi_0^{(s)}\rangle \;. \tag{21}$$

The expression containing the large parentheses in (20) can be simplified using the above definitions of γ_s and Δ_s,

$$\frac{|Q\Phi_s\rangle}{E - \mathcal{E}_s} \left[\gamma_s + \frac{\gamma_s\Delta_s}{E - E_s} \right] = \frac{|Q\Phi_s\rangle\gamma_s}{E - E_s} \;. \tag{22}$$

Thus we conveniently write our final expression for Ψ_u

$$|\Psi_u\rangle=\frac{\gamma_s\,|Q\Phi_s\rangle}{E-E_s}+\left[(1+G_Q^{(s)}H_{QP})\,|P\Psi_0^{(s)}\rangle+\frac{\gamma_s}{E-E_s}(1+G_Q^{(s)}H_{QP})G_P^{(s)}H_{PQ}\,|Q\Phi_s\rangle\right] . \tag{23}$$

The correctly normalized function Ψ to be used in the expression for q, Eq. (3), as is clear from (14) is

$$|\Psi\rangle=\cos\eta_r\,|\Psi_u\rangle . \tag{24}$$

On the other hand, the correctly normalized $\Psi_0^{(s)}=P\Psi_0^{(s)}+Q\Psi_0^{(s)}$ requires using the counterpart of (19) for $Q\Psi_0^{(s)}$,

$$|Q\Psi_0^{(s)}\rangle=G_Q^{(s)}QH\,|P\Psi_0^{(s)}\rangle . \tag{19$'$}$$

Thus we recognize that $\Psi_0^{(s)}$ has both a P and a Q part which together are

$$|\Psi_0^{(s)}\rangle=(1+G_Q^{(s)}H_{QP})\,|P\Psi_0^{(s)}\rangle . \tag{25}$$

$\Psi_0^{(s)}$ is the function Ψ_0 to be used in Eq. (1). Substituting (24) and (25) into Fano's basic expression (1) for the resonance profile, we find that the lhs of (1) does reduce to the form of the right-hand side (rhs), where in particular an explicit expression for q emerges. We shall write it in a form suitable for calculation in Sec. III.

We conclude this section with the following observation: $G_Q^{(s)}$ includes the effects of other resonances (ultimately on the shape parameter q) on the specific (s) resonance. However, the profile itself is given by a one-resonance–type formula, Eq. (1). Aside from the *ab initio* calculational aspect, this represents a somewhat different point of view of including the effect of other resonances from the one embodied in a many-resonance formula. Fano has derived the latter in Sec. V of his paper[11] leading to a formula which will automatically exhibit the usual resonant shape at each resonance, but which will also contain slight deviations in shape at any resonance coming from the other resonances. This comes down to describing the bound-state-like parts separately, but with a single nonresonant continuum. This is to be contrasted with the present approach of treating other resonances as a distortion of the nonresonant continuum associated with the single (sth) resonance.

As compared to a single profile formula (as is done here), it may be thought that the many-level formula is more accurate, because it allows deviations from the single profile formula. However, it should be emphasized that in a purely Feshbach approach, the shift, width, and finally q_s are energy *dependent*: $\Gamma_s=\Gamma_s(E)$, $\Delta_s=\Delta_s(E)$, and finally $q=q(E)$. To be sure, all these quantities depend only weakly on E in the vicinity of $E=E_s$. But to the extent that they do, the profile formula will deviate from a strictly one-level form with energy-independent parameters, and we believe it will do so in an experimentally meaningful way.

We remind the reader that the energy dependence of the Feshbach resonant quantities also leads to corrections from their energy independent (Breit-Wigner) counterparts; they are embodied in the formulas[8,13]

$$\Gamma_s^{(\mathrm{BW})}=\Gamma_s(E)\left.\left[1+\frac{\partial\Delta_s(E)}{\partial E}\right]\right|_{E=E_s} , \tag{26a}$$

$$E_s^{(\mathrm{BW})}=\left[[\mathscr{E}_s+\Delta_s(E)]+\frac{1}{4}\Gamma_s(E)\frac{\partial\Gamma_s}{\partial E}+\cdots\right]_{E=E_s} . \tag{26b}$$

Indeed our precision calculation[8] of the lowest ^1S autodetaching state of H$^-$ shows the second term of (26a) [but not (26b)] makes a small but important contribution to $\Gamma_s^{(\mathrm{BW})}$. One could in principle develop similar formulas for $q(E)$; however, they would be so complicated to derive and exhibit that it is better to calculate q numerically as a suitable mesh in E and then to assess the quantitative importance of its E dependence. We shall do that in Sec. III.

III. RESULTS

For calculational purposes we write the final formula in a manner similar to Ref. 7. (All quantities not given here are defined therein.) Specifically, we write

$$q=q_0+\delta q_c+\delta q_b+\delta q_r . \tag{27}$$

The new quantity here is δq_r,

$$\delta q_r=\frac{1}{\mathscr{V}}\sum_{n\,(\neq s)}\frac{\langle Q\Phi_n\,|T\,|\Psi_g\rangle}{E_s-E_n}\left[\frac{1}{\pi}\mathscr{P}\int\frac{\langle Q\Phi_n\,|H\,|P\Psi_0^{(s)}(E')\rangle\langle\Psi_0^{(s)}(E')P\,|H\,|Q\Phi_s\rangle K'dE'}{E_s-E'}+\sum_{\nu}\frac{\langle Q\Phi_n\,|H\,|P\Psi_\nu^{(s)}\rangle\langle\Psi_\nu^{(s)}P\,|H\,|Q\Phi_s\rangle}{E_s-E_\nu^{(s)}}\right] , \tag{28}$$

where

$$\mathscr{V}=k\langle\Psi_0(E_s)P\,|H\,|Q\Phi_s\rangle\langle\Psi_0^{(s)}(E_s)\,|T\,|\Psi_g\rangle . \tag{29}$$

Note the last factor in (29) involves $\Psi_0^{(s)}$ of Eq. (25) and not simply $P\Psi_0$ (although numerically the $Q\Psi_0$ contribution is found to be very small).

The calculation of q also involves quantities occuring in the nonresonant background, σ_B. The latter is the only significant contribution to the absorption for energies away from resonance; the formula for it is[14]

$$\sigma_B=4\pi\alpha_f K(I+K^2)\,|\langle\Psi_0^{(s)}\,|T\,|\Psi_g\rangle|^2 . \tag{30}$$

TABLE I. Convergence of δq_c and δq_r as a function of the number of mesh points in principal value integrals for doubly excited states of He and Li$^+$.

System	Number of points	$s=1$		$s=2$		$s=3$	
		δq_c	δq_r	δq_c	δq_r	δq_c	δq_r
He[$^1P(s)$]	175	3.676(−1)[a]	−9.895(−4)	1.674	−9.006(−2)	2.623(−1)	−4.325(−3)
	187	3.677(−1)	−9.892(−4)	1.678	−9.387(−2)	3.603(−1)	−4.537(−3)
	203	3.677(−1)	−9.892(−4)	1.678	−9.387(−2)	3.635(−1)	−4.595(−3)
Li$^+$[$^1P(s)$]	175	3.677(−1)	−4.329(−4)	1.749	−6.763(−3)	5.295(−1)	−6.438(−3)
	249	3.825(−1)	−4.024(−4)	1.706	−6.859(−3)	4.674(−1)	−5.884(−3)
	385	3.850(−1)	−3.972(−4)	1.685	−6.908(−3)	4.340(−1)	−5.587(−3)

[a] 3.688(−1) is an abbreviation for 3.688×10^{-1}.

α_f is the fine-structure constant, and I is the ionization potential. Note again that the effect of other resonances is incorporated in $\Psi_0^{(s)}$ [cf. Eqs. (18),(19),(25)] and hence in σ_B. Numerically we find that the contribution from the $Q\Psi_0^{(s)}$ to σ_B is small but not negligible. The total absorption cross section is given by[14]

$$\sigma_T=\sigma_B\frac{(\epsilon+q)^2}{1+\epsilon^2}\ . \tag{31}$$

Coming now to our actual calculation, we have used for the resonant wave functions 84-term Hylleraas functions of our previous papers.[4–7] The nonresonant continua are those of the exchange approximation. In addition to calculating δq_r itself we have concentrated in this calculation on refining the evaluation of the principal value integrals which occur in δq_c as well as δq_r. Note that in (28), all quantities referring to the nonresonant continuum are rigorously functions of s because each has a different potential constructed by omitting the s term from the full optical potential. Each nonresonant potential also gives rise to a bound-state spectrum ($P\Psi_v^{(s)}$). In practice we use the exchange approximation for which all these nonresonant quantities are independent of s. Nevertheless that approximation contains a bound-state contribution Ψ_v which is handled as discussed in Bhatia, Burke, and Temkin.[5]

Table I gives results for various numbers of mesh points used in evaluating the principal value integrals for the first three resonances in He and Li$^+$. The contribution for the principal value itself was handled by the usual device of Taylor expanding the numerator (retaining here as many as nine terms) and then analytically performing the integrals of the resultant sum between appropriate limits on either side of the singularity. The remaining part of the integral was done numerically and the "number of points" column refers to the number of mesh points in that portion of the integral plus the number of terms in the principal value expansion. Note δq_r also includes contributions from other resonances (n) in addition to its own bound-state spectrum. In Table I we also include a recalculation of δq_c which differs from Ref. 4 primarily by a factor of $\sqrt{2}$. (The polarized orbital value of δq_c in Ref. 5 is correct there and is negligibly different from the present δq_c. That appears to be true for all resonant quantities for the He$^+$ target and is the reason why we have restricted ourselves to the exchange approximation here.)

TABLE II. Calculation of resonance parameters and absorption cross sections for He**[$(2s\,2p)$ ^1P] as a function of E. (Cross sections are in the units of 10^{-18} cm^2.)

E	Γ (eV)	q	σ_B	σ_{tot}	σ_{tot}[a]	σ_{tot}[b]
59.6187	0.036 264		1.3610		1.640	1.531
59.7888	0.036 265		1.3686		1.799	1.669
59.9588	0.036 308		1.3761		2.226	2.046
60.0813	0.036 320	−2.8371	1.3816	4.178	4.193	3.578
60.1085	0.363 23	−2.8428	1.3829	6.456	6.470	5.136
60.1386	0.036 324[c]	−2.8471[c]	1.3834	12.597	12.605	9.801
60.1407	0.036 324[c]	−2.8474[c]	1.3843	12.470	12.476	10.079
60.1450	0.036 324	−2.8481	1.3845	11.231	11.231	10.212
60.1629	0.036 328	−2.8496	1.3853	2.451	2.447	3.707
60.1901	0.036 331	−2.8521	1.3865	0.0266	0.0260	0.0746
60.2989	0.036 340		1.3915		0.605	0.5813
60.6390	0.036 369		1.4071		1.126	1.095
60.8091	0.036 396		1.4150		1.202	1.170
60.9787	0.036 395		1.4230		1.251	1.220

[a] Using constant $q=-2.8481$, $\Gamma=0.036\,324$ eV at $E=E_r=60.1450$ eV from the present calculation.

[b] From Morgan and Ederer (Ref. 10) their parameters $q=-2.6$, $\Gamma=0.038$ eV, and $E_r=60.151$ eV, and their σ_B.

[c] Interpolated values.

TABLE III. Final results for resonance parameters.

		He			Li$^+$	
Parameter	$s=1$	$s=2$	$s=3$	$s=1$	$s=2$	$s=3$
			Present calculation			
q_0	-3.139	-3.556	-2.849	-2.507	-26.451	-2.294
δq_c	$3.677(-1)$	1.678	$3.635(-1)$	$3.850(-1)$	1.685	$4.340(-1)$
δq_b	$-7.631(-2)$	-2.636	$-1.129(-1)$	$-7.603(-2)$	-1.963	$1.704(-1)$
δq_r	$-9.892(-4)$	$-9.387(-2)$	$-4.595(-3)$	$-3.972(-4)$	$-6.908(-3)$	$-5.587(-3)$
q	-2.849	-4.606	-2.604	-2.199	-26.736	-2.033
E (eV)[a]	60.1450	62.7594	63.6610	150.2470	159.1453	161.0327
Γ (eV)[a]	0.0363	$1.06(-4)$	0.009	0.0593	$0.163(-3)$	0.0195
		Ref. b			Ref. d	
q	$-2.80\ \pm 0.25$		$-2.0\ \pm 1.0$	$-1.5\ \pm^{0.3}_{0.5}$		
E (eV)	60.133 ± 0.015	62.756 ± 0.010	63.656 ± 0.007	$150.29\ \pm 0.05$		161.06 ± 0.10
Γ (eV)	0.038 ± 0.004		0.008 ± 0.004	0.075 ± 0.025		
		Ref. c				
q	$-2.55\ \pm 0.16$		$-2.5\ \pm 0.5$			
E (eV)	60.151 ± 0.010		$63.655\ \pm 0.01$			
Γ (eV)	0.038 ± 0.002		0.0083 ± 0.002			

[a] Results for E and Γ for He from our preceding paper (Ref. 7). Compare Ref. 3 for other experimental and calculated results.

[b] Madden and Codling (Ref. 9). Results of Refs. 9 and 10 have been converted to eV using the latest values of $\hbar c = 1.973\,285\,8\times 10^{-5}$ eV cm from the compilation: Particle Data Group, Phys. Lett. 111B, (1982).

[c] Morgan and Ederer (Ref. 10).

[d] Carrol and Kennedy (Ref. 15); calculated results are with respect to the ground state of Li$^+$ which is taken as $-14.557\,86$ Ry.

In Table II we give the energy dependence of the various calculated quantities, including σ_B, which determines the total absorption cross section σ_T of Eq. (31). As we have indicated above, this includes the energy dependence of Γ and q. However, in practice we see that the effect on σ_T is negligibly different from using energy independent Γ and q evaluated at $E=E_r$, whose values are given in footnote a of Table II. The main difference from the experiment is in the maximum absorption, whose value at maximum is seen to be about 20% less than either of the theoretical values. The maximum absorption is in turn related to the value of q via

$$\sigma_{\max\,\mathrm{ab}} = \sigma_B(1+q^2)\ ,$$

thus it is clear that the experimentally inferred q is somewhat smaller in absolute value than our calculated result. In the following experimental paper,[10] Morgan and Ederer discuss the experimental significance of the error in this quantity specifically. From the theoretical point of view we would estimate the error of our result conservatively to be about 10%; however, it is clear from Table II that the deviation in shape of the resonance curve of Morgan and Ederer cannot be attributed to the energy dependence of the calculated resonance parameters.

In Table III we have collated our final results for all resonances we consider here. The various parts of q are included as well as our previous results for E and Γ. The lower part of Table III gives experimental results. First and foremost, observe the lowest ^1P state of He**. One sees that the central value of the new experimental result of Morgan and Ederer[10] is considerably closer to our value of E than the older result of Madden and Codling.[9] We emphasize that our result for E is here simply taken over from our previous calculation,[7] and that that result has not changed significantly since our earliest calculation of the shift.[3] It was in view of this constancy and its deviation from the central value of the older experiment that we had long been calling for a remeasurement of this basic autoionization state.[3,5,7] We are very grateful that a new measurement has now taken place.[10] [It should be noted from the table that both experimental results for E reflect the latest values of fundamental constants (viz., $\hbar c$), therefore, the Madden-Codling results (for E) differ slightly from their previously published values.] Taking a weighted average of the two measurements[9,10]

$$\bar{E} = \frac{\left[\sum_{i=1}^{2} E_i \Big/ (\Delta E_i)^2\right]}{\sum_{i=1}^{2} (\Delta E_i)^{-2}}\ , \quad \overline{\Delta E} = \frac{\prod_{i=1}^{2} (\Delta E_i)}{\left[\sum_{i=1}^{2} (\Delta E_i)^2\right]^{1/2}}$$

gives a weighted experimental value

$$\bar{E}_{\mathrm{expt}} = 60.145\pm 0.008\ ,$$

which can only be described as being in exceptional accord with our result[7] (60.145 eV).

The remaining comparisons in Table III are also seen to be within the experimental limits. The second resonance of Morgan and Ederer[10] clearly corresponds to the third ^1P resonance for the well-known reason that the second resonance is too narrow to be seen. The same also applies to the second resonance in Li$^+$ observed by Carrol and Kennedy,[15] hence we would also confidently associate it with the third resonance of the $\mathrm{Li}^{+}(^{1}P)$ series. Here as well as in $\mathrm{He}^{**}(^{1}P)$ the effect of the energy dependence of all resonance parameters can be calculated when the experimental accuracy warrants. But for the present we can say, with the possible exception of q, that the most accurate experimental observation and calculation are in quite satisfactory agreement for autoionization states of two-electron systems below the $n=2$ target threshold, in particular $(\mathrm{H}^{-})^{**}$ and He^{**}.

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