Addendum to "Autoionization states in He and H^- by the stabilization method"

A. K. Bhatia

National Aeronautics and Space Administration, Goddard Space Flight Center, Greenbelt, Maryland 20771

(Received 19 March 1974)

The positions of the resonances calculated by the stabilization method can be improved by inclusion of the shift as given by Hazi and Fels. It is also indicated that the phase shifts calculated by the Harris method at incident energies corresponding to the stabilized roots give the positions and the widths of the resonances reasonably well.

The positions and widths of the resonances in He and H^- have been calculated very accurately by several methods including the Feshbach–projection-operator (FPO) technique.[1] A method wherein projection operators are not needed is the stabilization method, and it was shown recently that quite reasonable results can be obtained by this method.[2] Though a single value of the width was obtained, there were three values of the positions, differing considerably from one another. It is possible, in all cases, to reduce this spread if a stabilization shift Δ_j is added to the previously calculated positions E_j by this method,[3] giving the resonance position

$$E_r = E_j + \Delta_j \ . \tag{1}$$

The shift is given by[3]

$$\Delta_j = \tfrac{1}{2}\Gamma^{1/2}(S_j \sin\delta_L - C_j \cos\delta_L) \tag{2}$$

and

$$\Gamma = \Gamma_j = (s_j \cos\delta_L + C_j \sin\delta_L)^2 \ . \tag{3}$$

Here δ_L is the nonresonant phase shift,

$$S_j = (2/\sqrt{k}) \int\int d\vec{r}_1\, d\vec{r}_2\, j_L(kr_1) Y_{L0}(\Omega_1) \times \phi_0(r_2)(H-E)\Phi_j \ , \tag{4}$$

and

$$C_j = (-2/\sqrt{k}) \int\int d\vec{r}_1\, d\vec{r}_2\, n_L(kr_1)(1-e^{-\gamma r_1})^{2+L} \times Y_{L0}(\Omega_1)\phi_0(r_2)(H-E)\Phi_j \ . \tag{5}$$

For charged targets j_L and $-n_L$ are replaced by F_L and G_L, the regular and irregular Coulomb functions as indicated in Ref. 2. The expression for the shift Δ_j involves the integrals C_j and S_j, which are already available from the calculation of the width. Therefore the shift can be obtained without requiring any new integrals. The previously calculated E_j and the shift Δ_j are given

TABLE I. Resonance positions including shifts (in eV).

State and system	γ	Stabilization method E_j	Δ_j	E_r	Γ	Harris method E	Γ	FPO technique results [a] E	Γ
^1S H^-	0.450	9.5322	0.1191	9.5514	0.046	9.552	0.047	9.549 [b]	0.041
	0.475	9.5422	0.0093	9.5517					
	0.500	9.5499	0.0020	9.5519					
^1S He	1.10	57.8140	0.0216	57.8356	0.128	57.834	0.133	57.830	0.125
	1.15	57.8333	0.0034	57.8363					
	1.20	57.8508	−0.0138	57.8369					
^3P H^-	0.300	9.7343 [c]	0.0018	9.7362	0.0055	9.734	0.0048 [d]	9.733	0.0063
	0.325	9.7334	0.0011	9.7348					
	0.350	9.7339	0.0003	9.7342					
^1P He	0.700	60.1429	0.0033	60.1462	0.0373	60.146	0.042	60.145	0.0374
	0.725	60.1451	0.0014	60.1465					
	0.750	60.1474	−0.0007	60.1468					

[a] See Ref. 2.
[b] See Ref. 1 and Erratum.
[c] This number is incorrectly given as 9.748 eV in Table I of Ref. 2.
[d] This width is obtained by using the values corresponding to $\gamma = 0.350$ and $\gamma = 0.375$.

TABLE II. Positions and widths from seven root (in eV).

State and system	N [a]	E_r	Γ
^1S H^-	65	9.5520	0.0559
^1S He	65	57.8375	0.1279
^3P H^-	75	9.7347	0.0049
^1P He	75	60.1494	0.0376

[a] Number of terms in the trial function.

in Table I along with corrected positions E_r. The inclusion of the shift significantly reduces the spread of resonance positions.

When the number of terms in the trial function is increased, the seventh root instead of the sixth root becomes stable in all cases. The positions, including the shifts, and the widths of the resonances are given in Table II. The two roots give the same results for the positions. We find that with the inclusion of the shift, the position of the ^1S H^- resonance is no longer closer to the results of Bhatia and Temkin[1] as indicated in Ref. 2. It should be noted that the present result for this state is the same as that obtained by Bardsley and Junker[4] and Doolen *et al.*[5] using the complex-rotation method.[6]

We feel that Feshbach formalism provides more rigorous framework for the solution of many-body problems; we therefore prefer the value coming from such calculations. A truly definitive scattering calculation, however, will be required to settle the issue.[7]

The positions and widths can also be calculated by knowing the phase shift in the resonance region. The phase shift can be calculated by the Harris method,[8] which again requires the same integrals C_j and S_j. This method has been used previously to calculate nonresonant phase shifts, especially the phase shifts[9] obtained for the scattering of positrons from hydrogen atoms agreed very well with the lower-bound calculations.[10] But this method has been used in the resonance region only for model problems.[11] The phase shift at an incident energy corresponding to the stabilized root is given by

$$\delta_j = \tan^{-1}(-S_j/C_j) \ . \tag{6}$$

In the resonance region, the phase shift can be written as

$$\delta_j = \delta_L + \tan^{-1}\left(\frac{-\frac{1}{2}\Gamma}{E - E_r}\right) \ . \tag{7}$$

We find for the ^1S H^- resonance state, $E_r = 9.552$ eV and $\Gamma = 0.047$ eV, in good agreement with the resonance parameters given in Table I. The results for other states are also given in Table I.

I wish to thank Dr. A. U. Hazi for bringing to my attention his paper with Dr. M. F. Fels.

[1] A. K. Bhatia and A. Temkin, Phys. Rev. A 8, 2184 (1973), and the references given therein; see also Phys. Rev. A 10, 458(E) (1974).
[2] A. K. Bhatia, Phys. Rev. A 9, 9 (1974).
[3] A. U. Hazi and M. F. Fels, Chem. Phys. Lett. 8, 582 (1971).
[4] J. N. Bardsley and B. R. Junker, J. Phys. B 5, L178 (1972).
[5] G. Doolen, J. Nuttal, and R. W. Stagat, Phys. Rev. A (to be published).
[6] G. Doolen, M. Hidalgo, J. Nuttal, and R. Stagat, in *Proceedings of the Third International Conference on Atomic Physics* (Plenum, New York, 1973), p. 257.
[7] A. K. Bhatia, V. L. Jacobs, and A. Temkin (unpublished).
[8] F. E. Harris, Phys. Rev. Lett. 19, 173 (1969).
[9] S. K. Houston and R. J. Drachman, Phys. Rev. A 3, 1335 (1971).
[10] A. K. Bhatia, A. Temkin, R. J. Drachman, and H. Eiserike, Phys. Rev. A 3, 1328 (1971).
[11] A. U. Hazi and H. S. Taylor, Phys. Rev. A 1, 1109 (1970).