

Variational close-coupling calculation for positron-hydrogen scattering at low energies

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The S -wave ($L=0$) and P -wave ($L=1$) phase shifts and the S -wave and P -wave elastic and positronium-formation cross sections for positron scattering from hydrogen at energies below the first excitation threshold are calculated in the close-coupling approximation, using the algebraic variational method. Four target-state coupling schemes ($H\ 1s-Ps\ 1s$, $H\ 1s-H\ 2s-Ps\ 1s$, $H\ 1s-H\ 2s-H\ 2p-Ps\ 1s$, and $H\ 1s-H\ 2s-H\ 2\bar{p}-Ps\ 1s$) have been considered for the calculation. It is found that the $H\ 2\bar{p}$ target channel significantly affects the S -wave positronium-formation cross sections.

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I. INTRODUCTION

The close-coupling method of approximation has been well developed and extensively considered by many researchers for the investigation of the various electron- and positron-scattering processes since it was introduced to atomic-collision physics by Percival and Seaton [1] and by Burke and Schey [2] more than three decades ago. While the relevant formalism has been developed by Smith [3], the close-coupling calculation with the consideration of the positronium-formation channel for positron scattering from hydrogen in the Ore gap [4] of energies (6.8–10.2 eV), strictly speaking, has only been carried out a decade later [5], even though the effect of this channel on the cross sections should be rather significant for scatterings at low energies. The absence of this calculation merely reflects the difficulty in handling numerically the positronium-formation channel in the close-coupling approximation. In the past decade or so, the calculation of the positronium-formation cross sections in general and the close-coupling calculation of positron scattering with the inclusion of the positronium-formation channel in particular have been very much revitalized [6], probably due to the fact that experimental data for some positronium-formation processes have now been available, and that research activities in positron collision with atomic targets have been vigorously pursued in laboratories worldwide [6] in recent years.

In most recent calculations [7,8] of e^+H scattering, the close-coupling results have been obtained by solving the coupled integro-differential equations in the momentum space. An interesting method of approach, the so-called algebraic variational method by Harris and Nesbet [9] which was successfully considered earlier by Seitler, Oberoi, and Callaway [10] for electron scattering from H and by Wakid [11] and Wakid and Lebahn [5] for positron scattering and positronium formation, has not yet been fully exploited subsequently. This method of approach has an advantage of being able to acquire the results fast, in terms of the computer time. It also provides more confidence in the results, since problems of numerical accuracy at some particular scattering energies are not present [10]. Wakid and Lebahn [5] have, however, carried out the calculation for the S -wave scattering only.

Furthermore, by comparing the results obtained by various authors for e^+H scattering at low energies [12–17] with each other, one can notice that these theoretical values, especially those for cross sections of positronium formation, are very sensitive to the different approximations considered, as well as to the different numerical methods employed for the close-coupling calculation. It is, therefore, worthwhile to use again the algebraic method of approach in a more detailed close-coupling calculation for comparison. In particular, we shall also carry out the algebraic calculation of P -wave scattering, whose relevant values of cross section, as will be seen subsequently, prove to be rather significant in comparison to those of S -wave scattering. Four coupling schemes, $H\ 1s-Ps\ 1s$, $H\ 1s-H\ 2s-Ps\ 1s$, $H\ 1s-H\ 2s-H\ 2p-Ps\ 1s$, and $H\ 1s-H\ 2s-H\ 2\bar{p}-Ps\ 1s$, have been considered in our calculation. In addition, we employed up to 20 basis functions for the bound part of the scattering wave in the case of S wave and up to 30 basis functions in the case of P wave. The use of such a great number of basis functions is expected to yield a much better accuracy for the calculated results. Relevant formulas which are required for our numerical calculation have been obtained by tedious derivations (and carefully double-checked) for both S - and P -wave scatterings in the different coupling schemes considered.

II. METHOD OF CALCULATION AND RESULTS

The variational method of close-coupling calculation by Harris and Nesbet [9] has been well known. In particular, the description of the relevant formalism for electron and positron scattering from hydrogen has been given by Seitler, Oberoi, and Callaway [10] and by Wakid and Lebahn [5]. A primary part of the method is to construct scattered waves for the scattering (and positronium-formation) channels. These scattered waves are composed of two parts, which are the so-called "internal" and "external" parts. The external part is included essentially to represent the scattered wave in the asymptotic region, while the internal part is to represent the scattered wave near the "scattering center." The external parts depend on two independent parameters (β , for the scattering channel and γ , for the positronium-

formation channel), whose values were fixed by the stability condition of the variational method. The internal bound parts are expanded over a complete set of square-integrable basis functions with parametrical exponents Z_i and Z_j . The sets of Z_i and Z_j were chosen over a wide range of values to secure a good convergence for the observables to be calculated. Let $\phi_L(1,2)$ be the trial wave function, corresponding to a total angular momentum L and a parity π , which is constructed in the L - S coupling scheme for the collision system. The Harris-Nesbet procedure requires that (H-E) $\phi_L(1,2)$ has no component in the subspace of state vectors spanned by the short-range bound functions. This condition provides a "linkage" between the internal and external parts for the scattered waves. Through the Kohn and inverse Kohn variational methods [18], the reactance matrix or the inverse reactance matrix of the process will be deduced. The partial-wave cross sections or the phase shifts (for scatterings with energies below the positronium-formation threshold) can then be evaluated.

One of the purposes of this work is to study the effect of the different target channels (which were included in the close-coupling expansion) on the elastic and positronium-formation cross sections at low energies. Four coupling schemes have, therefore, been considered for the calculation. They are (i) $H\ 1s + Ps\ 1s$, (ii) $H\ 1s + H\ 2s + Ps\ 1s$, (iii) $H\ 1s + H\ 2s + H\ 2p + Ps\ 1s$, and (iv) $H\ 1s + H\ 2s + H\ 2\bar{p} + Ps\ 1s$. Below the positronium-formation threshold, the coupling schemes $H\ 1s + H\ 2s + H\ 2p$ and $H\ 1s + H\ 2s + H\ 2\bar{p}$ have also been considered (but the calculation is now performed with a higher number of basis functions for the bound part of the scattered wave) to acquire the corresponding elastic cross sections and phase shifts for comparison with those previously calculated by other authors who used the same coupling schemes within the same method of calculation [10,11]. This latest calculation also served to double-check the convergence and accuracy of our computer codes. The form of the pseudostate $2\bar{p}$ by Damburg and Karule [19] has been chosen to represent the $H\ 2\bar{p}$ state in our calculation.

We considered values of Z_i and Z_j of different intervals and ranges for a great number of test runs until a satisfactory convergence of the results of calculation had been reached. A basis of either 15 or 20 functions was considered for the calculation in the case of S -wave scattering, and a basis of 20 or 30 functions in the case of P -wave scattering. However, all the results reported in this paper were those either obtained with a 20-function basis (S -wave scattering) or with a 30-function basis (P -wave scattering). In order to find the most appropriate values for the parameters β and γ , we adopted Schwartz's principle [20]. We varied the values of these parameters and searched for the area of values which yields stabilized results for our calculation. For the S -wave scattering, the solutions are stable in a large area around $\beta=2$ and $\gamma=2$. For the P -wave scattering, the elastic phase shifts are stable with values of β around 2, but above the positronium-formation threshold, the area for the stability of the solutions is around $\beta=6$ and $\gamma=6$. The agreement between the results obtained with the Kohn and in-

verse Kohn variational methods was also used as a convergence criterion for our calculation. In general, the two sets of values agree to about three figures.

The relevant matrix elements among the scattering channels alone (or among the positronium-formation channels alone) can be analytically reduced to closed forms, which can then be numerically evaluated with ease. The relevant matrix elements which involve both scattering and positronium-formation channels can only be reduced to a one- or two-variable integral. For convenience, we chose the two-variable integral form in the calculation. To verify the convergence of our numerical double integration, we have tentatively compared with each other the values of some of these matrix elements calculated by both simple and double quadratures, and we have found that they agree with each other at least up to the tenth figure of significance. The analytical derivations of the expressions for these matrix elements (as well as their numerical evaluations) have also been double-checked by a comparison of the values calculated with the use of the two completely different formulas which were independently obtained for these symmetric matrix elements. At times, the expressions for the closed forms were also double-checked for their correctness by comparing their numerical values to those calculated by numerical integration.

In Tables I and II we exhibit the elastic phase shifts for S -wave and P -wave scatterings (with scattering energies below the positronium-formation threshold) in different coupling schemes. The S -wave phase shifts were calculated with the use of a basis of 20 functions, and the P -wave ones with a basis of 30 functions. Both were obtained with the inverse Kohn variational method. We found that the elastic phase shifts for the P -wave scattering obtained by the Kohn variational method are, in particular, very sensitive to the value considered for the parameter β . We chose, therefore, to report the more stable values obtained in the inverse Kohn variational method, which are only slightly different from those obtained in the Kohn variational method. Also shown for comparison are the results previously obtained by Wakid and Lebahn [5], by Seidler, Oberoi, and Callaway [10], by Burke and Schey [2], by Cody *et al.* [14], and by Basu, Mukherjee, and Ghosh [7]. To prove that the convergence has been reached in our calculation, we calculated the Kohn and inverse Kohn phase shifts with the $H\ 1s - H\ 2s - H\ 2\bar{p} - Ps\ 1s$ coupling scheme for S - and P -wave scatterings, using different sets of basis functions, and we found that these values, obtained by the various calculations, approach each other when the number of basis functions reaches 20 for S -wave and 30 for P -wave scattering.

In Tables III–VI we present the results of elastic and positronium-formation cross sections calculated for the S - and P -wave scatterings in the Ore gap, with the employment of the various coupling schemes. Results obtained by Abdel-Raouf *et al.* [15], Basu, Mukherjee, and Ghosh [7], Hewitt, Noble, and Bransden [8], and by Brown and Humberston [12] are also shown for comparison. Again, we notice through the values, calculated with the employment of different numbers of basis func-

TABLE I. Elastic S -wave phase shifts in radians for e^+ -H scattering. (a), (b), (c), (d), (e), and (f), present calculation; (a1), (e1), Wakid and Lebahn [5]; (a2) Cody *et al.* [14]; (d1) Basu, Mukherjee, and Ghosh [7]; Burke and Schey [2].

	Positron momentum k (a.u.)						
	0.1	0.2	0.3	0.4	0.5	0.6	0.7
	H 1s - Ps 1s						
(a)	-0.0191	-0.0473	-0.0875	-0.1365	-0.1893	-0.2417	-0.2902
(a1)	-0.0191	-0.0472	-0.0874	-0.1365	-0.1894	-0.2415	-0.2901
(a2)	-0.0188	-0.0465	-0.0858	-0.1339	-0.1861	-0.2379	-0.2864
	H 1s - H 2s - Ps 1s						
(b)	0.0101	0.0031	-0.0262	-0.0723	-0.1270	-0.1836	-0.2366
	H 1s - H 2s - H 2p - Ps 1s						
(c)	0.0330	0.0212	-0.0163	-0.0672	-0.1234	-0.1802	-0.2328
	H 1s - H 2s - H 2\bar{p} - Ps 1s						
(d)	0.0661	0.0624	0.0234	-0.0313	-0.0905	-0.1488	-0.2023
(d1)	0.0924	0.0978	0.0607	0.0019	-0.0643	-0.1230	-0.1895
	H 1s - H 2s - H 2p						
(e)	-0.0048	-0.0421	-0.0929	-0.1471	-0.1986	-0.2465	-0.2876
(e1)	-0.0050	-0.0426	-0.0935	-0.1476	-0.1997	-0.2469	-0.2919
(e2)	-0.0054	-0.0426	-0.0931	-0.1472	-0.1990	-0.2461	
	H 1s - H 2s - H 2\bar{p}						
(f)	0.0466	0.0324	-0.0097	-0.0627	-0.1175	-0.1703	-0.2183

TABLE II. Elastic P -wave phase shifts in radians for e^+ -H scattering. (a), (b), (c), (d), (e), and (f), present calculation; (d1) Basu, Mukherjee, and Ghosh [7]; Seitler, Oberoi, and Callaway [10]; (e2) Burke and Schey [2].

	Positron momentum k (a.u.)						
	0.1	0.2	0.3	0.4	0.5	0.6	0.7
	H 1s - Ps 1s						
(a)	0.0008	0.0052	0.0134	0.0223	0.0286	0.0313	0.0339
	H 1s - H 2s - Ps 1s						
(b)	0.0010	0.0072	0.0189	0.0322	0.0428	0.0487	0.0543
	H 1s - H 2s - H 2p - Ps 1s						
(c)	0.0053	0.0182	0.0342	0.0494	0.0612	0.0687	0.0767
	H 1s - H 2s - H 2\bar{p} - Ps 1s						
(d)	0.0079	0.0265	0.0486	0.0683	0.0827	0.0911	0.0931
(d1)	0.0084	0.0294	0.0560	0.0802	0.0967	0.1045	0.1092
	H 1s - H 2s - H 2p						
(e)	0.0047	0.0134	0.0203	0.0221	0.0184	0.0099	-0.0016
(e1)	0.0045	0.0132	0.0201	0.0218	0.0180	0.0093	
(e2)	0.0020	0.0127	0.0201	0.0217	0.0183	0.0101	
	H 1s - H 2s - H 2\bar{p}						
(f)	0.0075	0.0234	0.0397	0.0517	0.0576	0.0574	0.0528

TABLE III. *S*-wave elastic cross sections in a.u. for e^+ -H scattering at energies in the Ore gap. (a) H 1s-Ps 1s, (b) H 1s-H 2s-Ps 1s, (c) H 1s-H 2s-H 2p-Ps 1s, and (d) H 1s-H 2s-H 2 \bar{p} -Ps 1s, present calculation; (a1) H 1s-Ps 1s, Abdel-Raouf *et al.* [15].

k (a.u.)	(a)	(a1)	(b)	(c)	(d)
0.710		2.1000			
0.7154	2.1048		1.4307	1.3911	1.0681
0.720		2.1038			
0.725	2.1076		1.4494	1.4094	1.0870
0.730		2.1066			
0.750	2.1113	2.1095	1.4935	1.4508	1.1320
0.775	2.1100		1.5306	1.4848	1.1710
0.780		2.1076			
0.800	2.1037	2.1025	1.5608	1.5120	1.2041
0.825	2.0934		1.5848	1.5331	1.2316
0.830		2.0896			
0.835	2.0880		1.5926	1.5398	1.2410
0.840		2.0840			
0.850	2.0790	2.0779	1.6025	1.5482	1.2535

TABLE IV. The *S*-wave positronium-formation cross sections in a.u. for e^+ -H scattering at energies in the Ore gap. (a) H 1s-Ps 1s, (b) H 1s-H 2s-Ps 1s, (c) H 1s-H 2s-H 2p-Ps 1s, (d) H 1s-H 2s-H 2 \bar{p} -Ps 1s, present calculation; (a1) H 1s-Ps 1s, Abdel-Raouf *et al.* [15]; (c1) H 1s-H 2s-H 2p-Ps 1s, (d1) H 1s-H 2s-H 2 \bar{p} -Ps 1s, Basu, Mukherjee, and Ghosh [7]; (c2) H 1s-H 2s-H 2p-Ps 1s, Hewitt, Noble and Bransden [8]; (f) Brown and Humberston [12]. Numbers in square brackets denote powers of 10.

k (a.u.)	(a)	(a1)	(b)	(c)	(c1)	(c2)	(d)	(d1)	(f)
0.710		0.00[-5]			1.91[-2]			1.75[-3]	
0.7154	1.503[-5]		1.829[-2]	1.116[-2]			1.138[-4]		
0.720		1.00(-5)							
0.725	4.058(-5)		2.429(-2)	1.297(-2)			9.084(-5)		
0.730		3.00(-5)							
0.750	1.703(-4)	1.20(-5)	2.966(-2)	1.244(-2)	1.31(-2)	1.27[-2]	7.974(-6)	8.86(-4)	0.0138
0.775	3.960(-4)		2.979(-2)	1.038(-2)			2.504(-5)		
0.780		3.40(-4)							
0.800	7.133(-4)	5.60(-4)	2.776(-2)	8.143(-3)	7.67(-3)	8.48(-3)	1.642(-4)	3.55(-3)	0.0154
0.825	1.108(-3)		2.475(-2)	6.090(-3)			4.113(-4)		
0.830		9.70(-4)							
0.835	1.287(-3)		2.339(-2)	5.344(-3)			5.359(-4)		
0.840		1.12(-3)							
0.850	1.569(-3)	1.29(-3)	2.130(-2)	4.300(-3)	4.90(-3)	4.30(-3)	7.467(-4)		0.0182

TABLE V. *P*-wave elastic cross sections in a.u. for e^+ -H scattering at energies in the Ore gap. (a) H 1s-Ps 1s, (b) H 1s-H 2s-Ps 1s, (c) H 1s-H 2s-H 2p-Ps 1s, and (d) H 1s-H 2s-H 2 \bar{p} -Ps 1s, present calculation; (a1) H 1s-Ps 1s, Abdel-Raouf *et al.* [15].

k (a.u.)	(a)	(a1)	(b)	(c)	(d)
0.710		0.1000			
0.7154	0.0741		0.1875	0.3723	0.6043
0.720		0.1038			
0.725	0.0752		0.1892	0.3731	0.6030
0.730		0.1034			
0.750	0.0709	0.0972	0.1768	0.3405	0.5599
0.775	0.0634		0.1579	0.3001	0.5043
0.780		0.0843			
0.800	0.0556	0.0758	0.1380	0.2605	0.4448
0.825	0.0490		0.1211	0.2287	0.3976
0.830		0.0646			
0.835	0.0467		0.1150	0.2171	0.3799
0.840		0.0614			
0.850	0.0436	0.0586	0.1065	0.2013	0.3552

TABLE VI. The P -wave positronium-formation cross section in a.u. for e^+ -H scattering at energies in the Ore gap. (a) H $1s$ -Ps $1s$, (b) H $1s$ -H $2s$ -Ps $1s$, (c) H $1s$ -H $2s$ -H $2p$ -Ps $1s$, (d) H $1s$ -H $2s$ -H $2\bar{p}$ -Ps $1s$, present calculation; (a1) H $1s$ -Ps $1s$, Abdel-Raouf *et al.* [15]; (c1): H $1s$ -H $2s$ -H $2p$ -Ps $1s$, (d1) H $1s$ -H $2s$ -H $2\bar{p}$ -Ps $1s$, Basu, Mukherjee, and Ghosh [7]; (c2) H $1s$ -H $2s$ -H $2p$ -Ps $1s$, (d2) H $1s$ -H $2s$ -H $2\bar{p}$ -Ps $1s$, Hewitt, Noble, and Bransden [8]; (f) Brown and Humberston [12]. Numbers in square brackets denote powers of 10.

k (a.u.)	(a)	(a1)	(b)	(c)	(c1)	(c2)	(d)	(d1)	(d2)	(f)
0.710		0.0206			0.0380			0.0252		0.0848
0.7154	7.548[-2]		0.1029	0.1388			0.1203			
0.720		0.1498								
0.725	1.920(-1)		0.2598	0.3547			0.3114			
0.730		0.2862								
0.750	4.578(-1)	0.5190	0.5956	0.7692	0.873	0.870	0.7198	0.685	0.804	1.15
0.775	6.526(-1)		0.8205	1.0009			0.9822			
0.780		0.7729								
0.800	7.918(-1)	0.8963	0.9678	1.1330	1.29	1.29	1.1439	1.08	1.27	1.51
0.825	8.979(-1)		1.0766	1.2315			1.2738			
0.830		1.0338								
0.835	9.323(-1)		1.1106	1.2624			1.3169			
0.840		1.0698								
0.850	9.772(-1)	1.1019	1.1542	1.3037	1.48	1.39	1.3769	1.26	1.51	1.76

tions in both Kohn and inverse Kohn methods, that the convergence of our calculation has apparently been reached when the number of basis functions is taken to be 20 for S -wave and 30 for P -wave scattering. In fact, the calculated values change very little when different numbers of basis functions are used in the calculation and when the Kohn variational method is switched to the inverse one. The values of the reactance matrix elements R_{12} and R_{21} (and those of the inverse reactance matrix elements R_{12}^{-1} and R_{21}^{-1}) are also found to agree with each other up to the eighth figure of significance.

It can be seen through Tables I and II that our elastic phase shifts for both S - and P -wave scatterings agree with available results obtained by other groups who employed the same coupling schemes, but different methods of approach. Our S -wave phase shifts agree with those calculated by Wakid and Lebahn [5] and by Cody *et al.* [14] in the H $1s$ -Ps $1s$ coupling scheme, and with those calculated by Wakid and Lebahn [5] and by Burke and Schey [2] in the H $1s$ -H $2s$ -H $2p$ scheme. Our P -wave phase shifts agree with those calculated by Seitler, Oberoi, and Callaway [10] and with those calculated by Burke and Schey [2]. However, there seems to exist a noticeable deviation of our results from those calculated by Basu, Mukherjee, and Ghosh [7] in the H $1s$ -H $2s$ -H $2\bar{p}$ -Ps $1s$ coupling scheme for both S - and P -wave scatterings. Our S -wave phase shifts obtained in the H $1s$ -H $2s$ -H $2\bar{p}$ -Ps $1s$ are found to be somewhat higher than those calculated by Wakid and Lebahn [5] using a slightly different H $1s$ -H $2\bar{p}$ -Ps $1s$ -Ps $2\bar{p}$ coupling scheme (not shown). This seems to indicate that in the e^+ -H scattering, the contribution from the H $2s$ target channel to the scattering phase shifts is more significant than that from the Ps $2\bar{p}$ channel.

With scattering energies in the Ore gap, our results of elastic cross section in the H $1s$ -Ps $1s$ coupling scheme are found to agree rather well with those calculated by Abdel-Raouf *et al.* [15] for S wave, but for P wave, there

appears to be a noticeable disagreement (see Table III and V). The cause for this disagreement is not apparent and worth investigating. In this connection, we wish to stress that our calculated values are expected to be reliable up to four or five figures of numerical significance for S -wave scattering and to two or three figures for P -wave scattering.

With regard to the positronium-formation cross sections, our results obtained with different coupling schemes are only in either fair or poor agreement with the corresponding ones calculated by the others who used different methods of approximation (see Tables IV and VI). The results obtained by other groups do not agree with each other either. In this connection, it should again be stressed that the significant figures of our values are expected to be about four for S -wave scattering and about three for P -wave scattering. It is difficult to assess the merit, one over the other, of these different methods of calculation. Our P -wave positronium-formation cross sections calculated with the H $1s$ -H $2s$ -H $2\bar{p}$ -Ps $1s$ coupling scheme tend to lie between the results acquired by Hewitt, Noble, and Bransden [8] and those by Basu, Mukherjee, and Ghosh [7].

The difference in the effects of the various target channels considered for the close-coupling expansion is, in particular, striking on the results of S -wave positronium formation (see Table VI). The H $2s$ channel significantly increases the values of cross section when it is added to the existing H $1s$, Ps $1s$ channels, whereas the inclusion of the H $2p$ channel depresses these values considerably. The use of the H $2\bar{p}$ channel, in place of the H $2p$ one, even more drastically decreases the positronium-formation cross sections to almost negligible values. Our values calculated in the H $1s$ -H $2s$ -H $2\bar{p}$ -Ps $1s$ coupling scheme for the S -wave positronium-formation cross sections are found to be of the same order of magnitude (and same shape) as those calculated by Wakid and Lebahn [5], who considered a slightly different coupling scheme

of $H 1s - H 2\bar{p} - Ps 1s - Ps 2\bar{p}$ (not shown). The strikingly similar characteristic of the two sets of values is that they are both very small. Since the $H 2\bar{p}$ target channel was included in the close-coupling expansion in both calculations, we conclude that the long-ranged polarization effects, through the $H 2\bar{p}$ target state, appear to play a significant role in depressing the S -wave positronium-formation cross sections. We have not, however, been able to figure out offhand a suitable physical picture to satisfactorily describe this situation.

III. CONCLUSION

We have employed in this work the algebraic method to calculate the elastic and positronium-formation cross sections of $e^+ - H$ scattering in the close-coupling approximation at energies below the first excitation threshold for S -wave and P -wave scatterings. The latter (P wave) has not yet been carried out in the literature. The algebraic method again proved to be rather convenient in handling

the positronium-formation channel in the close-coupling calculation. It is found that these close-coupling results, as usual, very much depend on the coupling schemes considered for the close-coupling expansion. In general, many sets of results obtained in our calculation agree with those calculated by others who used different numerical methods. However, for scattering energies in the Ore gap, the agreement among the results calculated by us as well as by others with the employment of different numerical methods is not quite good. The cause for this discordance is worth investigating.

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