J. Phys. B: Atom. Molec. Phys., Vol. 10, No. 5, 1977. Printed in Great Britain.

LETTER TO THE EDITOR

The scattering of s-wave positrons by helium

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Received 7 February 1977

Abstract. An attempt is made to reproduce theoretically the results of recent measurements of low-energy positron–helium total cross sections by Kauppila *et al*, which disagree with the earlier experimental results of Canter *et al* for positron energies below 6 eV. Positron–helium s-wave phaseshifts are calculated for a 14-term helium wavefunction, using similar techniques to those employed previously by the present authors. The results are only very slightly different from those obtained by Humberston for a less accurate helium wavefunction, and give cross sections in good agreement with the values of Canter *et al.* A significant discrepancy therefore remains between the theoretical cross sections presented here and the experimental results of Kauppila *et al* which, it is claimed, cannot be resolved by further improvements in the theoretical results.

Recently Kauppila *et al* (1976) presented the results of new measurements of the total cross section for positron–helium scattering in the energy range 0·3–28 eV, which established directly for the first time the existence of a Ramsauer minimum in the cross section at a positron energy of 2 eV. Above 6 eV their results are in good agreement with the earlier measurements of Canter *et al* (1973), but below 6 eV, and particularly in the vicinity of the Ramsauer minimum, they are significantly lower. Both sets of experimental results and various theoretical results, to be referred to later, are given in figure 1. Canter *et al* were unable to obtain reliable results below 2 eV, and so did not observe the minimum directly. However, an extrapolation of their data using a least-squares fit to the functional form

$$\sigma = a_0 + a_1 k + a_2 k^2 \ln k + a_3 k^2 + a_4 k^4 \qquad (1)$$

where k is the wavenumber of the positron, gave results of a similar form to, but larger than, those of Kauppila *et al*, with a minimum just below 2 eV followed by a sharp rise as the energy tended to zero (Bransden *et al* 1974, Humberston 1974).

The results of Canter *et al*, and their extrapolation, are in excellent agreement with the cross sections derived from one of the sets of phaseshifts calculated by Humberston (1973) and Campeanu and Humberston (1975). These authors used the Kohn variational method and the 'method of models' (Drachman 1972) to obtain s- and p-wave phaseshifts for two helium models, and the resulting cross sections are

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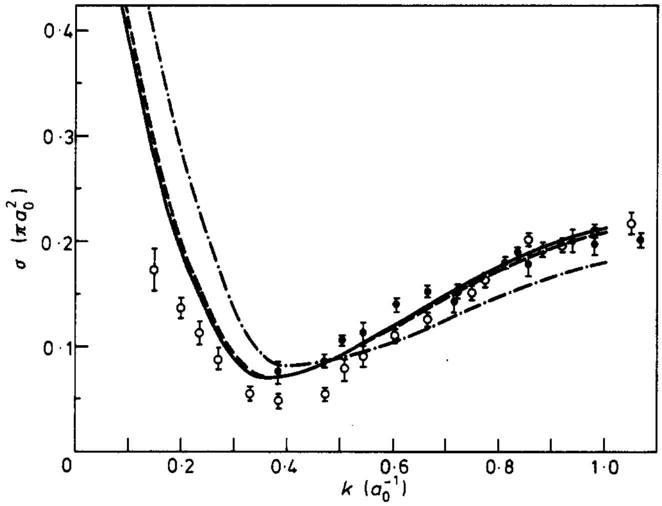

Figure 1. Total cross sections for positron–helium scattering: ♁ experimental results of Kauppila *et al* (1976), for clarity of presentation only a selection of these results are plotted; ● experimental results of Canter *et al* (1973); ----- theoretical results for helium model H14; —— theoretical results for helium model H5; –·–·– theoretical results for helium model DB. The theoretical results for helium models H5 and DB were calculated from the s-wave phaseshifts of Humberston (1973), the p-wave phaseshifts of Campeanu and Humberston (1975) and the lowest set of Drachman's (1966) d-wave phaseshifts. The theoretical results for helium model H14 were calculated from the present s-wave phaseshifts, the p-wave phaseshifts for model H5 and Drachman's d-wave phaseshifts.

given in figure 1. The wavefunction of each model was of the form (using the nomenclature of Humberston 1973)

$$\phi_{\mathrm{He}} = \exp[-\gamma(r_2 + r_3)] \sum_i d_i(r_2 + r_3)^{K_i}(r_2 - r_3)^{L_i} r_{23}^{M_i} \qquad (2)$$

with the summation over i including all terms such that

$$K_i + L_i + M_i \leqslant \omega_{\mathrm{He}}$$

where K_i, L_i, M_i and ω_{He} are non-negative integers and L_i and M_i are even. The two models, referred to as DB and H5, were generated by setting $\omega_{\mathrm{He}} = 0$ and 2 respectively. They both have the accurate value 1·38 a_0^3 (Dalgarno and Kingston 1960, Thomas and Humberston 1972) for the dipole polarizability, and their variational energies are −5·680 and −5·789 Ryd respectively.

The cross sections obtained with model H5 (so called because the number of terms in the summation over i in equation (2) is 5) are in good agreement with the values of Canter *et al* (1973) over the entire range in which calculations have been performed, and even in the region of extrapolation below 2 eV. The results for model DB (Drachman (1968) model B), however, are larger than those of Canter *et al* below 3 eV and smaller above 3 eV.

At energies below and just above the position of the minimum in the total cross section, the phaseshifts for $l \geqslant 1$ for any helium model with dipole polarizability P are given quite accurately by the formula (O'Malley *et al* 1961)

$$\delta_l = \frac{\pi P k^2}{(2l-1)(2l+1)(2l+3)}.$$

Hence, any errors in the theoretical cross sections in this energy region must be due mainly to errors in the s-wave phaseshifts. The s-wave phaseshifts for models H5 and DB are given in table 1. They are probably (Humberston and Wallace 1972) lower bounds on the exact values for each model, but they are not necessarily lower bounds on the exact phaseshifts for the exact helium wavefunction, as no bound principle is known to apply for variations of the model wavefunction. Therefore, although the results for model H5 are more negative than the corresponding results for model DB everywhere within the energy range considered, one cannot assume that the results for an even more accurate helium model would be everywhere more negative than the results for model H5. Indeed, the s-wave phaseshifts required to give cross sections in good agreement with those of Kauppila *et al* (1976) need to be less positive than those for model H5 at energies below 2 eV and less negative at energies above 2 eV.

In order to determine whether the phaseshifts for a more accurate helium model have this characteristic, the present authors have calculated the s-wave phaseshifts and the scattering length for such a model. The wavefunction of this new model is of the form given by equation (2) with $\omega_{He} = 4$, and it has 14 terms, including 5 electron–electron correlation terms. This model, hereafter referred to as H14, has a variational energy of $-5{\cdot}800$ Ryd and its dipole polarizability is again $1{\cdot}38\ a_0^3$.

Results have been obtained with scattering trial functions of the form used by Humberston (1973) containing 4 and 10 short-range correlation terms (corresponding to $\omega = 1$ and $\omega = 2$ respectively in Humberston's notation). Initially it was intended to increase the number of such terms to 70 ($\omega = 4$), as was done in the earlier calculations with models H5 and DB, but we believe that the results for 70 terms can be deduced from the present results and the earlier results for models H5 and DB in the following way, with considerable savings in computer time. Let us denote by $\delta(\text{model}, \omega)$ the s-wave phaseshift for a particular model obtained with a particular trial function, specified by ω. It was found that at each energy

$$\delta(\text{DB},\omega) - \delta(\text{H5},\omega) = \Delta(\text{DB},\text{H5},\omega)$$

was always positive and almost always decreased slightly with increasing ω. Where $\Delta(\text{DB},\text{H5},\omega)$ did not decrease, the increase was very slight. A similar behaviour was

Table 1. Positron–helium scattering lengths and s-wave phaseshifts for three helium models.

$k\ (a_0^{-1})$	DB	H5	H14
0	−0·524	−0·472	−0·48
0·1	0·037	0·031	0·032
0·2	0·051	0·040	0·041
0·3	0·044	0·029	0·030
0·4	0·027	0·007	0·009
0·5	0·001	−0·023	−0·021
0·6	−0·031	−0·057	−0·054
0·7	−0·066	−0·093	−0·090
0·8	−0·098	−0·128	−0·125
0·9	−0·133	−0·163	−0·160
1·0	−0·167	−0·195	−0·192

The $k = 0$ entries are the scattering lengths in units of a_0. Phaseshifts are in radians.

also found in the differences

$$\delta(\mathrm{H14},1) - \delta(\mathrm{H5},1) = \Delta(\mathrm{H14},\mathrm{H5},1)$$

and

$$\delta(\mathrm{H14},2) - \delta(\mathrm{H5},2) = \Delta(\mathrm{H14},\mathrm{H5},2)$$

as can be seen in table 2, although the magnitude of these differences are only approximately 10% of the corresponding earlier differences. Assuming that this

Table 2. Differences between the s-wave phaseshifts for three helium models.

$k\,(a_0^{-1})$	ω	$\Delta(\mathrm{DB},\mathrm{H5},\omega)$	$\Delta(\mathrm{H14},\mathrm{H5},\omega)$	$\delta(\mathrm{H14},\infty)$
0	1	−0·088	−0·014	
	2	−0·078	−0·010	
	∞	−0·052		−0·48
0·1	1	0·0083	0·00061	
	2	0·0078	0·00057	
	∞	0·006		0·032
0·2	1	0·0157	0·0008	
	2	0·0141	0·0010	
	∞	0·011		0·041
0·3	1	0·0208	0·0017	
	2	0·0186	0·0014	
	∞	0·015		0·030
0·4	1	0·0244	0·0020	
	2	0·0218	0·0016	
	∞	0·020		0·009
0·5	1	0·0264	0·0023	
	2	0·0259	0·0013	
	∞	0·024		−0·021
0·6	1	0·0272	0·0026	
	2	0·0254	0·0020	
	∞	0·026		−0·054
0·7	1	0·0272	0·0028	
	2	0·0269	0·0026	
	∞	0·027		−0·090
0·8	1	0·0266	0·0030	
	2	0·0268	0·0023	
	∞	0·030		−0·125
0·9	1	0·0260	0·0030	
	2	0·0268	0·0024	
	∞	0·030		−0·160
1·0	1	0·0250	0·0031	
	2	0·0263	0·0025	
	∞	0·028		−0·192

The $k = 0$ entries relate to scattering lengths, in units of a_0. Phaseshifts are in radians. The $\omega = \infty$ entries are calculated from extrapolated phaseshifts. These are obtained by considering the convergence of the phaseshifts as ω increases. The right-hand column gives the extrapolated phaseshifts for helium model H14 according to equation (3).

behaviour continués as ω increases, a reasonably accurate approximation to the fully converged phaseshifts for model H14 is given by

$$\delta(\mathrm{H14},\infty) \simeq \delta(\mathrm{H5},\infty) + 0{\cdot}1[\delta(\mathrm{DB},\infty) - \delta(\mathrm{H5},\infty)] \quad (3)$$

where $\delta(\mathrm{H5},\infty)$ and $\delta(\mathrm{DB},\infty)$ are the extrapolated phaseshifts for the two models (Humberston 1973). A similar relationship is assumed to hold for the scattering length. The scattering length and phaseshifts derived from equation (3) for model H14 are given in table 2, and also, for ease of comparison with the DB and H5 values, in table 1. These new phaseshifts are slightly more positive than those for model H5, although equation (3) probably gives an overestimate of the differences from the H5 results. The resulting total cross sections are slightly larger than those for model H5 below the minimum in the cross section and slightly smaller above it.

Hence, below the minimum, the discrepancy between the experimental results of Kauppila *et al* (1976) and the theoretical results for model H14 is slightly larger than it is for model H5 and above the minimum it is only slightly less. But model H14 is believed to be a rather accurate approximation to the exact helium wavefunction, and it is doubtful whether an even more accurate helium function could give s-wave phaseshifts sufficiently different from those for models H14 and H5 for the cross sections to be close to those of Kauppila *et al*. There may, therefore, be a systematic error in their measurements of the cross sections below 6 eV. It is possibly significant that in the energy range 0–6 eV the cross section for small-angle scattering is appreciable, whereas in the range 6–16 eV, where the results of Kauppila *et al* are in good agreement with those of Canter *et al*, the cross section for small-angle scattering is small (Massey 1976).

A further indication that the results of Kauppila *et al* may be in error below 6 eV is provided by the extrapolation of their data to zero energy. A least-squares fit of all their data below 18 eV to the functional form in equation (1) yields a cross section at zero energy of $0{\cdot}77\,\pi a_0^2$. If, however, only the data between 2 and 18 eV is used, as in the fit of the data of Canter *et al* referred to earlier, the zero energy cross section is $1{\cdot}39\,\pi a_0^2$. Neither result is as close to the zero-energy cross section obtained with either model H14 or H5 as is the extrapolated result of Canter *et al*, and the rather large discrepancy between these two results suggests that there are inconsistencies in the low-energy measurements. Further measurements of the total cross sections below 6 eV should therefore be made.

One of us (RIC) was in receipt of a grant from the Romanian Ministry of Education.

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