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LETTER TO THE EDITOR

The scattering of p-wave positrons by helium

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Abstract. Kohn's variational method is used to calculate low energy positron–helium p-wave phaseshifts and p-wave contributions to the annihilation rate parameter Z_{eff} for the two helium models considered previously by Humberston. The phaseshifts for both models are less positive than the lowest set of Drachman, but the cross sections and annihilation rates obtained from the present results and Humberston's s-wave results, for the more elaborate helium function, are in good agreement with the experimental values of Canter *et al* and Coleman *et al.*

In a previous publication (Humberston 1973 to be referred to as L1) results were given of variational calculations of positron–helium s-wave phaseshifts at several positron energies below the positronium formation threshold. The results for both helium models considered were found to be more negative than the lowest set of values obtained by Drachman (1966), who used a modified adiabatic approximation with the simpler helium model, DB, used in L1. It therefore seemed likely that the modified adiabatic approximation would also overestimate the higher partial wave phaseshifts. Further evidence was provided by a comparison (Humberston 1974) of the total cross sections measured by Canter *et al* (1973) with those calculated from the s-wave phaseshifts of L1, for the more accurate helium model H5, and the lowest set of Drachman's (1966) p- and d-wave shifts. The theoretical cross sections were found to be slightly larger than the experimental values, and since the s-wave phaseshifts for the model H5 are probably quite accurate and the partial waves with $l > 0$ are all positive in this energy region, it follows that Drachman's phaseshifts are too positive. We present here the results of variational calculations of the positron–helium p-wave phaseshifts which confirm this assertion. Calculations of the p- and d-wave phaseshifts have also been performed by Aulenkamp *et al* (1974), but an analysis of Bransden and Hutt (1975) suggests that the results are rather inaccurate.

The Kohn variational method

$$\frac{\tan \bar{\eta}_1}{k^2} = \frac{\tan \eta_1}{k^2} - \frac{2m}{\hbar^2}(\Psi_t, (H-E)\Psi_t)$$

is used with the 'method of models' (Drachman 1972), and the trial function is chosen to be, using the same nomenclature as in L1,

$$\Psi_t = \phi_{He}(\boldsymbol{r}_2, \boldsymbol{r}_3)\psi_t(\boldsymbol{r}_1, \boldsymbol{r}_2, \boldsymbol{r}_3)$$

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with

$$\psi_t(\boldsymbol{r}_1, \boldsymbol{r}_2, \boldsymbol{r}_3) = k^{-1/2} Y_{10}(\hat{r}_1)\left(j_1(kr_1) - \tan\eta_1 n_1(kr_1)(1-e^{-\lambda r_1})^3 + \sum_i c_i f_i \right)$$

and

$$f_i = (1+P_{23})\{\exp[-(\alpha r_1 + \beta r_2 + \beta r_3)] r_1^{k_i+1} r_2^{l_i} r_{12}^{m_i} r_3^{n_i} r_{13}^{p_i}\}.$$

The summation over i includes all terms for which

$$k_i + l_i + m_i + n_i + p_i \leqslant \omega$$

with $l_i \geqslant n_i$ and $m_i \geqslant p_i$ if $l_i = n_i$, where k_i, l_i, m_i, n_i, p_i and ω are non-negative integers. No dependence on the inter-electron coordinate r_{23} is included in ψ_t because it was found in L1 for s-wave scattering that the results were very insensitive to the introduction of such dependence into ψ_t. The total wavefunction Ψ_t will of course depend on r_{23} if the wavefunction of the helium model, ϕ_{He}, has such a dependence.

Results have been obtained at incident positron energies corresponding to $k = 0{\cdot}1(0{\cdot}1)1{\cdot}0 a_0^{-1}$ for the two helium models, DB and H5, defined in L1. The most elaborate trial functions used had 70 linear parameters ($\omega = 4$), in addition to $\tan\eta_1$, but by examining the convergence of the results with respect to ω we have attempted to extrapolate to the results corresponding to infinite ω. These extrapolated values are given in figure 1. Although the results at all energies converge monotonically with respect to ω from below, suggesting that they are probably lower bounds on the exact results for each helium model, the convergence at some energies is rather poor and the uncertainties in the extrapolated values are rather large. For example, at $k = 0{\cdot}9$ the uncertainty in the phaseshift is approximately $\pm 7\%$ for model H5 and $\pm 3\%$ for model DB, whereas at $k = 0{\cdot}3$ it is only $\pm 1\%$ for H5 and $\pm 0{\cdot}5\%$ for DB.

As with the s-wave phaseshifts in L1, the results for the more elaborate helium model H5 are lower than those for the model DB, and both sets of results lie below the

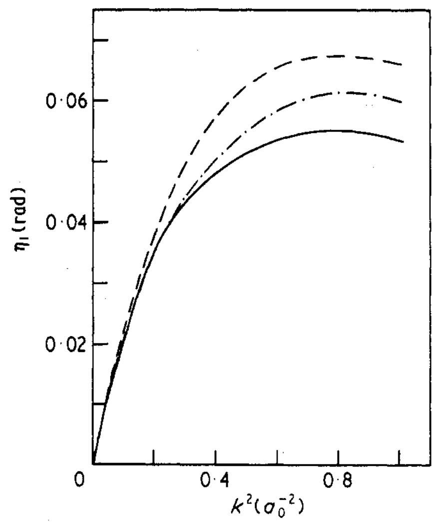

Figure 1. The energy dependence of the p-wave phaseshifts; full curve: present results for helium model H5; chain curve: present results for helium model DB; broken curve: the lowest set of Drachman (1966).

lowest set of Drachman (1966). It is, therefore, probable that more accurate d-wave phaseshifts will also be slightly more negative than Drachman's values.

Both helium models give very similar results at low energies, and this was to be expected because they have the same dipole polarizability, ($1{\cdot}38a_0^3$) and O'Malley *et al* (1961) have proved that the energy dependence of each partial wave phaseshift with $l > 0$ is determined by the dipole polarizability alone at low energies (where terms of order k^4 can be ignored).

The total cross section for the helium model H5, calculated from the s-wave results in L1, the present p-wave results and the lowest set of Drachman's (1966) d-wave phaseshifts, is plotted in figure 2. Partial waves with $l > 2$ make an insignificant contribution

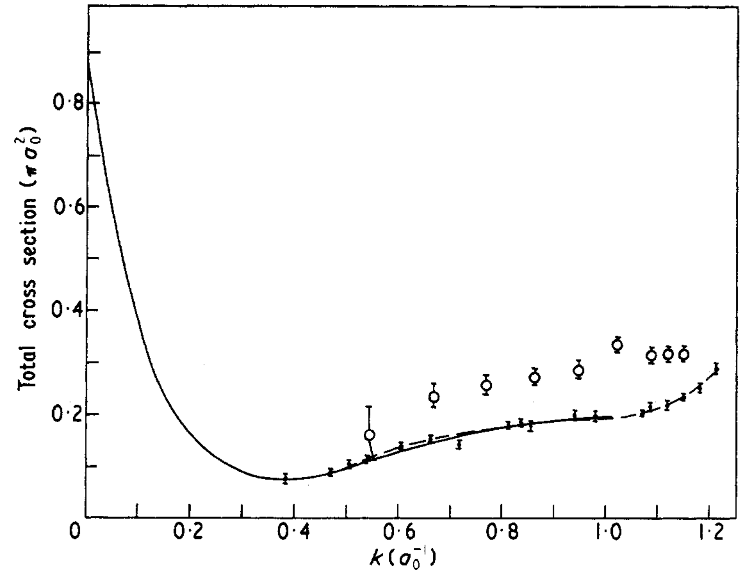

Figure 2. Variation of the total cross section with positron momentum. The full circles are the results of Canter *et al* (1973) and the open circles are those of Jaduszliwer and Paul (1973). The full curve is obtained from Humberston's (1973) s-wave phaseshifts, the present p-wave phaseshifts for the helium model H5 and the lowest set of Drachman's (1966) d-wave phaseshifts; the broken curve, which coincides with the full curve when it is not shown separately, is the least squares fit of Bransden *et al* (1974) to the data of Canter *et al* (1973).

to the cross section in this energy region. The agreement with the experimental measurements of Canter *et al* (1973) is very good, and is better than that obtained by Humberston (1974). There is, however, a slight deterioration at the higher energies in the agreement between the theoretical and experimental values of the real part of the forward scattering amplitude from that obtained by Bransden and Hutt (1975), but the uncertainties associated with the experimental values of the total cross sections at high energies (>200 eV) are such that this discrepancy is probably not significant.

The wavefunctions obtained from the variational method were used to calculate the p-wave contribution to the annihilation rate parameter Z_{eff}, and the results, combined with the s-wave contributions of Humberston (1974), are displayed in figure 3. Convergence with respect to ω was too erratic to permit reliable extrapolation to infinite ω and so the results for the most elaborate wavefunctions, with $\omega = 4$ (70 linear

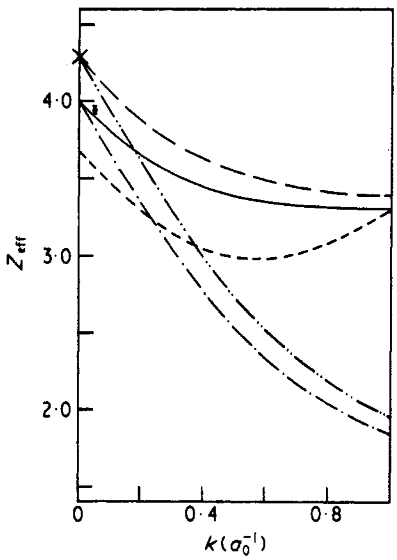

Figure 3. Variation of Z_{eff} with positron momentum; ——— combined s-wave (Humberston 1974) and present p-wave contributions for helium model H5; — — — combined s-wave (Humberston 1974) and present p-wave contributions for helium DB; –·–·– s-wave contribution for model H5; –··–··– s-wave contribution for model DB; - - - Drachman (1968), incorporating contributions from all partial waves, for model DB; ⧳ Coleman *et al* (1975); × Houston and Drachman (1971) for model DB.

parameters), are used. Also, contrary to the behaviour of the s-wave contributions, the p-wave contributions to Z_{eff} are slightly larger for the model H5 than for the model DB, but this may be due to the different patterns of convergence of the results for the two models. Figure 3 also contains the results of Drachman (1968), in which the s-wave contribution is obtained from his modified adiabatic wavefunction for model DB and all higher partial wave contributions are taken to be the same as for a plane wave. Most probably the addition of the partial wave contributions with $l > 1$ to the present results will also produce a rise in Z_{eff} beyond $k = 0{\cdot}5$.

Good agreement is obtained for Z_{eff} at thermal energies between the theoretical value, for helium model H5, and the experimental measurement of Coleman *et al* (1975). In addition, the rate of change of Z_{eff} with positron momentum at very low energies, for both models, agrees well with the experimental value.

Although the agreement between the theoretical result for model H5 and the experimental measurements of Canter *et al* (1973) and Coleman *et al* (1975) appears very satisfactory, further calculations, using even more accurate helium functions, are in progress.

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