CALCULATIONS OF SCATTERING CROSS SECTIONS AND ANNIHILATION RATES IN LOW ENERGY COLLISIONS OF POSITRONS WITH MOLECULAR HYDROGEN

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ABSTRACT

An analysis of the requirements for an accurate calculation of $Z_{\text{eff}}$, the effective number of electrons per molecule available to the positron for annihilation, for low energy $e^+H_2$ scattering using the Kohn method shows the importance of including basis functions which contain the positron-electron distance as a linear factor, i.e. Hylleraas-type functions. Such functions are very complicated to include as they are not separable, i.e. they cannot be expressed as a finite expansion of one particle functions. However, I have been able to extend the calculation of the lowest partial wave for low energy $e^+H_2$ scattering using the Kohn method and basis sets involving only separable functions, which I described at the last Workshop at Detroit in 1985, to include Hylleraas-type basis functions. The results for $Z_{\text{eff}}$ at very low energies are much closer to the experimental value than any that have been obtained previously. The inclusion of Hylleraas-type functions also has a very significant effect on the low energy phase shift and total cross section, bringing the cross section into agreement with experiment for incident positron energies up to about 2 eV. As far as I am aware, this is the first time that Hylleraas-type functions have been used in a molecular scattering calculation.

INTRODUCTION

At the last Workshop on positron-gas scattering in Detroit in 1985 I presented an application of the Kohn variational method to low energy positron-hydrogen-molecule scattering. The calculations were carried out using trial functions involving only separable functions, i.e. functions which can be expressed as a finite expansion of products of one particle functions. The use of such functions makes the evaluation of the matrix elements required in a variational calculation comparatively easy. For this reason they have been extensively used both in atomic and molecular bound state calculations and in electron-atom and molecule scattering calculations.

In the calculation I carried out on the lowest partial wave, i.e. the lowest partial wave of $\Sigma^+$ symmetry, I was able to obtain a good qualitative description of the behaviour of the phase shift by including sufficient
separable functions in the trial function. Similar results have also been obtained by Tennyson using the R-matrix method with separable basis functions. A description of his calculation appears elsewhere in these proceedings.

In the work I presented at Detroit, I drew attention to the inadequate description that the resulting wavefunction gave of the process of positron annihilation. Thus the calculated value of $Z_{\text{eff}}(k)$, the effective number of electrons per hydrogen molecule available to the positron for annihilation, at very low energies was found to be very much less than the experimental value.

The reason for this discrepancy is not hard to find. $Z_{\text{eff}}(k)$ measures the value of the wavefunction when the positron and an electron coincide. Suppose the electron concerned is electron $I$. As a consequence of the Coulombic attraction between the positron and the electron, the exact wavefunction, $\psi$, at points of coincidence must satisfy the cusp condition:

$$\left( \frac{\partial \psi}{\partial r_{13}} \right)_{r_{13}=0} = -\frac{1}{2}(\psi)_{r_{13}=0}$$

where

$$r_{13} = r_3 - r_1$$

and $r_1$ and $r_3$ are the positron vectors of the electron and positron, respectively. $\psi$ is the average value of $\psi$ taken over the sphere $r_{13}$ constant, with variables other than $r_{13}$ fixed.

The Kohn trial function can only be made sufficiently flexible so that it can take this condition into account adequately by including basis functions containing $r_{13}$ and $r_{23}$ as linear factors. These factors are not separable functions and their inclusion makes the calculation very much more complicated.

The inclusion of linear factors of the inter-particle distance in the trial function in variational calculations has a long and interesting history. As early as 1929, Hylleraas showed that their inclusion brought about rapid convergence in variational calculations of the ground state energy and wavefunction of helium. Soon afterwards, James and Coolidge showed that this was also the case for the hydrogen molecule. The rapid convergence is due to the increased flexibility of trial functions containing such functions. This enables them to take into account adequately the cusp condition similar to equation (1) when the two electrons coincide. In what follows I shall refer to basis functions which contain the inter-particle distance as a linear factor as Hylleraas-type functions.

Schwartz showed in 1961 that the Kohn variational method with a basis set made up of functions containing linear and higher powers of the inter-particle distance gave accurate results for low energy positron-hydrogen-atom scattering. Basis sets of this type have subsequently been employed in Kohn and other variational calculations on low energy positron-hydrogen-atom and positron-helium scattering. For details, see the review article by Humberston. It has not so far been possible to compare the results obtained for atomic hydrogen with experiment but the results obtained for helium are in good agreement with experiment, both in the case of the total cross section and $Z_{\text{eff}}(k)$. The spherical symmetry of atomic targets made it possible to incorporate the inter-particle distance directly into the variables of integration, as was done by Hylleraas. This made it possible to evaluate all