THE EFFECT OF A CHANGE OF CHARGE: THE SCATTERING
OF LOW ENERGY POSITRONS BY HYDROGEN MOLECULES

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ABSTRACT

The lowest partial wave is calculated for low-energy $e^+ - H_2$ scattering using the Kohn method. In order to obtain accurate results, it is necessary to use a trial function which includes basis functions containing the positron-electron distance as a linear factor, i.e. Hylleraas-type functions. The inclusion of such functions has a very significant effect on the low-energy total cross section, bringing it into agreement with experiment for incident energies less than about 2eV. It also brings the calculated value for the annihilation rate of thermal positrons much closer to the experimental value. Progress is also reported on the calculation of the lowest partial waves of $\Sigma_u^+$ and $\Pi_u$ symmetry. As far as we are aware, this is the first time that Hylleraas-type functions have been used in a molecular scattering calculation.

INTRODUCTION

It has been well known since the work of Hylleraas and James and Coolidge that the inclusion of the interelectronic distance as a linear factor in the trial function brings about rapid convergence in variational calculations on bound states of two-electron atoms and molecules. However, trial functions involving only separable functions i.e. functions which can be expressed as a finite expansion of products of one-particle functions, are much easier to work with. The required matrix elements can be evaluated straightforwardly using Slater’s rules for one and two electron operators. The speed of modern computers makes it possible to include a very large number of Slater determinants constructed from separable functions. This has made it possible to obtain satisfactory accuracy in variational calculations on atomic and molecular bound states (see, for example, Schaefer). Trial functions of this type have also proved very successful in electron-atom and electron-molecule scattering calculations (see, for example, Burke et al., Schneider and Collins and Lima et al).

The advent of intense low-energy positron beams has made possible many positron-atom and molecule scattering experiments, and further experiments can be expected in the near future. The change of sign in positron as opposed to electron scattering has very important consequences. The
The positron is distinguishable from the target electrons and therefore exchange effects with the incident particle are absent. In contrast to the electron, the positron is attracted by the target electrons and repelled by the nuclei. In this situation an expansion for the wavefunction in terms of separable functions converges very slowly. The calculations by Armour, using a generalization of the Kohn method, and Tennyson, using the R-matrix method, show that it is possible to obtain a good qualitative description of the behaviour of the phase shift of the lowest partial wave in low-energy positron-hydrogen molecule scattering by including sufficient separable functions in the trial function.

However, such calculations are incomplete. As the positron is the antiparticle corresponding to the electron, it may annihilate with a target electron to form 2 or 3 gamma rays. The calculation of the annihilation rate provides a particularly stringent test of the accuracy of a wavefunction. Only the region of configuration space where the positron is very close to a target electron is sampled and the error in the annihilation rate is first order in the error in the wavefunction. Armour and Baker have shown that the wavefunction obtained in the Kohn calculation gives a value of the annihilation rate for thermal positrons which is much smaller than the experimental value.

The use of separable basis functions corresponds to including only even powers of the positron-electron distance in the trial function. Schwartz showed in 1961 that the Kohn variational method with a basis set made up of functions containing linear and higher powers of the interparticle 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.

Calculations of this type are greatly facilitated by the spherical symmetry of atomic targets. Nevertheless, Clary has succeeded in carrying out very accurate variational calculations of the energy of $\text{He}_2^+$ and $\text{He}_2$ for a given internuclear distance by using basis sets which included functions containing the interelectron distance as a linear factor.

In this paper we describe how, following a method similar to that used by Clary, we have carried out an accurate calculation of the lowest $L_g^+$ partial wave in positron-hydrogen-molecule scattering by using Kohn trial functions which include basis functions containing the positron-electron distance as a linear factor. We also report on progress on the extension of the method to the lowest partial waves of $L_u^+$ and $\Pi_u$ symmetry. As far as we are aware, this is the first time that Hylleraas-type functions have been used in a molecular scattering calculation.

**CALCULATION**

The basic form of the calculation was similar to earlier calculations using separable basis functions (Armour,18). The lowest partial wave is of $L_g^+$ symmetry and the trial function was taken to be of the form

$$\Psi_T = \Omega(c, \lambda_3, \mu_3; \tau, a) \Psi_G + \sum_{i=1}^{M} g_i \chi_i \Psi_G$$  \hspace{1cm} (1)

where $\tau$, $a$ and $\{g_i\}$ are variable parameters and $c = \frac{1}{2} k R$, where $k$ is the wave number of the incident positron and $R = 1.4 a_0$ is the separation between