THEORETICAL ASPECTS OF POSITRONIUM COLLISIONS

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INTRODUCTION

From its former position as a mathematical curiosity, study of the positronium atom (Ps) has gradually evolved into a subject of quite active experimental and theoretical interest. Ps, especially in the ortho (triplet spin) state, is relatively long-lived and can be considered just like any ordinary atom in most of its interactions with other systems. The unique characteristic of Ps, its annihilation into gamma rays, can usually be treated as a small perturbation superimposed on the dominant Coulomb interaction which determines its static properties and the cross-sections for collisions with electrons, various atoms, molecules, and ions. Although Ps is an atom, in some sense an isotope of hydrogen, its mass is so much less than that of any other that the standard techniques of atomic scattering theory are not applicable, and those of electronic scattering theory may be more appropriate. Nevertheless, the internal structure of Ps, its extension, and the Pauli principle combine to complicate the theory. In this report I will try to summarize the calculations already performed on the scattering of Ps from the simplest atomic systems, describing some of the methods used to analyze the collisions. I will also discuss the long-range effective potential acting between Ps and these other systems; here the low mass of Ps brings about some interesting modifications of the conventional van der Waals force. Next, the interesting "poly-electrons" Ps and Ps₂ will be described. Finally, some astrophysical and exotic applications will be mentioned.

THE POSITRONIUM–HELIUM SYSTEM

Although this system contains three electrons and is therefore rather difficult to handle theoretically, it is easy to describe and may be a good introduction to the general subject. At collision energies below 5.10 eV (the first excitation energy of Ps) only elastic scattering is energetically permitted, so only a single channel formalism is needed. Since the helium atom has a spin-singlet ground state no spin-exchange is possible, and our non-relativistic approximation omits spin-orbit coupling. In addition, there is no bound state of the He⁻ ion or of PsHe.

Fraser¹ carried out the first ab initio calculations of the low-energy scattering of Ps from helium using the static-exchange approximation. In this approximation a variational trial function is constructed from an anti-
symmetrized product of the ground-state wave functions of the two atoms:

\[ \psi = v \left( \frac{1}{2} \left( \sum_{1}^{n} + \sum_{p} \right) \right) \psi(\vec{r}_1, r_3) \psi(\vec{r}_2, r_3) \chi_1^1(s_1, s_1) \chi_0^0(s_2, s_3) + \ldots \]  

where electron 1 is bound to the positron (p), electrons 2 and 3 are in the Helium atom, and the spin functions represent the triplet state for Ps and the singlet state for helium. The function \( v \) represents the motion of the center of mass of the Ps atom relative to the fixed nucleus of the other atom. It is from the necessity of describing the Ps this way when the potentials do not depend on the center of mass coordinate that much of the difficulty and the challenge of Ps calculations arises. Fraser and Kraidy\(^2\) used the simplest one-term Hylleraas closed-shell function to describe the helium ground-state and derived variationally the integro-differential equation satisfied by \( v \), retaining three partial waves. Since the helium function is not exact, there is some ambiguity concerning the formation of the integral equation. This leads to a spread in the calculated cross-sections; at zero energy the variation is between 14.2 and 11.8, in units of \( \alpha \); the latter is perhaps the better value although the very existence of the spread is a measure of the inaccuracy of the helium wave function.

This calculation is incomplete since it does not include the effect of the distortion or polarization of the two colliding atoms. Two quite different attempts to rectify this omission have been reported. The first\(^3\) concentrated on the long-range distortion due to the van der Waals potential acting between the two systems. This was found to have the approximate asymptotic form \(-19.3/R^6\) and to approach zero following a certain variational form for small \( R \). In fact, the original motivation for performing this calculation was the measurement of pickoff annihilation in Ps-He collisions, that is, the observation\(^4\) of a density dependence of the lifetime of ortho Ps in helium gas due to the bound positron annihilating with one of the helium electrons during the collision. It was the disagreement between the pickoff rate calculated from the static-exchange approximation and the observed value that clearly showed the inadequacy of that approximation. By adding this potential term to Fraser's integro-differential equation it was possible to increase the pickoff rate but not enough to give good agreement with experiment.

The same motivation led Houston and me along another path.\(^5\) We concentrated on the short-range distortion induced in the Ps by the exchange force acting between the helium closed shell and the Ps electron. This force is expected to re-orient and stretch the Ps, and thus to reduce the scattering length; it is easy to see qualitatively that the sort of distortion described above also increases the overlap between the positron in Ps and the atomic electrons and leads to an increase in the annihilation rate. Both effects should be included in a correct calculation, and I will return to the van der Waals problem later.

Instead of adding correlation terms to the trial function (1), the rigorous way to proceed, we modeled the exchange interaction as a local potential, \( V(r) = V_0 \exp(-ar) \), where \( r \) represents the electron in the Ps atom, the helium atom is frozen, and antisymmetry between the incoming and target electrons is not included. The two parameters were adjusted to give the no-correlation values of the scattering length and the pickoff rate (at zero energy) obtained previously by Fraser and Kraidy.\(^2\) Then correlation was introduced and the parameters of the resulting wave function were determined by the Kohn variational method. That is, we chose a trial function of the following form: