# POLARIZATION AND FORWARD SCATTERING EFFECTS IN LOW-ENERGY POSITRON INTERACTIONS WITH $H_2$

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**Abstract.** Positron physical-chemistry has been a significant area of scientific investigation in recent decades. However, low-energy positron scattering by atoms and molecules still presents several open questions, particularly regarding the effects of low-angle scattering on measured cross sections and the role of target polarization in the comparison between theoretical and experimental results. In this study, we examine low-energy positron collisions with $H_2$ molecules, focusing on the convergence of the polarization contribution in the scattering potential.

The interaction between the positron and the molecule is represented by a model potential, which combines a free-electron gas correlation term with an asymptotic polarization potential derived from perturbation theory. Specifically, we analyze how polarization effects beyond second-order perturbation influence scattering observables. Our findings indicate that a model incorporating up to the quadrupole polarization contribution shows improved agreement with recent experimental data when corrected for forward scattering effects, as these measurements were obtained using a transmission beam technique.

We also examine angular distributions by comparing our results with available folded differential cross-section measurements. A simple correction scheme is proposed for experimental folded differential cross sections at energies below 1 eV, which we argue aligns well with the quadrupole polarization model. Finally, a comparison between our phase shifts and scattering lengths with recent many-body **ab initio** calculations—including virtual positronium effects—suggests that these effects are inherently accounted for within the adopted model correlation potential.

**Keywords:** molecular hydrogen, positron, elastic scattering, polarization.

## Introduction

Positron scattering by atoms and molecules is widely recognized as a challenging problem. Despite its many applications in fields such as material science, medicine, and astrophysics, the fundamental nature of positron interactions with atomic and molecular targets remains a subject of debate. Unlike electron scattering, positron scattering requires careful treatment of correlation and polarization effects, as the absence of exchange interactions makes the balance between electrostatic and distortion effects crucial for determining scattering cross sections. One such correlation effect, virtual positronium formation, plays a complex role in scattering dynamics that is not yet fully understood.

The case of the hydrogen molecule is no exception. Numerous experimental and theoretical studies on low-energy positron scattering with $H_2$ have been conducted. However, even for elastic scattering, the agreement between theory and experiment remains limited. One major source of discrepancy is the limited angular resolution of transmission-based spectrometers, which count positrons elastically scattered below a certain angle as unscattered, leading to an underestimation of the total cross section (TCS). This issue can be addressed by incorporating reliable differential cross-section data, either from experimental measurements or theoretical calculations. However, experimental data on this subject remain scarce, and the choice of the most suitable theoretical approach remains a challenge. While some theoretical methods offer more convincing results than others, achieving a systematic theoretical description that aligns with experimental data remains an ongoing effort and a significant open problem.

Among the various theoretical approaches for positron-molecule scattering, two predominant methodologies exist: ab initio many-body calculations and model potential approaches. Each method has its own advantages. While an ab initio approach aims to compute a many-body wave function for the positron-molecule system with minimal approximations, model potential approaches rely on simplified scattering potentials that are easier to interpret and adjust to match experimental cross sections.

For positron scattering with $H_2$, there is a wealth of theoretical and experimental data, though still not sufficient for a complete understanding of the problem. On the theoretical side, both ab initio calculations and model potential approximations have been employed. The agreement between theoretical predictions and experimental results continues to evolve as new experimental data become available. For instance, when Zecca et al. published their experimental results for positron energies between 1 eV and approximately 10 eV, they significantly influenced the theoretical understanding of positron scattering in this energy range. Prior to this, no data were available for positron energies below 1 eV, and their study remains the only one providing data below 0.5 eV—an energy region critical for theoretical comparisons.

The data from Zecca et al. were obtained using a transmission-based positron spectrometer, which, as mentioned earlier, tends to underestimate cross sections due to the exclusion of elastically scattered positrons below a certain angle. These cross sections were later corrected for low-angle scattering effects using a full ab initio treatment. However, the experimental data were not enhanced as much as expected, likely due to incomplete treatment of correlation and polarization effects, as indicated by the comparison of their folded differential cross sections (FDCS) with available measurements. This discrepancy becomes even more intriguing when compared with recent many-body calculations that incorporate full correlation effects, yielding significantly higher cross sections.

Within this context, we propose to study positron scattering by $H_2$ using a model potential approach, with the aim of understanding how the inclusion of correlation and polarization effects influences the calculated cross sections and the forward scattering corrections for available experimental data. Following our previous work, we will apply the positron correlation polarization (PCOP) approach**,** modifying the polarization term to include not only second-order perturbation theory contributions but also relevant hyperpolarizabilities. This study will assess how these additional effects impact integral and differential cross sections.

## Theoretical Approach

The scattering model used in this study is based on the static plus correlation polarization (SCP) approximation, defined as:

Accurately describing the positron-electron interaction requires a reasonable representation of the occupied molecular orbitals φi(ri)\phi_i(\mathbf{r}_i)φi(ri) in the given molecular state (in this case, the ground state). It is well known that the Hartree-Fock (HF) representation of molecular orbitals provides a sufficiently accurate description for this purpose, particularly within a model potential approach, as electronic correlation effects can be incorporated through an external potential.

For the correlation and polarization term, we adopt the approach proposed by Jain and

This matching scheme was originally introduced in the context of electron scattering and was justified based on its effectiveness in reproducing accurate phase shifts. While it lacks direct physical interpretation, it has been observed that the cut radius correlates with the spatial extent of the electronic cloud. This suggests that correlation effects in the outer molecular region, such as virtual positronium formation, predominantly occur near this point.

**Numerical Details**

The polarization potential defined in Equation (7) depends on the molecular polarizabilities. In this study, we utilized the CISD/D6Z values determined by Miliordos and Hunt. Since these polarizabilities act as parameters in our calculations, we selected values that provide the most accurate long-range polarization function. Additionally, for convenience, we chose tabulated data corresponding to equilibrium geometry. It appears that the quadrupole polarizability value used by Frighetto et al. contains an error by a factor of 2. Equation (7) aligns with Dalgarno’s definition; however, the relationship between Dalgarno and Buckingham quadrupole polarizabilities is given by αq=2C0\alpha_q = 2C_0αq=2C0, as noted by Buckingham, Thakkar and Lupinetti, and Maroulis and Thakkar. This discrepancy is significant and should be carefully considered when comparing results and analyzing potentials.

All scattering calculations were performed using the MCF method, employing 800 radial grid points spanning from 0.002 to 125.35 a.u. Special attention was given to the molecular region when distributing these points, and we determined that 295 grid points within 10.0 a.u. are sufficient to ensure that the electronic wave function normalizes within 1.0000±1×10−41.0000 \pm 1 \times 10^{-4}1.0000±1×10−4. Additionally, this grid setup adequately supports the electrostatic potential expansion described in Equation (3), as the obtained SCF quadrupole moment compares well with reference values.

Since the differential cross sections calculated in this study cover the full angular range 0∘0^\circ0∘ to 180∘180^\circ180∘ for all considered energies, we report folded differential cross sections (FDCS) for direct comparison with experimental data from Sullivan et al. and Machacek et al. These experimental DCS measurements are mirrored and summed around

Experimental total cross-section (TCS) data are typically uncorrected for forward-angle scattering, as is the case for the TCS measurements by Zecca et al. We compare these results with our present calculations, along with the data from Machacek et al., both of which were corrected for forward-scattering effects using theoretical data from Zammit et al. However, since the measurements from Zecca et al. extend to very low energies (as low as 0.1 eV), and our theoretical approach differs fundamentally from that of Zammit et al., we opted to use our own calculated cross sections to correct this dataset. Given that the Zecca et al. cross-section data extends to such low energies, these corrections may provide valuable insights into the positron-$H_2$ scattering system, particularly in analyzing properties such as the scattering length, as previously explored by Zhang et al. The conclusions drawn by Zhang were later questioned by Brunger et al., so further discussion of these data may help clarify aspects of this ongoing debate.

**Conclusion**

In this study, we examined the scattering of low-energy positrons by $H_2$ molecules using a polarization correlation model (PCOP) and analyzed the effects of second, third, and fourth-order perturbation theory polarization. An evaluation of the scattering potential indicates that including polarization up to fourth order is essential for achieving convergence. However, the calculated cross sections are larger than the most recent many-body ab initio calculations, which explicitly incorporate virtual positronium effects. The agreement between our PQ model and the results reported by Rawlins et al. suggests that the overcorrelation introduced by the PCOP functional near the van der Waals radius effectively models virtual positronium formation.

Particular emphasis was placed on correcting for forward scattering effects in the total cross-section (TCS) measurements **of** Zecca et al**.**, as well as on comparing our results with the folded differential cross-section (FDCS) measurements of Sullivan et al. and Machacek et al. Since the FDCS measurement technique is influenced by the angular resolution of the spectrometer, we proposed a correction to the magnitude of the experimental FDCS at 0.5 eV, based on the direct correction of the TCS data from Machacek et al. for forward scattering effects, as well as an estimated correction for the TCS data from Zecca et al. Despite the simplicity of the correction methodology, the adjusted FDCS aligns quantitatively with both the PQ model and the modified effective range theory (MERT) model, which was extracted from forward-corrected data from Machacek et al. This consistency suggests that the correction is both necessary and reliable**.**

At other energies, comparison of our results with the measured FDCS from Machacek et al. indicates that including anisotropic terms in the polarization interaction is essential for the calculated integral and differential cross sections to reach the correct magnitude**.**

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