Low energy positron-methane scattering

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Introduction

Positron molecule scattering is a delicate phenomenon to consider theoretically. Unlike electron molecule scattering, there is no need for an exchange potential, since the positron is distinguishable from the molecular electrons. This is very convenient in order to solve the scattering equations. However, it makes the interaction potential very sensible to relatively small variations in the polarization potential. So, a well-determined polarization potential is central for the determination of good cross sections curves for collisions between positrons and molecules.

In order to account the short range polarization, the PCOP model was developed [1], using the correlation of a positron in a free electron gas, modeled by [2]. So, in PCOP model, the short range polarization is described as

$$2V_{cor}(r) = \begin{cases} \frac{-1.82}{\sqrt{r_s}} + (0.051\ln(r_s) - 0.115)\ln(r_s) + 1.167 & r_s \leq 0.302 \\ -0.92305 - \frac{0.09098}{r_s^2} & 0.302 \leq r_s \leq 0.56 \\ -\frac{8.7674 r_s}{(r_s+2.5)^3} + \frac{-13.151+0.9552 r_s}{(r_s+2.5)^2} + \frac{2.8655}{(r_s+2.5)} - 0.6298 & 0.56 \leq r_s \leq 8.0 \end{cases}$$

where $r_s = \sqrt[3]{\frac{3}{4\pi\rho(r)}}$ and we do not worry about the $8.0 \leq r_s \leq \infty$ region, as it is beyond the point where $V_{cor}(r)$ crosses $V_{pol}(r)$. Then, the polarization interaction $V_{cor-pol}(r)$ in any position is

$$\begin{aligned} V_{cor-pol}(r) &= V_{cor}(r) \qquad r \leq r_c \\ V_{cor-pol}(r) &= V_{pol}(r) \qquad r \geq r_c \end{aligned}$$

where r_c is the crossing point between $V_{cor}(r)$ and

$$V_{pol}(r) = -\frac{\alpha_0}{2r^4}.$$

Once determined the polarization potential, the interaction potential between positron and molecule is well determined, since the interaction is

$$V(r) = V_{cor-pol} - \sum_i \frac{1}{|\vec{r_i} - \vec{r}|} + \sum_j \frac{Z_j}{|\vec{R_j} - \vec{r}|}$$

and the problem is just solve the scattering equation in order to obtain the scattered positron wave function, i.e., solve the Lippmann-Schwinger equation

$$|\psi\rangle = |u\rangle + G_0 U |\psi\rangle .$$

In order to perform such a task, we used the Method of Continued Fractions [3] which iterative and, in the N^{th} iteraction, the LS equation is

$$|\psi_N\rangle = |u_N\rangle + |\psi_{N+1}\rangle \frac{\langle u_N| U^{(N)} |u_N\rangle}{\langle u_N| U^{(N)} |u_N\rangle - \langle u_N| U^{(N)} |\psi_{N+1}\rangle}$$

with

$$\begin{aligned} |u_{N+1}\rangle &= G_0 U^{(N)} |u_N\rangle \\ |\psi_{N+1}\rangle &= |u_{N+1}\rangle + G_0 U^{(N+1)} |\psi_{N+1}\rangle \end{aligned}$$

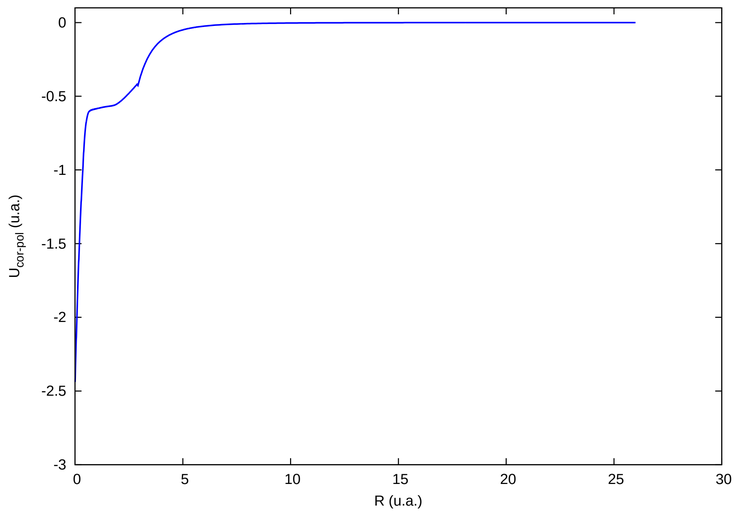

FIGURE 1: Correlation polarization potential, obtained using the PCOP model. Note that r_c (see text) is in about 3 a_0.

The calculations for CH_4 molecule begin with the polarization interaction potential determination, which is represented in figure 1. Note in that figure that r_c is in about 3 a_0, which is beyond the radial point where are the hydrogen atoms (R_{CH} =1.0837 a_0).

$e^+ - CH_4$ cross sections

The method found the scattered positron wave function in no more than 6 iterations. With that, the cross sections were determined and compared with those in [4, 5, 6]. In figure 2, we show the Integral Cross Sections compared with theoretical and experimental data.

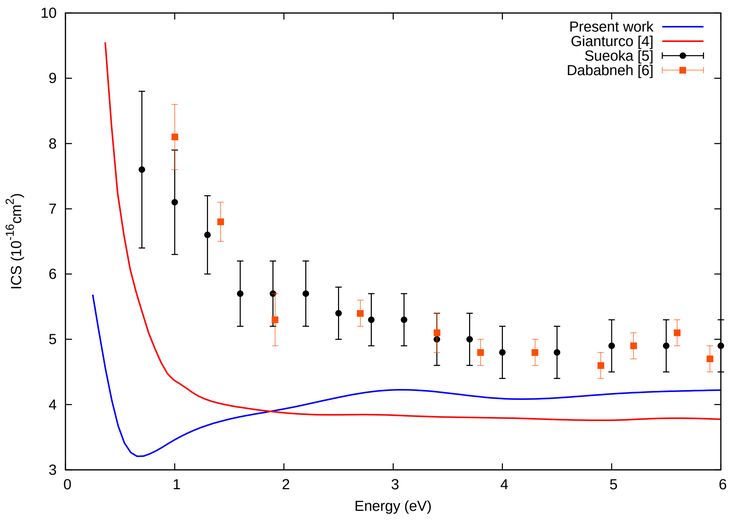

FIGURE 2: Integral cross section (ICS) for $e^+ - CH_4$ scattering. Note the minimum at about 0.8 eV in the present results that do not exist on data [4]. No theoretical result agree with the experimental values.

The present work shows a minimum in the ICS, that is absent in the oter calculation. Considering other cross sections obtained with the PCOP model [7], we expected the existence of the minimum, as CH_4 is an apolar molecule and there is no dipole interaction to hide possible imprecisions in the PCOP model. In order to obtain more information about the difference of the calculations, we show the Differential Cross Section (DCS) for a incident energy of 0.8 eV.

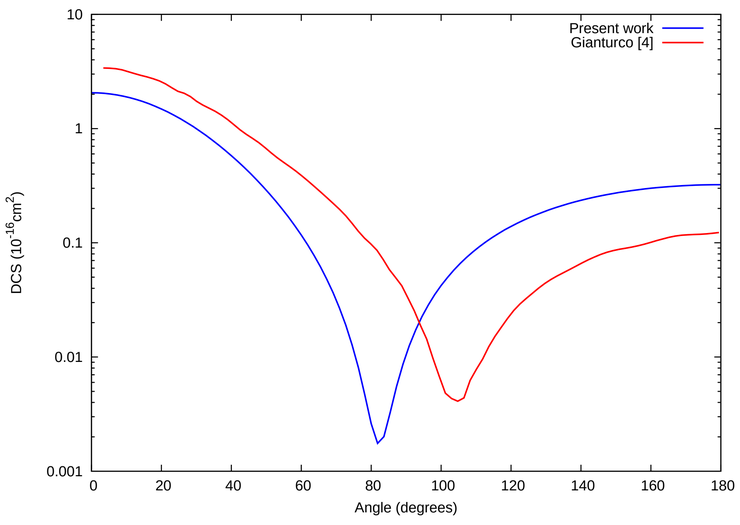

FIGURE 3: Differential cross section (DCS) for a incident positron with 0.8 eV. Blue line represents the present work, and the red line is from reference [4].

In the DCS's there is a clear difference in the position of the minimum. The magnitudes of the cross sections are almost equal, considering all angular region, but the point of the minimum define the difference in the ICS. There is no experimental data to compare, so there is no way to know which minimum is closest to real position.

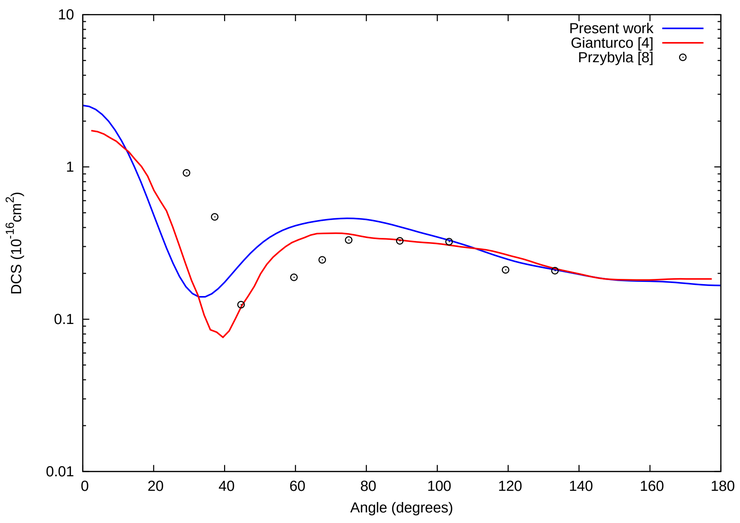

FIGURE 4: Differential cross section (DCS) for a incident positron with 6.0 eV. Blue line represents the present work, the red line is from reference [4] and the points are the experimental data from reference [8].

In figure 4 we show the DCS for a positron with energy equal to 6 eV, and observe again a distinction between the theoretical cross sections. The experimental data from reference [8] are normalized to DCS(90) value of reference [4]. Again the minimum of the present work is shifted to the low angle region, but now can be compared to experimental values. The results from reference [4] agree better with the experiment in a qualitative way, since the points are normalized, but no theoretical data reproduces the position of the minimum or the low angle behavior. In reference [4] there is a mention about the discrepancy theory and experiment, which occurs at low angle region, justified by tha fact that the polarization is fundamental to describe the cross sections in this angular region, and the short range polarization should be better described in order to obtain cross sections that agree better with the experimental data.

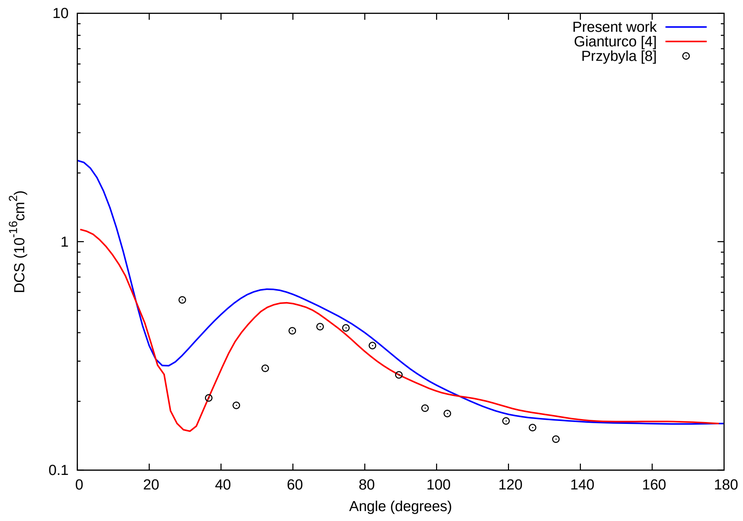

FIGURE 5: Differential cross section (DCS) for a incident positron with 10.0 eV. Blue line represents the present work, red line is from reference [4] and the points are the experimental data from reference [8].

The same discussion made on figure 4 can be made on figure 5. The behavior of the theoretical results are equivalent for incident energies of 6 and 10 eV. The only difference is that the low angle behavior becomes more explicit, as the divergence of the minima is more clear, for all three data.

Conclusions

We presented the integral and differential cross sections for positron methane scattering at low energies (1-10 eV) obtained with PCOP model, and compared with other results of the literature, theoretical and experimental. We see clearly that the PCOP model presents a disability in the determination of the polarization potential, and improvements are necessary in order to determine low angle corss sections more accurately.

Acknowledgments

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